

**NEURAL NETWORKS APPROACH TOWARDS
DETERMINING FLAX - BIOCOMPOSITES
COMPOSITION AND PROCESSING PARAMETERS**

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ABSTRACT

This research introduces neural networks (NN) as a novel approach towards aiding biocomposite materials processing. At its core, the aim of the research was to investigate NN usage as a tool for advancing the field of biocomposites. Empirical data was generated for compression-molded flax fiber and High Density Polyethylene (HDPE) matrix based biocomposite materials. In an attempt to create the NN model, tensile strength, impact strength, hardness, bending strength, and density were provided to the NN as inputs. These inputs were processed through multiple layers of the NN, and contributed to the prediction of the composition (fiber loading percentage) and operating parameter (pressure in MPa) as output. In précis, NN's use was investigated to predict composition and operational parameter for biocomposites production when the desired mechanical properties of the biocomposites were available.

Flax (*Linum usitatissimum*) fiber biocomposite boards were manufactured using chemically pretreated flax fiber and high density polyethylene (HDPE). After extensive preprocessing (combing and size reduction to 2 mm particles) and pretreatment regimen - flax fiber was mixed with HDPE and extruded using a laboratory scale single screw extruder. Extrudates generated from the extruder were again ground to 2 mm particles. Ground extrudates from different sample sets were exposed to a compression molding unit. The mold was put under two sets of pressures, (variable operating parameters) for all individual fiber loading. These boards were used to determine the mechanical properties tensile force, impact force, hardness, bending, and density.

For verification and analysis of the mechanical properties, Microsoft Office Excel and a statistical software package SAS were used. After verification five different multilayer neural networks, i.e., cascade forward neural network, feedforward backpropagation neural network, neural unit (single layer, single neuron), feedforward time delay neural network and NARX, were trained and evaluated for performance. Ultimately, the feedforward backpropagation NN (FFBPNN) was selected as the most efficient. After rigorous testing, the FFBPNN trained by the TRAINSCG algorithm (Matlab ®) was selected to generate prediction results that were the most suitable, fast and accurate.

Once the selection and training of the NN architecture was complete, biocomposite materials prediction was performed. From 9 separate input sets, NNs provided overall prediction error between 2 - and 4%. This was the same amount of error that was observed in the training of the neural network. It was concluded that the neural network approach for the experimental design and operational conditions were satisfied.

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DEDICATION

This thesis is dedicated

to

my loving mother Mazedra,

caring father Wahab,

and

wonderful sister Luna

who are an inspiration, guidance and a blessing to my life.

-- Mubashshar

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CHAPTER I

INTRODUCTION

1.1 Biocomposites

Biocomposites are composites that are created with the mixture of two compatible elements such as a biological fiber and a synthetic polymer, both of which contribute to the strength while maintaining the structural integrity of the new material. Biocomposites have shown immense potential towards creating a sustainable alternative to augment plastics and replace synthetic composite materials in different consumer applications. Global research is ongoing, to decrease petrochemical consumption, reduce plastics use, reuse waste plastics, and cut operating costs in the polymer products production cycle (Burger et al., 1995). Natural fiber composites or, simply, biocomposites have come close to satisfying all of the aforementioned constraints and provide a cost-effective, sustainable, green, and renewable solution. The attractiveness of biocomposites is due to the different materials properties that can be attained by natural fiber and polymer composition.

From an environmental standpoint, consciousness and concerns over biodegradability continue to create industry attention and public interest towards biocomposites (Averous et al., 2003). Construction applications, civil engineering structures, furniture, packaging, interior components of vehicles and automobiles, and daily household products can be efficiently and cost-effectively produced from biocomposites (Fowler et al., 2007). Effective uses of biocomposites result in cutting of material costs, development of green materials, and reduction of fossil fuel dependence.

In creating novel natural fiber materials, researchers have found that fiber properties are varying, non-homogeneous, and inconsistent (Bauer et al., 2005). Often within the same species, fibers collected from two independent sources have different mechanical properties and chemical composition. As a result of the natural component of biocomposite materials, the consistency required for quality control in industrial products is dismayingly absent. This inconsistency, together with lack of policies and industrial standard requirements, has proven to be a hindrance in developing biocomposites for the consumer market. Further hindrance has occurred due to high research cost, expensive labor requirements, and slow product development cycle. However, it is expected that research work and effective use of computational tools can assist in the realization of biocomposites true potential.

In this research project, the focus was biocomposites with compression-molded high density polyethylene (HDPE) matrix reinforced by flax fiber. There are numerous types of biocomposites based on the fiber type, polymer matrix, and the production process. However, for Saskatchewan the most commonly available and abundant fiber source is the flax fiber. In an attempt to provide increased crop value to Saskatchewan farmers, oilseed flax fiber was considered in this research. In the development of biocomposite materials, Panigrahi and coworkers (2002) have commented that the use of flax fibers would make the most environmental sense for renewable biocomposites. At the same time, High Density Polyethylene (HDPE), a commonly used polymer matrix with uses ranging from household appliances to industrial products, was selected for the matrix.

1.2 Neural network aided biocomposites formulation

Biocomposites design and new biocomposite products development is a new field. It will take time to recognize the true potential of biocomposites. Novel biocomposite product development has been deemed expensive, complicated, and time intensive. This has created the need for complex computation and different numerical modeling to supplement and expedite biocomposites formulation. Due to its inherent structure and parallel processing capabilities, neural networks can be used as an effective tool towards predicting biocomposites materials property, composition, structure, etc. Neural networks can aid the appropriate modeling of biocomposites by mapping real world data to develop an expert system within the precise domain. The mapping of relevant information with input versus output data over a large knowledge base can create an effective tool for biocomposites design.

NN have already shown promising results towards coherently modeling materials property in different fields. Research results show that with the aid of an appropriate NN and a good research knowledge base – fast prediction, characterization, and modeling of novel composites and materials can be possible. Hence, research work should be undertaken to replicate successful use of NN in biocomposites and advance this field.

Neural units are effective representation of the human neuron. They are effective mathematical representation of the neural network (Jones et al., 1997). Neural units are clustered together within an architecture to accomplish a particular task are commonly known as the neural network NNs have evolved and spanned across multiple disciplines providing unique solutions to complex problems. Today, they are successfully being used in many different areas ranging from

Agriculture and Agrifood (Yang et al., 2000) to neural hardware, software, and even financial and business forecasting (Zhang, 2004). These are powerful mathematical tools (Zhang et al., 2002) that are often capable of providing better results than conventional algorithms, models or processes due to their massive parallel processing capability, competitive learning ability, and adaptation to new information. Provided an exhaustive set of inputs and corresponding outputs, the neural network can be trained to exert intelligent decision making capabilities using its knowledge base (Schocken et al., 1994). There are different types of NNs depending on the learning, adaptation and neural structure, as well as, the problem domain definition. Some networks are effectively created with the merger of two or more different networks. However, all NNs follow the common principle of learning and adaptation. They all show the capability to solve complex problems by using efficient parallel processing algorithms. Figure 1.1 provides the mathematical morphology of a neuron that participates in a neural network. It represents the

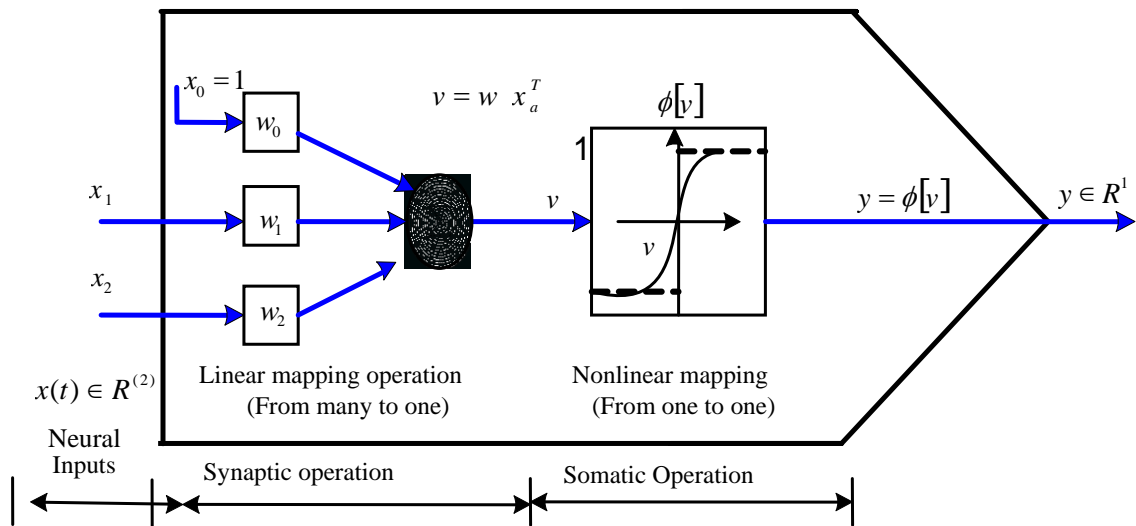


Figure 1.1 Mathematical representation of a neural unit with sections describing synaptic and somatic operation of the neural network (Gupta, 2006).

linear neural unit (LNU). In comparison to a human neuron, this neural unit can take two inputs x_1 and x_2 . The synaptic operation or the connection of the dendrites with neighboring relevant neurons is represented with weights w_1 and w_2 . Nonlinear mapping or the somatic operation generates the output. The output for the LNU is represented by y . The mathematical representation of a generalized neural unit with n inputs can be formulated with the following equations:

1. Neural inputs: $x_1 \dots x_n$
2. Neural outputs: y_N
3. Every input has corresponding weight: $w_1 \dots w_n$
4. Bias x_0 and corresponding weight w_0
5. Synaptic operation: $v_a(k) = \sum_{i=0}^n w_i(k)x_i(k)$

$$\Rightarrow v_a(k) = w_0(k)x_0(k) + w_1(k)x_1(k) + \dots + w_n(k)x_n(k)$$

$$\Rightarrow v_a(k) = w_a^T \cdot x_a$$

6. $w_a^T = [w_0(k) \ w_1(k) \ \dots \ w_n(k)] \in \mathbb{R}^{n+1}$
7. $x_a = [x_0(k) \ x_1(k) \ \dots \ x_n(k)]^T \in \mathbb{R}^{n+1}$ [where bias $x_0 = 1$] (Gupta, 2007)

Finally, like their human neural counterparts, NNs can learn from example. This attribute allows them to continuously learn and be trained towards finding solutions for complicated nonlinear, multi-dimensional functional relationships without any prior assumptions (Zhang et al., 2003). A well-trained neural network is able to effectively find the relations in a host of information and deduct a conclusion from that information. This allows the NNs to be a powerful tool in information development, data mapping, and knowledge filtering.

1.3 Organization of the thesis

This thesis has been organized into 6 distinct chapters. These are: Chapter I - Introduction, Chapter II - Objectives, Chapter III - Literature Review, Chapter IV- Materials and Methods, Chapter V - Results and Discussion and Chapter VI - Conclusion.

Chapter I - Introduction, provides an overview on biocomposites, NNs potential in aiding biocomposite design, biological neural networks and their mathematical counterpart, the NN. This chapter also provides a short section describing the organization of the thesis. Chapter II- Objectives, outlines the research questions that we have attempted to answer within the body of this thesis. Chapter III - Literature Review describes, in depth, the existing works on biocomposites and NNs. This chapter also provides the very reason for undertaking the research for this thesis, which is, the absence of actual work on biocomposites design using NNs. Chapter IV - Materials and Methods explains the different materials and equipments that were used for producing the biocomposites for this research and the overall method of developing the neural networks for the biocomposites. Chapter V - Results and Discussion presents the results that were obtained through testing of the biocomposites boards and discusses how the data was used to create and train the NN. Chapter VI - Conclusion provides a short review of the entire thesis and draws conclusions based on the observed results. It also outlines the potential research opportunities that may stem from this research work.

CHAPTER II

OBJECTIVES

The use of natural fibers for the creation of industrial products provides additional value to agricultural producers and secondary industries. It is important to realize the need to devise automation and intelligent tools that allow fast and economical production of natural fiber biocomposites. Attempt has been made to introduce NN as a tool for advancing biocomposite research. The research described in this thesis has the following three objectives:

1. To provide an effective process of creating neural networks for biocomposite materials;
2. To determine the appropriate training algorithms that are best suited for the modeling of biocomposites using neural networks; and
3. To develop a neural network for predicting the composition of a biocomposite board and the pressure (operational parameter) required to produce that board using tensile, impact, hardness, bending, and density data as inputs.

CHAPTER III

LITERATURE REVIEW

This review focuses on: i) contemporary biocomposites research; ii) neural networks as used in materials science; and iii) the need for neural networks for advancing the field of biocomposites. It will also consider the research gap that this project may fill using a neural network approach towards biocomposites design.

3.1 Biocomposites

Biocomposites use can result in the effective reduction of plastic consumption and may curb greenhouse gas production. Although biocomposites are environmentally friendly, inherent problems exist with respect to the variability of properties and composition within the same natural materials. This must be resolved before biocomposites will be a true alternative to pure polymers.

3.1.1 Flax fiber

Canada is the largest flax producer in the world accounting for approximately 40% ~ of the entire world production. Flax is also grown in different parts of the United States, Europe and Asia. In Canada, Saskatchewan is the largest producer of flax ranging from oilseed to flax fiber (Saskflax.com, 2007). Oilseed flax, *L. usitatissimum*, is an important part of the crop rotation in Saskatchewan's vast farm land (47% of Canada's arable land). Post-harvest - oilseed flax straw is commonly left in the field to be decomposed naturally or may be burnt which may cause environmental damage. It is important that this natural product be used in the development of

multiple products to generate value for farmers. The use of oil seed flax fiber can assist in creating composite materials with novel properties. They can be used to curtail the use of polymer. The flax straw goes through decortications and mechanical processes until the fiber is separated from the shive. After the mechanical process, the processed fiber has a lot of dust and shives particles in it. There is also waxy material on the surface of the fiber. These contaminants prevent it from being a good candidate in the fiber and polymer mix.

Mohanty et al. (2001) determined the chemical composition of flax fiber in their research. Table 3.1 provides their results:

Table 3.1 Selected composition of flax fiber Mohanty et al. (2001)

| | |
|--------------------------------------|-------------|
| Density (g/cm³) | 1.5 |
| Cellulose % | 71 – 78.5 |
| Hemicellulose % | 18.6 – 20.6 |
| Ash % | 1.5 |
| Pectin % | 2.2 |
| Wax % | 0.5 |
| Moisture Content % (w.b.) | 10.0 |

From Table 3.1, we can see that the composition of agriculture fibers varies, even within the same species. Depending on the weather, time in the year, soil condition and harvesting conditions, the fibers can have varying mechanical strength. From the chemical composition, we can see that there are substantial amounts of pectin, wax, hemicellulose, ash, etc. present in the flax fiber. A pretreatment regimen using NaOH chemically removes these constituents from the outer surface of the fiber by an oxidization process.

3.1.2 High density polyethylene (HDPE)

There is a wide variety of polymeric materials. These are both synthetic and natural. Polymers even exist within the human body as well as the in plants. Essentially, polymers are a string of molecules that are connected together to create a continuous chain. HDPE, Linear Low Density Polyethylene, Poly Vinyl Chloride, etc. are some common polymers. In this experiment, we used HDPE as the polymer matrix. The HDPE was purchased from Exxon Mobil, Toronto, Ontario, Canada. Injection grade HDPE was provided in the form of small pellets. Some mechanical properties of HDPE are: density = $0.935 - 0.1 \text{ g/cm}^3$, tensile strength = $14.5 - 38.0 \text{ MPa}$, Young's modulus = $0.413 - 1.490 \text{ GPa}$, ultimate tensile strain = $12 - 1000 \%$ (Van de Velde et al., 2001).

HDPE-based materials are extremely resilient against any form of wear and tear. It is most commonly used for heavy duty applications where high tensile strength and advanced mechanical properties are required. From water pipes to heavy duty furniture and appliances, HDPE is a commonly used polymer that has few branches in its structure. At the same time, HDPE is also widely used in the composites industry. Due to extensive use of HDPE, it has been selected as the matrix in this research

3.1.3 Biocomposites - the future for polymeric compounds

Polymeric materials (e.g. plastics, resins) contribute to a huge amount of today's household and industrial goods. From vehicle components to boats, tanks, agricultural equipment, handheld tools and playing equipments; composite materials, as well as, biocomposites are being used everywhere. Karmaker et al. (1996) commented on the growing interest in the use of agricultural

fibers towards polymer reinforcement and the development of novel products. Researchers around the world, as well as at the University of Saskatchewan, have taken on the task of developing novel biodegradable and eco-friendly biocomposite materials. Natural fiber sources for reinforcing the polymer matrix include fibers such as jute, flax, sisal, hemp, banana fiber, cotton, coconut, etc. Using cellulosic materials in polymer matrix has produced favorable composites consisting of a wide range of desirable properties that were previously unexplored.

Biocomposites have an extensive history in industrial usage dating back to the early 20th century (1941). Henry Ford used them for automotive applications (Mohanty and coworkers 2004). Today structural, semi-structural, packaging products, etc., effectively utilizes biocomposites. Wang et al. (2003) have reported that with further research, innovation, and development in the area of agricultural fibers, there is a potential to replace expensive synthetic fibers.

Based on an extensive review by Kolybaba et al. (2003), use of biodegradable polymer composites or biocomposites is faced with the challenge that their properties are varying, non-homogeneous, and inconsistent. Industry applications dependent on rigorous quality control cannot tolerate these inherent variations. Fibers, even within the same species, collected from independent sources often show varying mechanical properties and chemical composition. This inconsistency has proven to be a challenge in developing biocomposites for a competitive consumer market that requires consistency and stringent standards on material properties.

3.1.4 Natural fibers

Fiber is the natural component in biocomposites. A significant number of plant fibers have been selected as candidates for biocomposite production. All plant fibers contain cellulose, lignin,

pectin, hemicellulose and ash. Lignin, pectin, and ash are fiber components that act as contaminants and decrease the structural strength of biocomposites. However, pectin and lignin, natural resins, creates structural strength for plants. Chemical and mechanical treatments are performed on natural fibers to get better surface contact of the synthetic resin with the cellulosic material. Observations made by Li et al. (2007) clearly showed different amounts of cellulose, lignin, hemicellulose, pectin and ash within different plants. From their study, it is interesting to note that even within the same plant fiber type there is significant variation in the composition percentage. This is due to nutrition and different environmental factors that the plants are exposed to. Ranging from the use of wood chips, flax, jute or hemp - even pistachio shells, date pits (Ghazanfari et al., 2005, 2008) - different compositions contribute to difference in their mechanical property that can be used towards different applications and products development. Natural fibers are significantly weaker when compared to synthetic fibers such as carbon fiber, glass fiber, etc. Natural fibers have certain limitations due to their natural origin. These limitations are: a hydrophilic nature, weak resistance to high temperature, inconsistent properties and short length (Nystrom, 2007). Although they are weaker, their use could be maximized for certain applications, thereby eliminating the usage of fiberglass. Li et al. (2007) also compared synthetic and natural fibers. Their work showed significant weakness of natural fibers compared to synthetic fibers. In their work on the use of chemical treatments for natural fibers, they concluded that to achieve better mechanical properties, chemical treatment is required

Chemical treatments have become a well-investigated mechanism towards enhancing biocomposites property through increased surface fusion capacity. It is gradually becoming a common procedure to subject the natural material to numerous chemical treatments that radically

alter the chemical makeup, composition and ultimately, contributes to better surface contact with the polymers. Chemical pre-treatment can range from a simple alkaline or silane treatment to the use of plasma or even ultraviolet radiation to modify the surface layer of the composite material (Kafi, 2006). Studies also show that different chemical treatments can significantly change the material properties of the composite (Wang, 2004).

3.1.5 Considerations for making biocomposites

In making a biocomposite or any other plastic composite material, there are a number of considerations. First, the natural fiber has to be selected. Upon selection of the fiber, the next task is to look into an optimal polymer matrix. At the same time, inspection has to be done to see whether the polymer will be useful for the particular application. In addition, the amount of fiber in the composite, the orientation of the fibers, and the production costs must also be considered.

In selecting a fiber, careful consideration must be given to its properties, as well as, its availability in the local market. For Saskatchewan and Canada, flax fiber and, specifically, oilseed flax fiber is the most abundant and therefore is the best choice for creating a biocomposite. Table 3.2 provides a complete set of flax fiber mechanical properties which were determined by Panigrahi et al. (2002) when they were creating their biocomposite product.

Table 3.2 Flax fiber properties

| Properties | Flax |
|---|---|
| Density, g/cm ³ | 1.5 |
| Tensile Strength (10E6 N/m ²) | 800 – 1100 |
| E-modulus, (GPa) | 40 –100 |
| Thermal Reaction | Gradual Decomposition after exposure at 150°C |
| Breaking Elongation (%) Dry Elongation | 2.7 – 3.3 |
| Fiber tenacities at 20°C and 65 RH | 2.6 – 7.7 |

(from Panigrahi et al., 2002a)

Flax fiber, has good E-modulus compared to other fibers. This fiber can tolerate high temperature thermal reactions making it suitable for use as reinforcement in biocomposites. Based on industrial requirements, – it has been found that flax-based biocomposites have acceptable mechanical properties for the plastics industry (Siaotong et al., 2004; Oksman, 2001; Burgueno, 2004).

Mwaikambo (1999) found that the properties of the cellulose fibers depend mainly on the nature of the plant, i.e., where it is grown, and also the age of the plant. According to their findings, sisal fibers with cellulose content of 67% and micro-fibril angle of 10 to 222 degrees have a tensile strength and modulus of elasticity of 530 MPa and 9 to 22 GPa, respectively. In their study, they also observed that chemical pre-treatments allow fibrils to be exposed and give a rough surface topography to the fiber.

Wang et al. (2003) found that the lack of chemical pre-treatment results in very poor adhesion between fiber and matrix. However, chemically-treated fiber shows better fiber and matrix interaction. In studying chemical pretreatment, it was observed by Franco et al. (1996), that the silane deposited on the surface of the fiber has a considerable impact on the composite strength. Figure 3.1 shows that there are very few interfacial bonds created when there is are high amounts of contaminants such as pectin, lignin, etc. However, after the silane treatment is performed notice that there are reduced contaminants in the biocomposite material which always results in

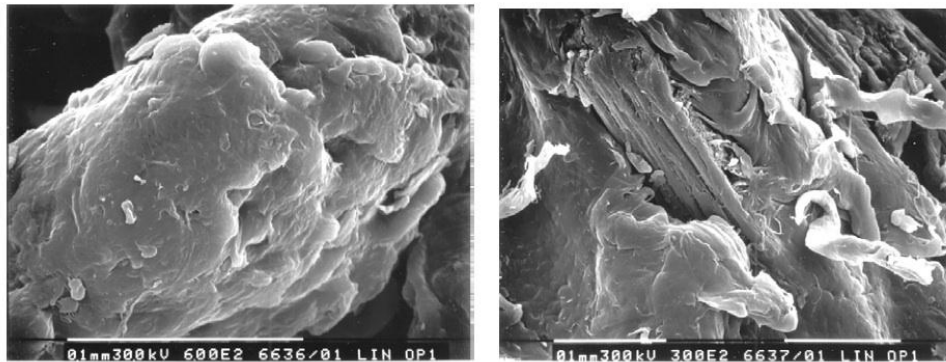


Figure 3.1 Left hand image is of SEM micrograph of LLDPE with 10% untreated flax in composites. Right hand image is SEM micrograph of LLDPE with 10% silane treated flax in composites (Wang, 2003). (printed with permission)

overall increased strength and quality. Once the fiber is selected, the polymer resin is selected next. Commonly, high density polyethylene (HDPE) and linear low density polyethylene (LLDPE) materials have been used for biocomposites. These polymer resins are used in numerous products and multiple industries. In Table 3.3, common properties of HDPE and LLDPE are given as reported by Panigrahi et al. (2002b).

Table 3.3 Properties of polyethylene used for production of flax-based biocomposites.

| Properties | Unit | Test method | LLDPE 6501 | HDPE 8760.29 |
|---------------------------------------|-------------------|--------------------|-----------------------|-------------------------|
| Melt index | g/10 min | ASTMD-1238 | 5.0 | 5.0 |
| Density | g/cm ³ | ASTMD-4883 | 0.937 | 0.942 |
| Melting point | °C | °C | 127 | 129 |
| Tensile strength | MPa | ASTMD-638 | 17.6 | 20.3 |
| Flexural modulus | MPa | ASTMD 790 | - | 1060 |
| Impact strength | J | ARM | 77 | 79(58) |
| Environmental stress crack resistance | Hr | ASTMD-1693 100% | >100 | 9 |

(Panigrahi et al., 2002b)

The polymers have lower melting points than the flax fiber. This allows the creation of polymer and fiber interfacial bonds, without affecting the fiber properties. From mechanical tests by Panigrahi et al. (2002a), it was observed that the tensile strength of biocomposites increases as the natural fiber (reinforcement filler) loading in the polymer matrix is increased. Therefore, for polymer resins, the fiber works as a strengthening component instead of decreasing the polymer property. The major drawback to the use biocomposite materials is their hygroscopic nature, resulting from the presence of cellulose which is hydrophilic. Moisture from the environment can easily damage the microstructure of biocomposite materials. An increase in moisture content adversely affects the mechanical properties of biocomposite materials.

Finally, the last consideration to be made is the type of manufacturing process that is going to be employed. Some common manufacturing methods are: compression molding, injection molding, and rotational molding. Depending on the application, the manufacturing process is selected based on speed, economic feasibility, and ease of production. The most common and diverse

creations of polymer products have been performed with compression molding for biocomposites.

3.2 Neural networks

Neural networks are a fascinating toolset that allows simulation, modeling and prediction in a wide variety of complex domains using weighted adaptation methods. They have an input layer which allows the input of a dataset or a set of parameters for the particular model. The outputs are effectively the results of adaptive training and validation of input parameters. Rao and Gupta (1993) stated that neural networks are parallel distributed processing units, uniquely capable of morphing human neurons. Conventional neural models deal with extremely simplified mathematical representations of the human neurons. In general, only a very simple linear summation of the weighted neural inputs is considered when performing neural applications. Some very simple examples of these NNs' are feedforward neural networks (FFNN), backpropagation neural networks (BPNN), self organizing map (SOM) neural networks, etc. The growth of neural networks as a research field was not a smooth one. In their earliest stages of evolution, neural networks, used as a single neuron, were almost abandoned. This was - due to the failure to simulate the XOR gate (Figure 3.2). From Russian mathematician Kolmogorov's proof (Kolmogorov, 1957), it was found that a three-layer neural network could learn any function, provided there are a sufficient number of neurons in it. In Figure 3.2, Gupta (2006) provides a XOR operation that uses three neurons to create a neural network.

Within an uncertain environment, species have the capability of learning, adaptation, and self organization (Gupta et al., 2003). Neural networks are highly adaptive to uncertainty and noisy

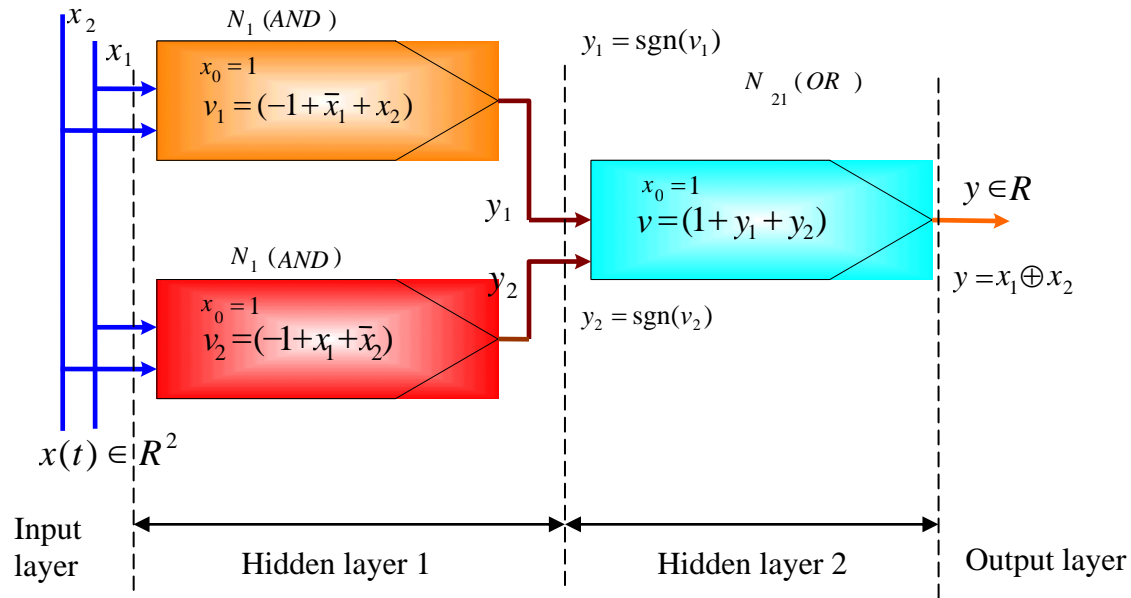


Figure 3.2 Mathematical representation of feedforward neural network (Gupta, 2006).

data. Neural networks provide a fascinating set of mathematical tools, which can be used to simulate a wide variety of circumstances and accurately predict all events in different knowledge domains through means of learning and adaptation. NN theory has been developed in the form of parallel distributed network models based on the learning process of the human brain (Anijdan et al., 2004). NNs have now become a commonly used research tool in many different fields. With the ability to learn from input in a defined environment, NNs are fast becoming prominent tools in industrial research and product development. As a novel tool in the area of biocomposites, NNs can assist in the development and fast prototyping of biocomposites. Ultimately, NNs will be able to design materials for multiple variables and conditions in the biocomposites domain.

3.2.1 Neural network in materials science

This review is a step towards understanding the current work that has been committed in the use of neural networks for materials science. No work has been done in the area of biocomposite materials characterization using neural networks thus far.

3.2.1.1 Modeling

Wu (1990) has looked at the common approaches towards materials analysis and characterization. He has stated that until now materials analysis has been done using mathematical models of material behavior derived from observation and reasoning. Wu (1990), from his observation, believes that the non-conventional and less used neural network-based method of materials behavior modeling can be done in the unified environment of the neural network.

Kusiak et al. (2002), have modeled the microstructure and mechanical properties of steel using neural networks. Their NN model was capable of effectively predicting ferrite grain size, ferrite fraction, etc. They found that the microstructure and mechanical properties of the considered steel is in agreement with experimental data.

3.2.1.2 Novel materials

Gotlib et al. (2000) found that when neural networks are properly scaled, have relevant bounds and are trained on small but well-defined experimental sets, they may provide a useful insight into the effective behaviour of the heterogeneous materials. They opined that neural networks are effective tools for materials development.

Ashida et al. (2003) worked on multilayer composites plates. In their study, they tried to determine the thickness of each pero-ceramic layer using neural networks so that the maximum value of the applied electric potential distributions is minimized subject to stress constraints.

Figure 3.3 provides the hierarchical neural network as used by Ashida et al. (2003).

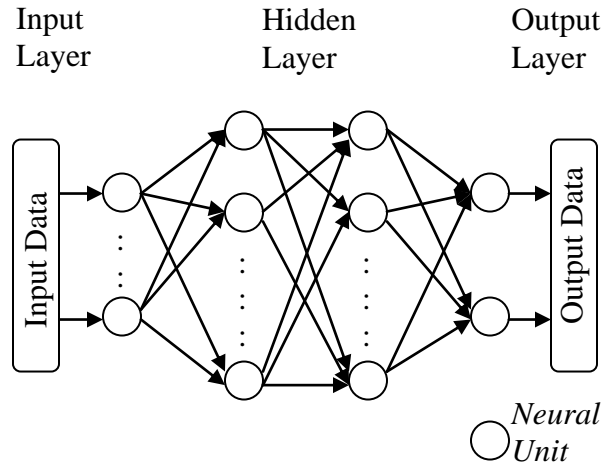


Figure 3.3 Hierarchical neural network as used by Ashida et al. (2003) (adapted image)

The neural network has two hidden layers. Malinov et al. (2002) conducted research on optimizing composition and processing parameters. They have found that NN are convenient and powerful tools. In order to obtain the desired combination of properties at different working temperatures for titanium alloys, they observed that NN can contribute to process optimization. Hosseini (2004) modeled the effects of heat treatment parameters using NN. In this study, the resulting mechanical properties of Si–Mn TRIP steels were used for creating a back propagation neural network. Hosseini (2004) concluded that to achieve accurate results using NN, a committee of models is preferable to, a single model.

3.2.1.3 Mechanical strength

Calcaterra et al. (1999) used a number of different compositions to create a number of different castings with different cooling times and different inoculation temperatures. Their tests went into dealing with tension property. Finally, the derived data was used to test different neural structures. Their work progressed from a simple perceptron (also known as a neural unit) to multilayer perceptrons and finally, their data was validated.

3.2.1.4 Composites degradation

Friere et al. (2006) stated that, the main problems found in the analysis and study of the fatigue behavior of composite materials is the poor understanding and prediction of the test results. For fatigue, a huge number of tests is required to evaluate the fatigue behavior of the material. Fatigue lives of composites were also predicted using neural networks by Lee et al. (1999). In their experiment, they were able to find the fatigue life for the composite materials.

Friere and coworkers (2006), go on to state that the main problems found in the analysis and study of the fatigue behavior of composite materials is the poor understanding and prediction of the test results. They have also gone to state that there is a need to do a huge number of tests to evaluate the fatigue behavior of the material. In an ideal case, they suggest using the least possible number of tests for the design to make preliminary predictions about the products fatigue life.

The use of neural networks as a tool for modeling fatigue life of multidirectional composite laminates has been performed by Vassilopoulos et al. (2006). They concluded that the modeling

efficiency of the network was satisfactory for both on and off axis coupons life,— irrespective of the test condition.

3.2.2 Neural networks for biocomposites advancement

Human inspired neural networks provide a fascinating set of mathematical tools which can be used to simulate biocomposite materials production, processing, and modeling. Zeng (1998) in his review of NN and their use in mechanics, stated that NN is the most rapidly expanding area across many disciplines. With the push from the market, the complexity in modeling natural materials renders a state where the use of neural networks as an alternative and fast modeling tool provides an extremely viable option that can maintain quality and cut cost.

3.2.2.1 Faster product development cycle

For development of a shingle, to have the product marketable, there is the need for extensive lab research work. First of all, the required properties or standards must be known for the composition. In this case, the use of ASTM standards greatly reduces the production downtime. Once the properties are known, the next step is to create a consistent mixture. Then through step by step processes that lead to extrusion, molding, and finally cooling, the composite product is made into an initial product. Once the product is created, the material is subjected to a

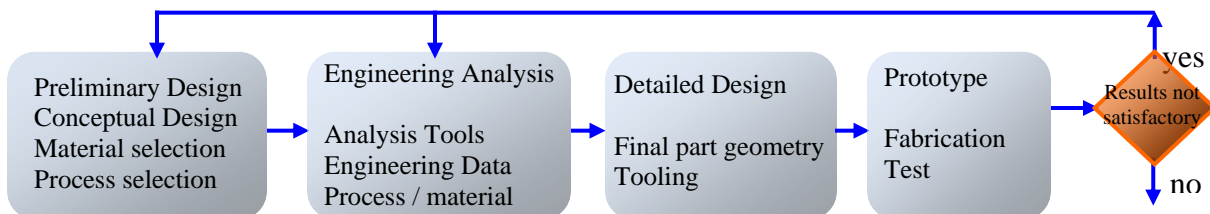


Figure 3.4 Design Engineering Process. (adapted from Characterization and Failure Analysis of Plastics, 2003)

number of mechanical and rheological tests. These tests allow the engineer to know about the properties of the composite. Once the property of the composite has been characterized, a comparison is made with the ASTM standard of the desired product. Rosentrater et al. (2005) have explored all of the different ASTM standards that are involved in composite testing and manufacturing. This is a long and exhaustive process. Figure 3.4 provides further illustration on the use of actual engineering development processes that are done repetitively to lead to the development of a final biocomposite product.

Zhang et al. (2003) reported that NN techniques are extensively used to create better materials with a shorter product research time span. At this point it becomes apparent that the best way to minimize the product development time and cost is the use of in-situ modeling techniques and algorithms. The in silico nature of neural networks contribute to; cost effective, alternative, optimal and fast solutions for products development, systems engineering and processing in multiple industries.

Bhadeshia, (1999), in his review, extensively reiterated the potential of neural networks in the creation and characterization of novel materials. Neural networks can aid in creating optimized structural quality for biocomposites. They can also contribute towards developing new natural fiber-based composites and greatly advance the field of biocomposites as a whole. Large NN knowledge base developed from continuous research can aid the biocomposites industry by contributing to swift product development, product optimization, R & D cost crunching and fast delivery of products to the consumer.

3.2.2.2 Solutions to material sciences inherent complexity

Drawing the focus to materials science itself, it is observed that, biocomposites are not only very ill-understood, but materials science, itself, also has problems that are complex and the general concepts are not yet amenable to scientific treatments (Bhadeshia, 1999). The sciences allow the understanding of material properties, but seldom, effectively, state their characteristics. Often, there are formulations and models to quantify material properties, but they run short of providing a complete representation of the actual biocomposites. Often they are put in the context of mathematical models that do not correlate. Hence, the interaction of different models in the description of biocomposites is hard to decipher. This has been repeatedly underpinned by Bhadeshia, (1999).

In their paper, Shtrauss et al. (1999), provided a number of reasons, for using neural networks to predict or evaluate material structural property rather than conventional methods. One reason mentioned was that huge complexity renders non-destructive testing almost impossible in accurately predicting material properties. Another reason as stated is the problem of structural evaluation is a typical inverse problem which is characteristically ill conditioned.

Composite materials and its specialized natural fiber-based biocomposite materials subset are complex in nature and often very hard to model due to their non-homogenous component structure and the different changes associated with it them during the production and processing phases. At the same time, there are 50 different groups of plastics with hundreds of different varieties (wasteonline.org.uk, 2008). The different natural materials that can be used for the development of biocomposite material are also numerous.

For an individual to know all of their properties and then also to know the effect of composition of different natural material exposed to different variable conditions is almost impossible. Continuous changes in the components through heat, pressure, moisture absorption, etc., and external asymptotic variables that are involved directly in developing the composition matrix, renders the modeling process into a precarious scenario where it is hard to model individual components or even the entire component.

3.2.2.3 Market drive

The NN approximates the laws of mechanics within the actual novel material (Wu et al., 1990). This allows characterization of the material for new product development. Furthermore, it enables fast prototyping as research time decreases. Other pertinent manufacturing parameters can also be derived with the aid of the NN algorithms. As a result, biocomposites can evolve faster and NN can become an efficient tool in this field.

Due to the variation in different types of natural fiber, the prerequisite knowledge base is currently absent for biocomposites. As a result, problems such as modeling, property prediction, composition prediction, operating parameter determination etc., cannot be concluded for novel biocomposite products. Often NN results outperform existing finite element methods and common statistical approaches towards engineering design.

The key to any product development is the optimization of different variables that contribute to the design parameters, product development, and allows effective materials production. In the consumer market, natural fiber-based biocomposite materials are exposed to extreme

competition in the development of new eco-friendly products. To be competitive, the development of biocomposite materials needs fast prototyping and an extensive knowledge of the materials used in the composition. This is absent in the case of natural materials since the mixture of natural fibers and polymers is not age-old or well-tested. Desired material properties used as inputs to the NN can generate a good initial composition percentage between fibers and matrix. It is assumed that if a neural network can be trained on a comprehensive set of experimental data derived from the real world with appropriate representation scheme, the model can approximate all the laws of mechanics within the actual novel material (Wu et al., 1990). This would allow characterization of the material and new products development.

3.4 Summary

The mixture of fibers into polymers results in an overall increase of strength for the polymer and fiber matrix or, simply, the biocomposite. The mixture creates improved properties provided that the fiber is pretreated. Therefore, for manufacturing biocomposites, sufficient care has to be given towards the fiber selection, fiber pretreatment and polymer selection.

Through this review, it is apparent that researchers who have used neural networks in the areas of composite materials, new materials development, structural property analysis and prediction, all have had satisfactory results with the use of neural networks. NN have already contributed to advancing multiple sciences and engineering disciplines. Research reviews from metal composites stipulate that, the inherent complexity in materials modeling can be removed with the aid of neural network tools.

An extensive literature review has not revealed use of NN for biocomposite materials applications. Hence, biocomposite materials analysis, prediction and development using NN - is an attractive area that can unfold many unknown features of biocomposites that may otherwise possibly remain unexplored. It is therefore important that research in this new field is commenced and supported.

CHAPTER IV

MATERIALS AND METHODS

Within this chapter, different materials and methods are described. The biocomposites principle constituents, - flax fiber and HDPE polymers, are also discussed briefly in this chapter. The five tests completed according to ASTM standard are presented here. Finally, the method of creating NNs for biocomposites using Matlab is described in this chapter.

4.1 Biocomposites formulation

In the experiment, oilseed flax fiber and HDPE plastic were used to create the biocomposite. The flax fiber was collected from a Saskatchewan based company Biofiber, Canora, Saskatchewan. The fiber was used to strengthen the polymer matrix and increase the mechanical quality of the composite material.

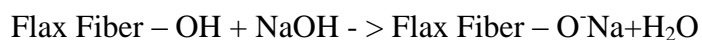
In order to create biocomposite materials, - the first step is to pre-treat the flax fiber and then both pre-process the flax fiber and HDPE. To ensure that the composite materials are well-mixed, the mixture is extruded, and again pelletized and fine ground. The materials preparation processes are described in detail in this section.

4.1.1 Fibre pretreatment

Fiber collected from Canora, SK was first combed clean and washed thoroughly. This was done to remove any dirt and dust that was present in the fiber. This was further cleaned with regular dish detergent. After cleaning the fiber, it was filtered to remove any excess water. Chemical

modification, as well as surface modification, was then done through the process of fiber pretreatment.

There have been a great number of studies carried out in the areas of fiber pretreatment. The benefits of alkali pretreatment have been studied by many researchers (Ray et al., 2001; Mishra et al., 2001; Sreekala et al., 2000). At the same time, considerable progress has been achieved in the use of alkali or mercerization for the fiber pretreatment process in the College of Engineering, University of Saskatchewan (Panigrahi et al., 2009; Panigrahi et al., 2008; Panigrahi et al., 2006; Ghazanfari et al., 2006; Li et al., 2008; Li et al., 2007; Wang et al., 2007; Wang et al., 2008; Soleimani et al., 2008). As performed in previous studies, the pretreatment for the fiber was done with the use of alkali. The cleaned and washed fiber was exposed to a 5% NaOH solution as recommended by Sreekala et al. (2000). The time of exposure was 3 hours. During this time the following reaction takes place:



This reaction results in the removal of wax and oily materials from the fiber. At the same time, mercerization also contributes to the breaking down of lignin and pectin compounds. This ensures decreased fiber diameter, enhanced aspect ratio, better mechanical properties, such as increased strength, etc. and improved exposure of the fiber surface to the polymer resulting in good interfacial bonds. Due to this oxidization process, the fiber gradually turns yellow. After 3 hours, it was transferred to another container and thoroughly rinsed. Continuous rinsing was performed so that no NaOH is present in the fiber. Presence of water results in poor mechanical

properties and fast degradation of the material. Prior to any further steps, the fiber was dried thoroughly in a drying chamber at 30°C for 72 hours. The low temperature ensured that the fiber did not experience surface degradation or localized burning.

4.1.2 Material preprocessing

The fiber treated with NaOH was removed from the drying chamber. At this point, the flax fiber has a bright yellow hue. The fiber was then ground into fine particles using a 2 mm screen to ensure good surface contact between the fiber and polymer. Upon grinding they were again stored in two separate plastic bags for later use. This was done to ensure that the surface of the fiber was sufficiently modified so that the fiber and polymers mix efficiently.

The fiber and the biocomposite strands were ground into lengths of 2 mm by passing the fiber and the small biocomposite pellets through a 4 mm screen, first, and then through the 2 mm screen. At the same time, the HDPE pellets were also passed through the grinder to make shorter pieces. The reason for cutting the fiber into fine size was to increase the aspect ratio. This ensures better mixing of the fiber with the polymer. Tests were performed to see if fibers cut into larger pieces were capable of mixing with the polymer well enough to create good bonding with the polymer matrix. The 2 mm particle size was deemed the optimal size.

The treated fiber samples were mixed with HDPE in amounts of 5% - 35% fiber (at 5% fiber intervals). A rotating mixer was used to thoroughly mix the short fiber and the ground HDPE pieces to ensure that the mixture was fairly homogeneous prior to extrusion. It was important that the two mix well, since the fiber is natural and the HDPE is a synthetic product.

4.1.3 Extrusion

The barrel temperatures for the two types of samples were maintained at temperatures of 130°C in the 1st barrel zone, 143°C in the 2nd barrel zone, 150°C at the third barrel zone and 150°C at

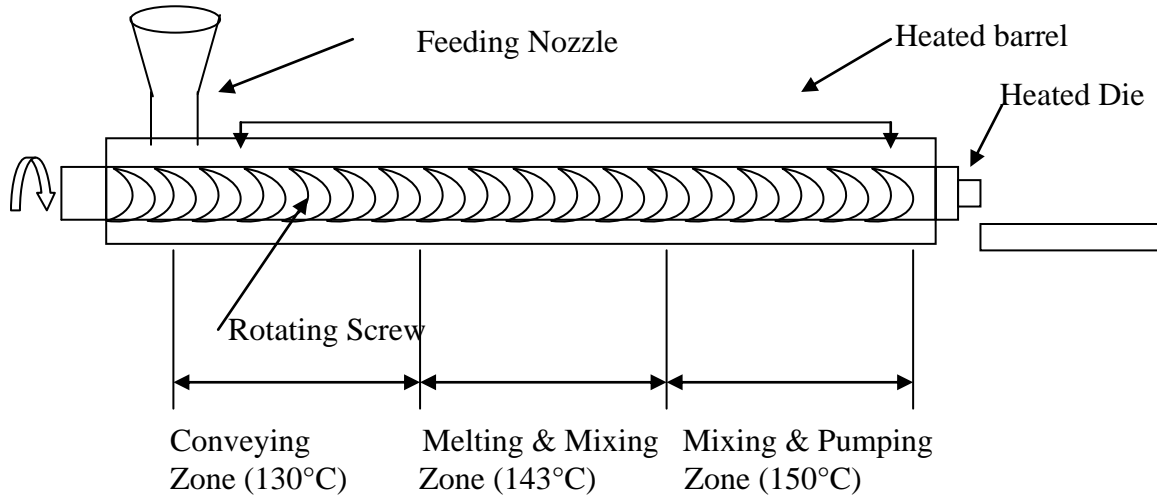


Figure 4.1 Single screw extruder diagram displaying different extruder components.

the die zone, the screw was rotating at 20 rpm. Figure 4.1 shows a line diagram of a single screw extruder. The mixture when passing through the extruder, due to high amounts of heat, the polymer and fiber mixture is turned into a molten biocomposite in the extruder. The extrudate was then cooled in cold water to convert the biocomposite from a molten state to a solid state. Prior to cutting into smaller pellets, the strands were thoroughly shaken so that the extra water was removed. At this point, the extrudate was passed through the chopper to create small pellets. The extrusion process was carried out to create a cohesive mixture of fiber and polymer. A number of test biocomposite boards were made without the involvement of any extrusion process. However, in all cases, the biocomposites boards were of poor quality with lots of air pockets and the mixture of fiber and polymer was non-homogenous. Therefore, the use of

extrusion prior to creating the sample boards was considered a crucial step. It should be noted that prior to starting the experiment, - the extruder was purged using linear low density polyethylene (LLDPE) to remove any contaminants from the extruder screw.

4.1.4 Compression mold

A novel mold, shown in Figure 4.2, was designed for creating the biocomposite samples. The

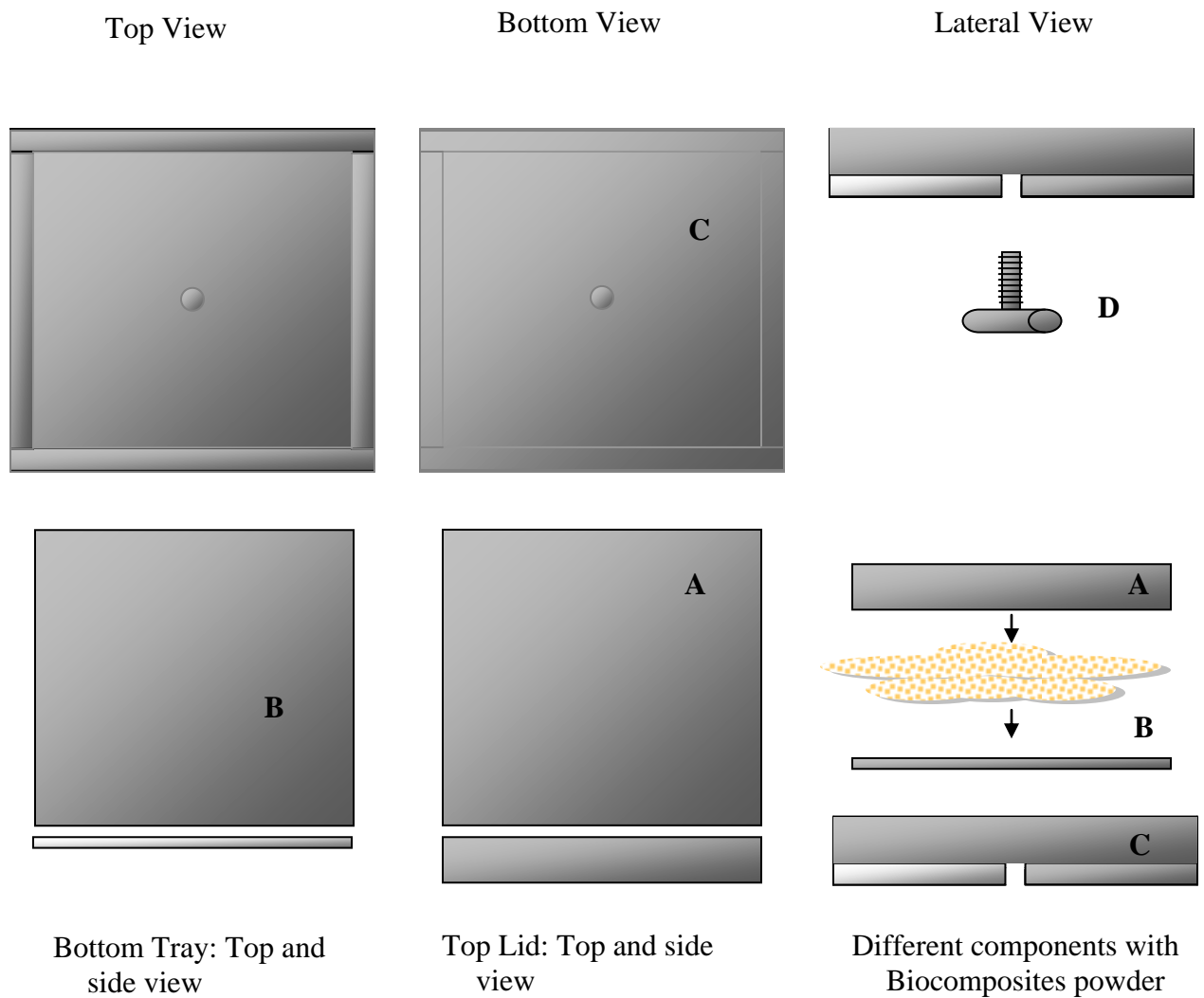


Figure 4.2 Compression mold diagram with different lids and sides being displayed

mold has a metal casing “C” with a hole in the bottom. A thin aluminum plate “B” is placed inside the casing to hide the hole present in the metal casing. A thicker aluminum plate “A” is used to cover the bottom plate as well as compress the ground biocomposite particles. This ensures that the biocomposites are level with respect to the mold. The plate “A” works as a lid that fits tightly inside the metal casing. Using the property of aluminum, when the entire mold is heated, the layers A and B create a tight fit within the casing

C, due to fast expansion. Once the production process is complete, the temperature is gradually lowered. At the same time, the tight fitting also decreases, making it easier to remove A and B.

Prior to any activity with the mold, - it was sprayed with a mold release (Si base) agent to ensure that the biocomposite material would come off easily. Bottom tray B was fitted into the tray C. The ground composite materials were spread on the top of tray B. In all cases 150 g of ground composite material was used. The composite material was leveled. Finally the top lid A was placed on top of the leveled biocomposite powder. The ground mixtures of extrudates were compressed in a compression mold, using a hydraulic press device. The composite mix was spread evenly in the mold that has a silicon based spray spread on the mold, working as a releasing agent. The ground materials of each sample category were exposed to two different pressures of 1.6 MPa and 1 MPa. The biocomposites particles were cooked at 150°C for 25 min. Once the production of biocomposite board was complete, the mold was air cooled.

Once the mold had cooled and it was possible to be in contact without protective gloves, a screw “D” as displayed in Figure 4.2 was used to gradually remove plates A and B. Once the top plate

was removed, – the biocomposite board was exposed to the outside environment and the board and inner plate were also completely removed. The sample was labeled and kept inside of a plastic bag to avoid any environmental contamination. The boards were cut into different pieces as required to create different samples.

4.1.5 Experimental sample replicates

Nine test samples were created based on fiber composition and operating pressure. Reasoning behind the sample numbers are provided in Appendix A. Table 4.1 contains the different sample naming conventions as well as complete number of samples that were used for this experiment.

Table 4.1 Total sample names, sets and numbers.

| Treatment Numbers | Pressure in MPa (P) | Fiber (F) Composition Percentage | Sample (S) Name (based on pressure – fiber % - sample number) | Number of Replicates | Data Points (for 5 different mechanical property: T, I, B,H,D) |
|--------------------------|----------------------------|---|--|-----------------------------|---|
| 1 | 1 | 5% | P1F05S1..P1F05S9 | 9 | 9 x 5 |
| 2 | 1 | 10% | P1F10S1..P1F10S9 | 9 | 9 x 5 |
| 3 | 1 | 15% | P1F15S1..P1F15S9 | 9 | 9 x 5 |
| 4 | 1 | 20% | P1F20S1..P1F20S9 | 9 | 9 x 5 |
| 5 | 1 | 25% | P1F25S1..P1F25S9 | 9 | 9 x 5 |
| 6 | 1 | 30% | P1F30S1..P1F30S9 | 9 | 9 x 5 |
| 7 | 1 | 35% | P1F35S1..P1F35S9 | 9 | 9 x 5 |
| 8 | 1.6 | 5% | P2F05S1..P2F05S9 | 9 | 9 x 5 |
| 9 | 1.6 | 10% | P2F10S1..P2F10S9 | 9 | 9 x 5 |
| 10 | 1.6 | 15% | P2F15S1..P2F15S9 | 9 | 9 x 5 |
| 11 | 1.6 | 20% | P2F20S1..P2F20S9 | 9 | 9 x 5 |
| 12 | 1.6 | 25% | P2F25S1..P2F25S9 | 9 | 9 x 5 |
| 13 | 1.6 | 30% | P2F30S1..P2F30S9 | 9 | 9 x 5 |
| 14 | 1.6 | 35% | P2F35S1..P2F35S9 | 9 | 9 x 5 |
| | 2 P type | 7 types of F loading % | 9 sample sets for pressure and fiber loading % | 9x14 = 126 Sample sets | 9 x14x5= 630 Total data points |

A separate data cluster consisting of 100% HDPE was also created for this experiment. This was used as a control data set. In this data set, for 1.6 MPa and 1 MPa, two data sets with 5 different

mechanical properties were created. This data was not used for NN training, but rather to compare with experimentally generated biocomposite data. All biocomposites data that have been derived from the research is presented in Appendix B.

4.2 Mechanical properties measurement

Data collection is the most important part of developing the neural network. Data has to be representative of the investigation domain.

4.2.1 Tensile test (ASTM D638 - 08)

Tensile tests were conducted on each type of sample with both 1.6 MPa and 1 MPa pressure compressed biocomposites, according to standard ASTM D638-02a. The standard equation for the tensile test is

$$\sigma_{ty} = \frac{F_{max}}{A}$$

where σ_{ty} is the tensile strength at yield, F is the maximum load value attained and A is the cross sectional area of the specimen.

4.2.2 Bending test (ASTM 5023 - 07)

Bending is the behavior of a structural element subjected to an external load applied perpendicular to the axis of the element. The test was done according to the ASTM 5023 specification. The specimen was tested in the Instron machine (Model 1011). In this case, the specimen is placed on two supports - while a force is exerted perpendicularly from the top.

4.2.3 Hardness test (ASTM D2240 - 05)

The ASTM D2240 testing standard was used for the hardness test. Each of the samples was placed on a flat surface, then a durometer was placed on the sample and ten readings were taken. The average of the readings is considered the output for a single data for the sample.

4.2.4 Impact test (ASTM D1822 - 06)

The impact test was done in accordance with ASTM D1822. In this case with a single swing of a pendulum (Impact test specimen was attached to this pendulum), the sample was allowed to be broken upon impact. This moves a dial from its initial resting point to a point where the applied impact force is indicated. The impact test samples were again of the dog bone structure but significantly smaller. The Tinius tensile impact test machine was used for this experiment.

4.2.5 Density test

Density is defined as mass per volume and expressed in the following equation

$$\rho = m/V$$

where ρ is the density of the composite material, m is the mass of the material and V is the volume of the material.

In calculating the density, an individual biocomposite board was cut into nine strips. From these strips nine other smaller pieces were cut and their weight was taken. After taking their weight, their dimensions (length, width and height) were measured. These are the nine data points for density as collected for the individual test specimen.

4.3 Neural networks

This section describes the neural network algorithms used for the training, as well as the process of creating the neural network for biocomposites using Matlab.

4.3.1 Backpropagation neural network training algorithm

Given a finite length input patterns $x_1(k), x_2(k), \dots, x_n(k) \in \mathbb{R}$, ($1 < k \leq K$) and the desired patterns $d_1(k), d_2(k), \dots, d_m(k) \in \mathbb{R}$,

Step 1: Select the total number of layers M , the number n_i ($i = 1, 2, \dots, M - 1$) of the neurons in each hidden layer, and an error tolerance parameter $\varepsilon > 0$.

Step 2: Randomly select the initial values of the weight vectors $w_{aj}^{(i)}$ for $i = 1, 2, \dots, M$ and $j = 1, 2, \dots, n_i$.

Step 3: Initialization:

$$w_{aj}^{(i)} \longleftarrow w_{aj}^{(i)}(0), E \longleftarrow 0, \quad k \longleftarrow 1$$

Step 4: Calculate the neural outputs

$$s_j^{(i)} = (w_{aj}^{(i)})^T x_a^{(i-1)}$$
$$x_j^{(i)} = \sigma(s_j^{(i)})$$

for $i=1, 2, \dots, M$ and $j = 1, 2, \dots, n_i$.

Step 5: Calculate the output error $e_j = d_j - x_j(M)$ for $j = 1, 2, \dots, m$.

Step 6: Calculate the output delta's $\delta_j^{(M)} = e_j \delta'(s_j^{(M)})$.

Step 7: Recursively calculate the propagation errors of the hidden neurons

$$e_j^{(i)} = \sum_{l=1}^{n_{i+1}} \delta_l^{(i+1)} w_{lj}^{(i+1)}$$

from the layer M-1, M-2, ..., to layer 1.

Step 8: Recursively calculate the hidden neuronal delta values:

$$\delta_j^{(i)} = e_j^{(i)} \sigma' (s_j^{(i)})$$

Step 9: Update weight vectors

$$w_{aj}^{(i)} = w_{aj}^{(i)} + \eta \delta_j^{(i)} x_a^{(i-1)}$$

Step 10: Calculate the error function

$$E = E + 1/k \sum_{j=1}^m e_j^2$$

Step 11: If $k = K$ then go to Step 12; otherwise $k \longleftarrow k + 1$
and go to Step 4.

Step 12: If $E \leq \varepsilon$ then go to Step 13; otherwise goto Step 3

Step 13: Learning is completed. Output the weights. (Gupta, 2003)

4.3.2 Steps involved in the training process

The steps involved in implementing a simple neural network are as follows:

- i) Assemble training data. ii) Create the neural network. iii) Train the network.
- iv) Simulate the network response to new inputs. (Matlab NN guide mathworks.com, 2008)

i) Assembling training data

For assembling the training data, – the biocomposites boards were created. These boards were then cut into different test specimens and five different mechanical tests were performed on these boards, as described previously. Once the tests were completed the data were stored in Excel and transferred to Matlab in different corresponding variable names.

ii) Creation of neural network

The neural networks were created with the aid of Matlab. While coding with C/C++, it was observed that there is the need for standardization and also comparison with other research work. In this view, the most commonly used application, Matlab's NNTOOL functionality, was used. This ensured standardization with regards to NN development, – allowing the comparison of error to other research.

Towards developing the neural network, - first, the appropriate neural network type was selected. Five different NNs were selected for the initial experiment. This was done by using the same number of neurons and the same number of layers for all of the NNs. Once the NN was complete, the network object was tested with a number of rigorous experiments. After testing, it was found that the feedforward backpropagation NN with TRANLM training algorithm was most suitable for this project.

The performance of the NN greatly depends on the neural architecture itself (Zhang et al., 2006). So, selecting an appropriate architecture for the selected neural net was done next. In this case, - a reduced number of neurons and layers were used. An increased number of neurons were used

to see the performance of the neural net. After observation of the increase or decrease in error, - the architecture and number of neurons that contributed to a decrease in error was selected.

iii) Training the network

Once the data creation and network object creation was complete, – the network object was trained with the aid of the experimentally acquired data. This ensured that the NN was aware of the actual data domain and could provide accurate results based on the design of the problem. In some cases, researchers use simulated results for the research work. However, data obtained directly from the experimental domain is preferable to simulated data. Finally, the NN was studied and observed to check its network response from different independent inputs representative of the application domain. If the results were successful, the creation of the neural net was complete. Otherwise, more data and more training was required.

iv) Simulation of the network response

Finally, the network response to the known dataset and the unknown dataset must be taken. The known data were design variables to inspect whether the NN was performing accordingly. The unknown variables were simply to provide output to different user inputs that are representative of the problem domain.

4.3.3 Using Matlab for creating neural networks for the biocomposites domain

Matlab® and its neural network libraries were used to model the neural network for this research project. The learning algorithms, NN training, NN validation and finally, the prediction tool all were all developed using the neural network. The neural network toolbox for neural network

development in Matlab is known as NNTOOL. It is accessed by typing NNTOOL in the MATLAB command prompt. The Graphical User Interface is structured in 7 different boxes. The input data uses all the data that was provided for training. The target data is the output data for the NN. The Input Delay states were used for Time Delay NNs. The Networks allows the user to create a new NN. The output data is the output provided once the simulation is being carried out. The error data provides all of the errors that were incurred while simulating the responses for input and output. The Layer Delay States were not used for this research purpose.

Based on the desired requirement for neural network type, input ranges, training function, performance function, number of layers and neurons, – a neural network with specific attributes can be created from this “Create Network or Data” child window . The neural network of choice can be further trained, validated and its weights realized by clicking on “view”. From here, a new child window was created. This is presented in figure 4.3. This child window allows the user the capacity to train, simulate and initialize and or view or edit weights for the neural network.

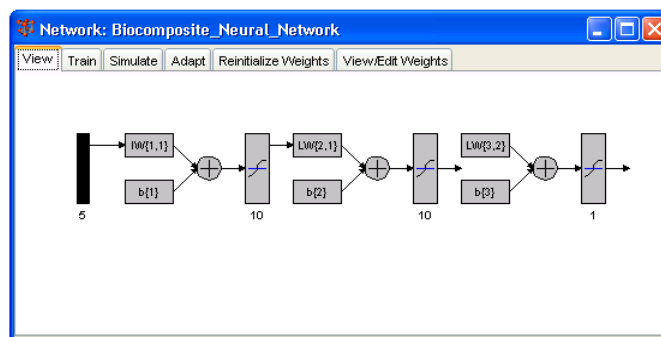


Figure 4.3 Neural network training window from Matlab® NNTOOL application

4.3.4 Design of feedforward backpropagation NN as used in the project

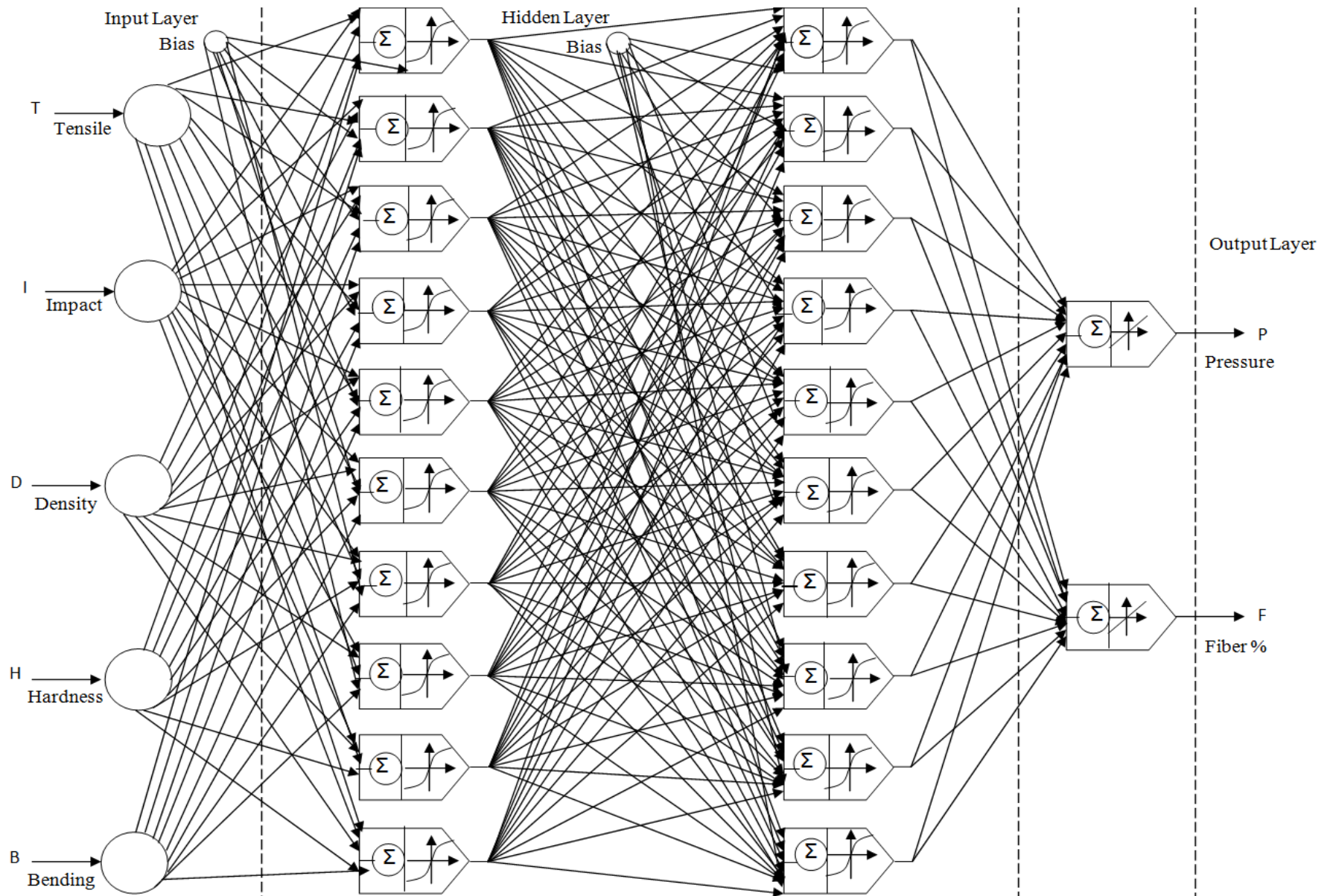


Figure 4.4 Three layer feedforward neural network with 5 inputs (tensile, impact, density, hardness, bending) and 2 (pressure, fiber) outputs

4.3.5 Training data size

At first, out of the 126 datasets 60% was allocated for training 20% for testing and 20% for the prediction. Upon doing the initial training, performance error was 0.16. At this point, the allocation was changed; training data was increased to 70%, test data remained at 20% and prediction data set was reduced to 10%. In this case, there was an increase in overall performance and it came to 0.10. Upon changing the dataset to training data set to 80%, testing data to 10% and 10% for the prediction dataset, there was a further increase in the performance to 0.06. This was still further away from the desired performance of 0.04 that is being attempted to achieve. Finally, a single data set from the seven fiber percentages and two pressures (7x2) were taken for the prediction and 112 datasets were used as the training data set. For testing, the Leave one out approach was taken as is described in the following section.

4.3.6 Testing approach

The general testing approach for neural networks has been to use 70% of training data set and 30% for testing dataset. However, this became a problem when all of the datasets were required for the training. For this research, 126 input datasets with 5 data points containing the tensile, impact, hardness, bending and density data were created. There were also 126 output datasets with 2 data points containing fiber percentage and pressure created. Due to the small number of datasets and the large number of weights for the neural network training, the maximum number of datasets possible was required for the training. However, to observe that the neural network was capable of predicting biocomposites fiber loading and operational pressure, 26 data sets were kept separate, for validation purposes.

In a scenario where there is a small number of training data sets, a number of algorithms such as cross-validation (Van H. et al., 1990), leave-one-out / jackknife (Spitz et al., 1999) and bootstrapping techniques (Efron et al., 1993, Guisan and Harrell, 2000) are available for testing models. For this research work, LOO (Leave one out, Capen et al., 1986. Osborne and Tigar 1992) was used. LOO is a special case of k-fold partitioning (Stockwell, 1992). In this type of testing methodology, one case was taken as a testing case and the remaining cases were used as the training set. In the LOO process for n data sets, n accuracy errors were calculated. Therefore, out of the 126 datasets, for every testing, 125 datasets were used as training sets and 1 set as the validation set. Five percent error or less was considered acceptable performance from the testing of the neural networks.

4.4 Software used for data analysis

Microsoft Excel 2003® has been used to store the initial data. It has also been used to generate graphs and figures that provided visual validation of different data generated from the research project. SAS software was used for the statistical analysis of the five mechanical properties.

4.5 Summary

The materials and methods section elaborates on the steps that were taken to create the biocomposites, as well as the development of neural networks. Different action blocks provided in Figure 4.5 shows all activities that were performed in order to complete this research project.

4.5.1 Steps in creating data from biocomposite boards

- Oilseed Flax fiber *L. usitatissimum*, was collected (Source of the flax fiber for this experiment was from Biofiber Industries, Canora, Saskatchewan).

- Contaminants (shive, dirt etc.) were removed by combing the fiber.
- Pretreatment with 5% NaOH by soaking fiber in solution for 3 - 4 hrs and continuous rinsing in distilled water for 3 h. (Alkaline treatment) (Sreekala et al., 2003).
- Water was removed by leaving the fiber in a container with porous bottom. Extra water was removed by extensively wringing the water out of the fiber.
- Treated fiber was dried in a drying cabinet for 3 days until fiber moisture content was lowered to 2% - 3%. Moisture content was calculated by repeatedly taking samples from the dryer and further drying it in an oven overnight to study the loss of moisture.
- Dried fiber was ground to 2 mm size using a bench top grinder. The ground fiber once fine ground was kept in sealed plastic bags.
- Injection grade HDPE pellets (Exxon Mobil) was ground using bench top grinder.
- Ground HDPE and flax fiber were mixed with 5% - 35% fiber loading at 5% intervals.
- Ground HDPE and ground flax fiber (oil seed flax) mix was extruded using a lab scale extruder with temperatures of 130°C in the 1st barrel zone, 143°C in the 2nd barrel zone, 150°C at the third barrel zone and 150°C at the die zone, the screw was rotating at 20 rpm. The extrudates were water cooled and dried in the drier for 48 hours.
- Ground extrudates were compressed at 1 MPa and 1.6 MPa (variable operating parameters) with a compression molding unit at 150°C (top and bottom plate).
- 5 different types of samples for testing were created.
- After testing, the data was stored in Microsoft Excel.

4.5.2 Steps in creating neural network from Matlab for biocomposites

- Stored individual data (input data), transferred from Excel to Matlab. They are given the variable names T - tensile force, D - density, I - impact force, H - hardness, B - bending.
- Corresponding pressure and fiber % data is transferred from Excel to Matlab. They were given the variable names P - pressure, F - fiber %.
- NNTOOL application was loaded in Matlab.
- 5 different types of neural networks were selected to investigate their best fit towards the biocomposite domain (cascade forward, feedforward backpropagation, feedforward time delay, neural unit (perceptron), nonlinear autoregressive exogenous model (NARX)). Based on training results and fastest to achieve the least error within shortest time frame, the NN model (feedforward backpropagation) was selected.
- Selected NN was tested for five different training algorithms.
- Based on selected NN and selected training algorithm (feedforward backpropagation neural network with TRAINSCG (scaled conjugate gradient backpropagation)) – training was done to reach desired performance.
- Data validation was done using Leave one out, (Capen et al., 1986. Osborne and Tigar 1992) algorithm.
- The training that provides the best validation result was accepted with the NN model that best satisfies the biocomposites domain.

4.5.3 Design layout

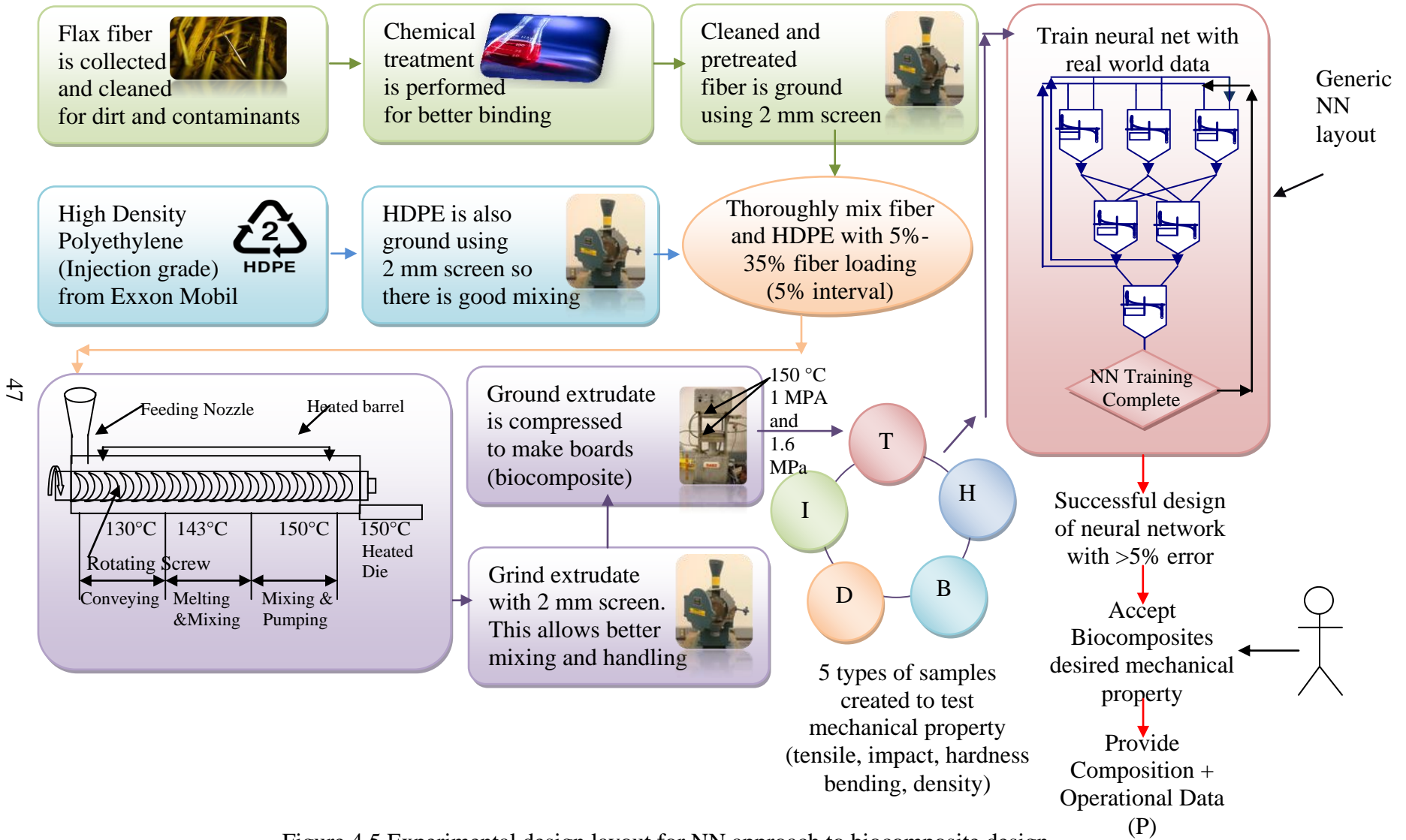


Figure 4.5 Experimental design layout for NN approach to biocomposite design

CHAPTER V

RESULTS AND DISCUSSION

The results and discussion chapter provides reasoning behind individual results and trends found from the experiments. The first section – “Experimental Data Validation” looks into validation for the experimentally obtained mechanical properties of the biocomposites. In this section, –the mechanical properties of the biocomposite materials have been analyzed, data trends highlighted and compared with 100% HDPE (control data).

The “Neural Networks Design” provides simulation results obtained from five commonly used neural network models. Analysis is provided on the most suitable neural network for this experimental domain. This section determines the optimal NN for the biocomposites domain.

The “Neural Network Results” section provides analysis on the results obtained from training and testing of the selected neural network architecture. It also looks into the prediction of the composite materials composition. Conclusions of the success of the NN are determined based on the results of composition prediction and operating parameter.

5.1 Experimental data validation

Data is important for neural network training. Without data fidelity, the model is not a good representation of the research domain. For neural networks, it is important to know that the data that is being used is authentic and representative of the domain. Hence, the analysis in this chapter tries to discuss that validity of data obtained from the research are valid and can be satisfactorily used towards neural network training.

Towards, data validation, all five (tensile, impact, hardness, bending, density) different types of mechanical tests for the biocomposite materials were considered. All individual samples were compared with their corresponding sample counterparts. Three-dimensional (3D) surface graphs were generated from this data. This did not include the 100% HDPE. The 3D graph provides a visual representation of the data domain, as well as, data trends and data anomalies.

The 100% HDPE was shown with respect to the averages of the nine samples for every individual mechanical property set in the line graphs. The 100% HDPE was created so that there were a set of control variables to compare with the biocomposites data. The data trends, when compared with HDPE materials, contributes to the data's representation within the research domain.

5.1.1 Tensile test

Towards establishing the validity of the tensile data, it was observed that pressure and fiber content % percentage had an effect on the biocomposites. With an increase in fiber content there was an increase in tensile strength. This was true until the fiber content reached 20% for biocomposites produced at 1.6 MPa pressure and 15% fiber loading at 1 MPa pressure. This was likely due to a reduction in good interfacial bonds between the fiber and polymer as a result of excess fiber. This is provided in figure 5.1

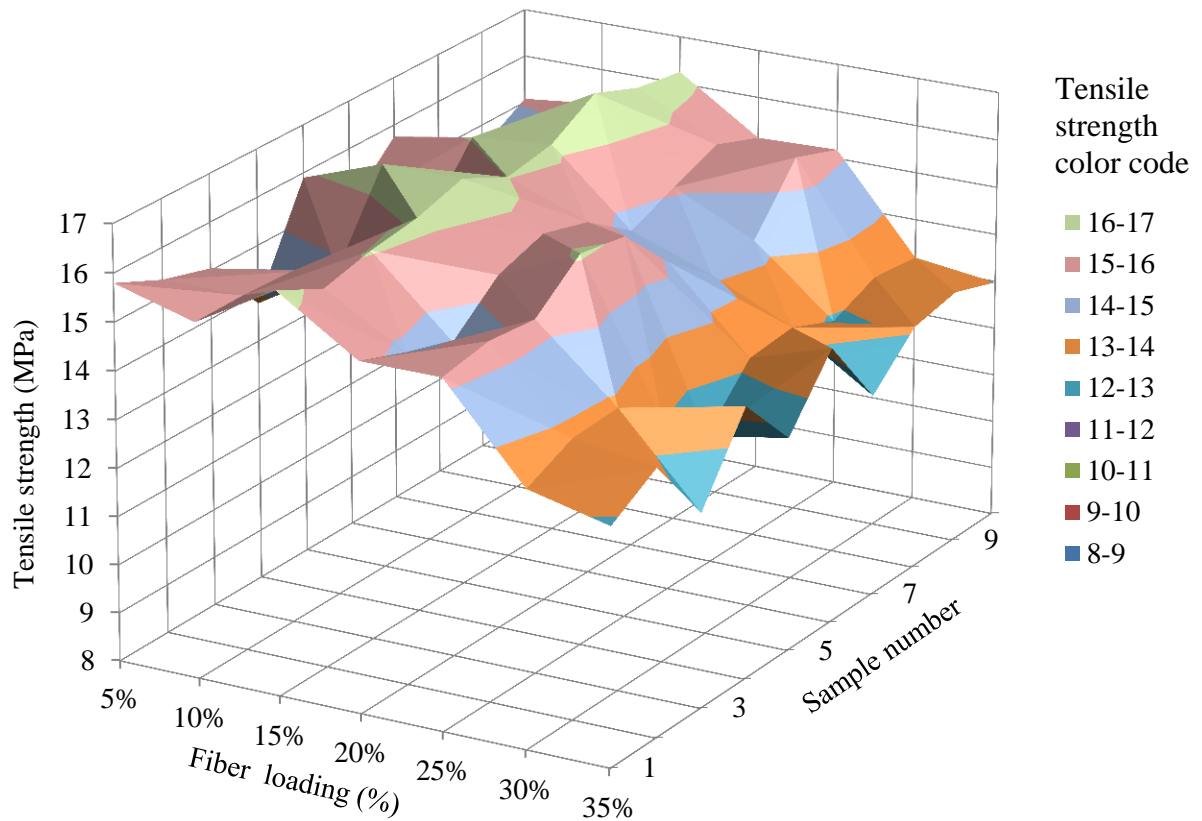


Figure 5.1 3-D graph presenting surface image of tensile strength vs. fiber loading % with regards to sample number. The samples were created at 1 MPa pressure.

At a pressure of 1 MPa the tensile strength varied from 13.01 MPa to 16.78 MPa (actual data is provided in Appendix B). At a pressure of 1.6 MPa, the tensile strength varied from 10 MPa to 19.24 MPa (actual data is provided in Appendix B). Higher pressure resulted in higher tensile strength for the composite material with increased fiber loading capacity. Mwaikambo et al. (2003) found similar results in their research of biocomposites. The increase in pressure and same residence and production temperature means that more HDPE molecules were exposed to the fiber which created better surface spread.

It was also important to notice that increased pressure meant that there was less variability in the data. With increased pressure, the tensile strength values were closer to each other. As shown in Figure 5.2, at 1.6 MPa, there is a significant amount of composite materials that are within the range of 14 – 16 MPa. The 16 – 18 MPa range was a result of increased fiber content and pressure. When the average of the different samples was considered,(9) a consistent trend line

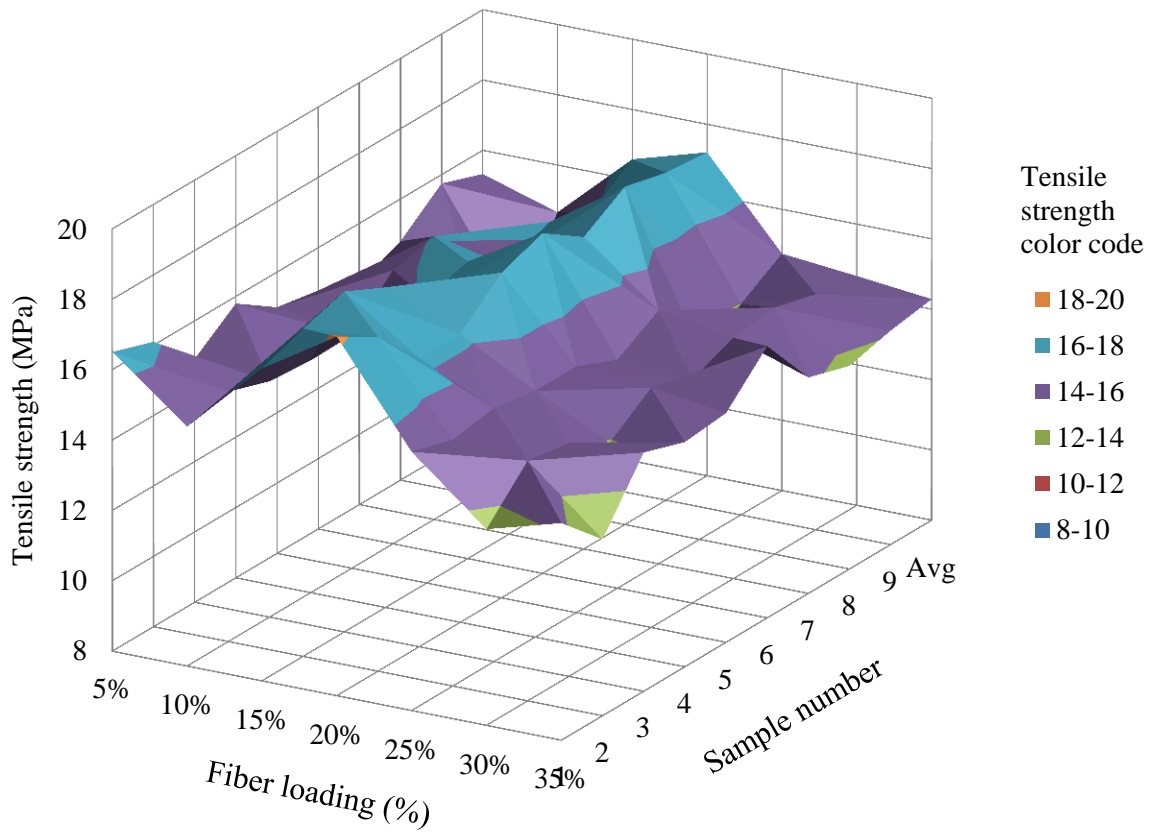


Figure 5.2 3-D graph presenting surface image of tensile strength vs. fiber loading % with regards to sample number. The samples were created at 1.6 MPa pressure.

was visible. The sample averages were compared with 100% HDPE. A gradual increase in tensile property was observed when compared with 100% HDPE. A number of studies also concluded that increase of fiber contributes to increased tensile property (Panigrahi et al., 2002a;

Wang et al., 2003; Wang et al., 2004). Figure 5.3 shows that the tensile strength for an operating pressure of 1.6 MPa is the highest (17.6 MPa) for a fiber content of 20%. For an operating pressure of 1 Mpa, the highest tensile strength (16.0 MPa) occurs at a fiber content of 15%.

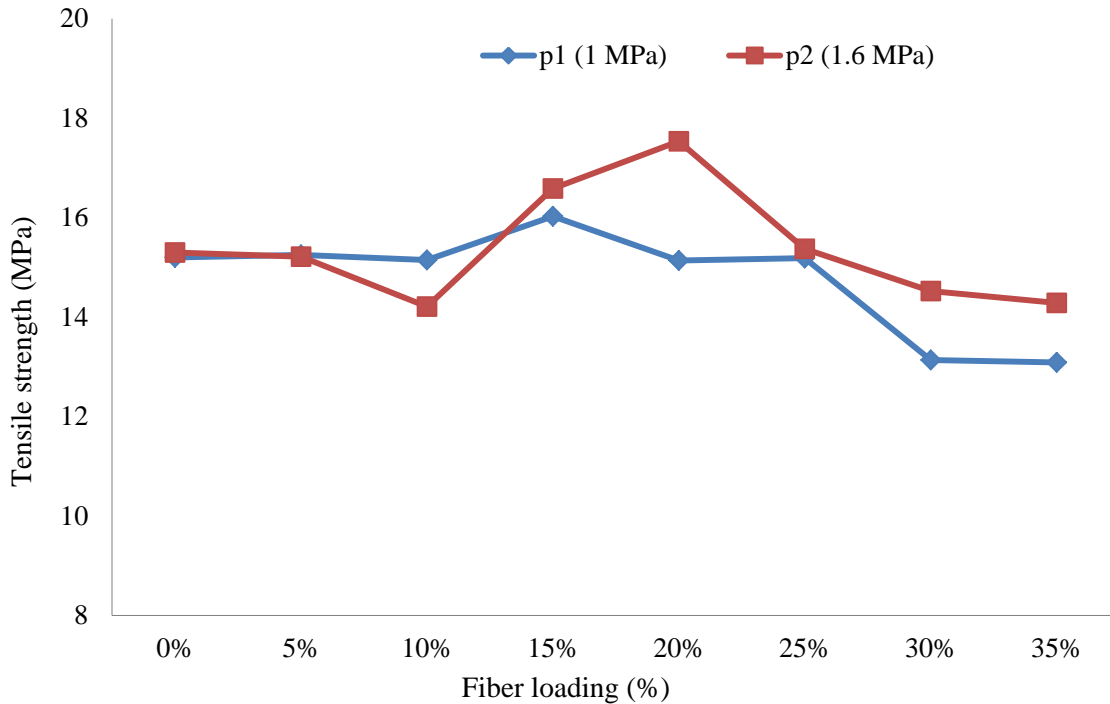


Figure 5.3 Average tensile strengths of different samples manufactured at pressures p1 (1MPa) and p2 (1.6MPa) with respect to different fiber contents loading %.

As the fiber content corresponding to the highest tensile strength was surpassed, the tensile strength decreased. This is a result of the higher fiber content creating weaker interfacial bonds.

5.1.2 Bending

Bending is a test to determine the ductility of the biocomposites. Within the scope of the 9 sample sets from Figures 5.4 and 5.5 it may be seen that as the fiber quantity increases there is an increase in bending strength. After fiber content reaches 25%, - the biocomposites samples show

a decrease in overall bending strength. Through physical observations, – it was noticed that when the fiber content passed 20%, the samples became increasingly brittle.

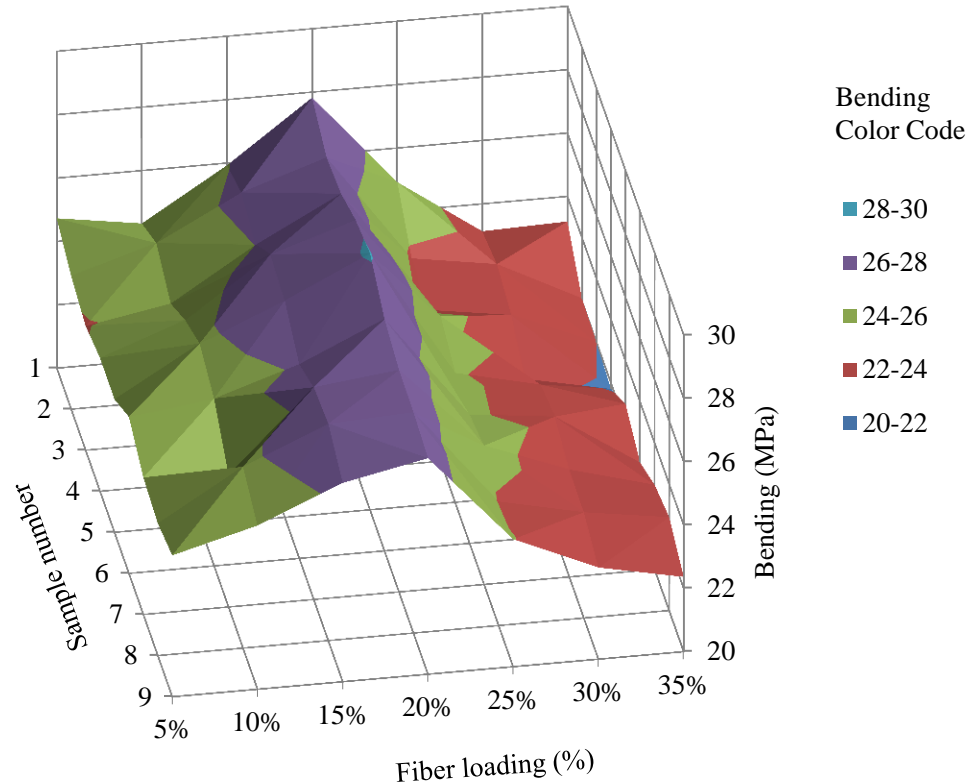


Figure 5.4 3-D graph presenting surface image of bending strength vs. fiber loading% with regards to sample number. The samples were created at 1 MPa pressure.

However the overall bending strength increase was not very significant. In fact, for both pressures 1 MPa and 1.6 MPa, the bending values were between 24 and 28 MPa. For the 1 MPa samples, the bending value significantly decreases for fiber contents of 30 and 35%. The samples with 35% fiber had almost no elasticity within them and would effectively snap into different segments.

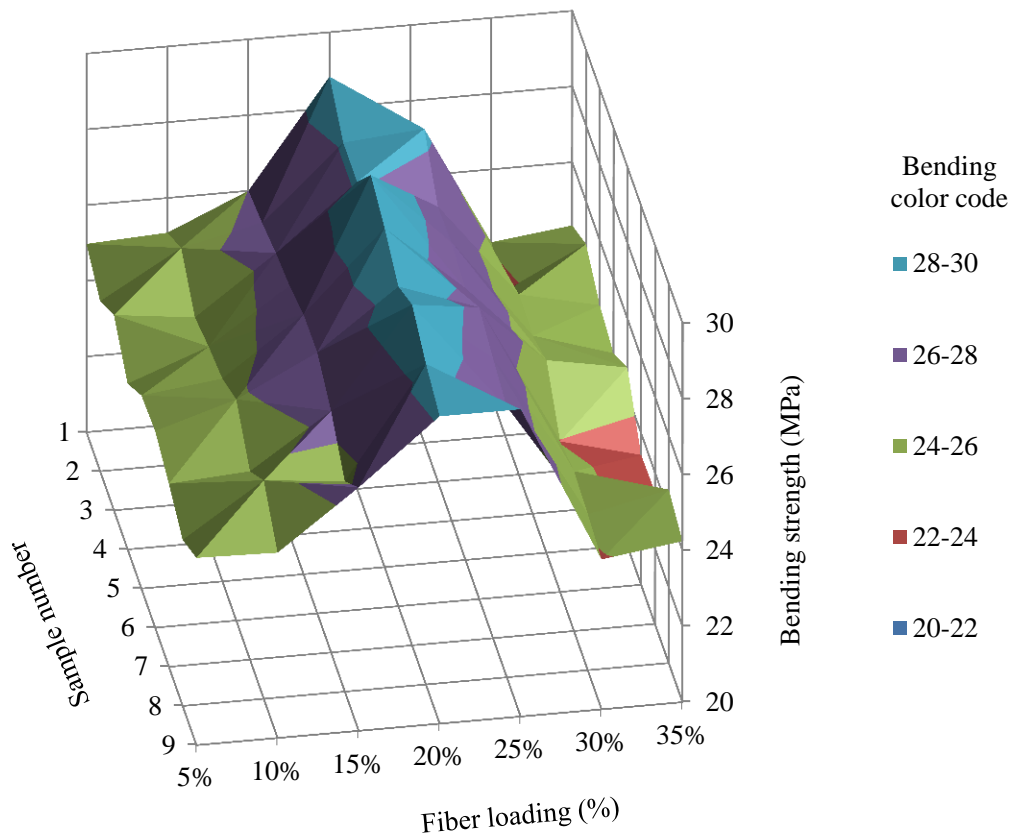


Figure 5.5 3-D graph presenting surface image of tensile strength vs. fiber loading% with regards to sample number. The samples were created at 1.6 MPa pressure.

The maximum bending strengths for both the 1 MPa and 1.6 Mpa pressure samples occurred for a fiber content of 20%. The values were 28.1 MPa and 29.3 Mpa, respectively. Figure 5.6 shows a graph of the averages of the bending strengths for the nine samples. For both

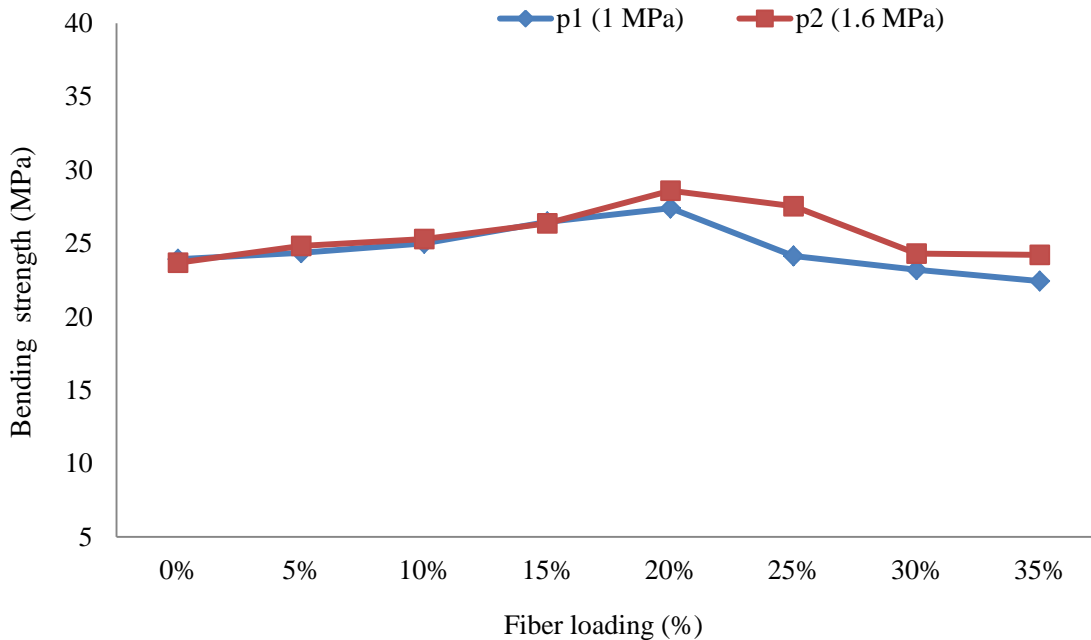


Figure 5.6 Bending strength of different samples manufactured at pressure p1 (1 MPa) and p2 (1.6 MPa) with respect to different fiber loading %.

1 MPa and 1.6 MPa processing parameters, – the bending strength gradually increased from 0% fiber load to 20% fiber load. At 25% there was gradual decrease and sharp decrease of bending strength starting at 30%. The maximum value for the average bending strength was 27.39 MPa for a processing pressure of 1 MPa and 28.59 MPa for 1.6 MPa. Both of these were higher than the 100% HDPE bending value. Also, there was no significant change in the bending property from 100% HDPE to a fiber content of 10% or 15%. This was due to the fact that the biocomposites with lower fiber concentrations retained some of the polymeric bending characteristics. The bending results presented here follow the trend that had been reported by other researchers in this field.

5.1.3 Hardness

The hardness test was done according to the ASTM 2240. In both pressures, the hardness was determined by the use of small sample specimens cut off from the board. The Shore durometer

type D was used to calculate the hardness. The results show that the hardness increased until the fiber content reached 20%. Again, the effect of pressure was apparent. For both operating pressures, with the increase in fiber, the hardness increases to a certain extent. However, beyond fiber contents of 20%, there was a gradual decrease of indentation. For the processing pressure of 1 MPa, the hardness did not change significantly between fiber contents of 15% and 20%. These are presented in figures 5.7 and 5.8.

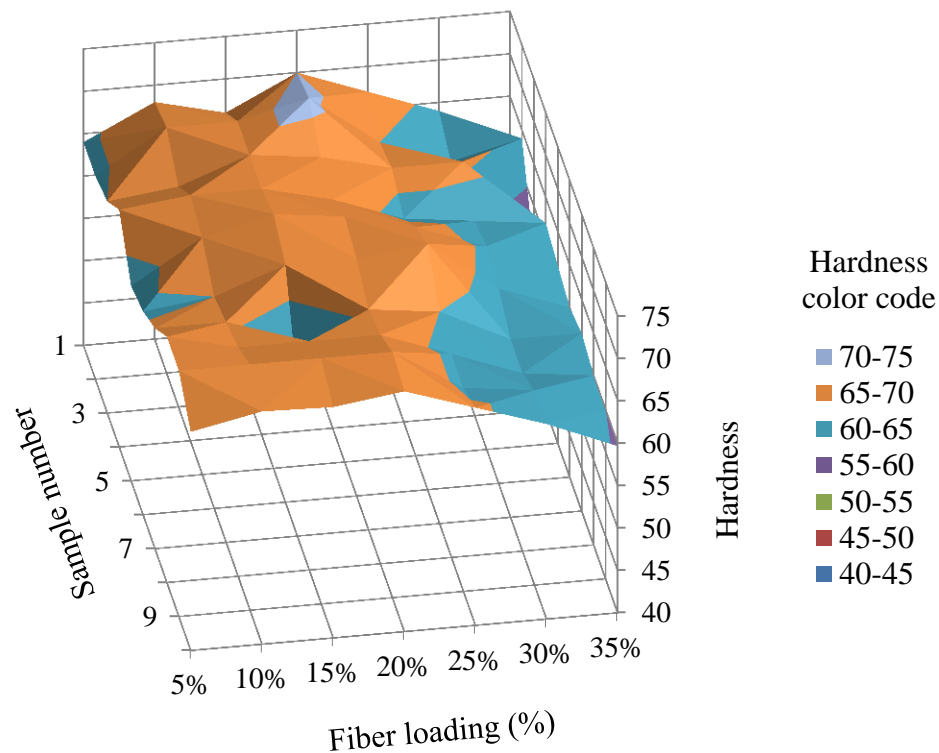


Figure 5.7 3-D graph presenting surface image of hardness vs. fiber % with regards to sample number. The samples were created at 1 MPa pressure.

However, as with the change in elasticity, there was also a change in the material’s hardness. In this case, the hardness gradually decreased. This was also true as many pores appeared in the boards. The micro pores contributed to hardness and increase of brittleness. Also the boards

increased fiber concentration decrease the overall hardness of the material. As the gradual increase of fiber occurs there was the gradual decrease of the biocomposites hardness.

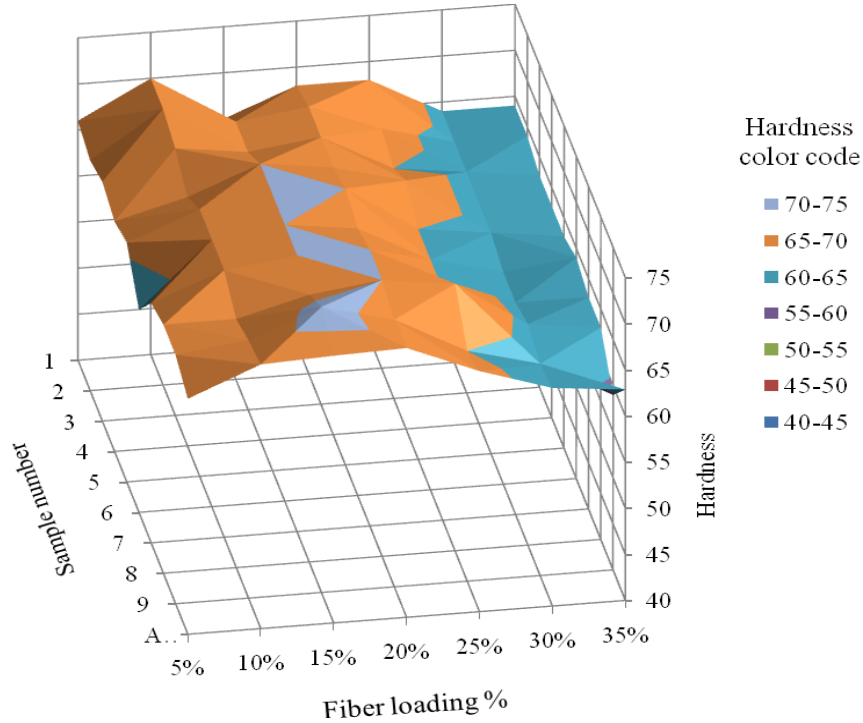


Figure 5.8 3-D graph presenting surface image of Hardness vs. Fiber % with regards to sample number. The samples were created at 1.6 MPa pressure.

From the trendline presented in Figure 5.9, it was seen that the hardness increases gradually with the increase in fiber loading. At 0% fiber, the hardness remained almost unchanged. The value of 65.0 for 1 MPa and 1.6 MPa can be simply attributed to the variability of the data collection process. This also points out that at 0% fiber, with variable pressure there was no change in the hardness of the material.

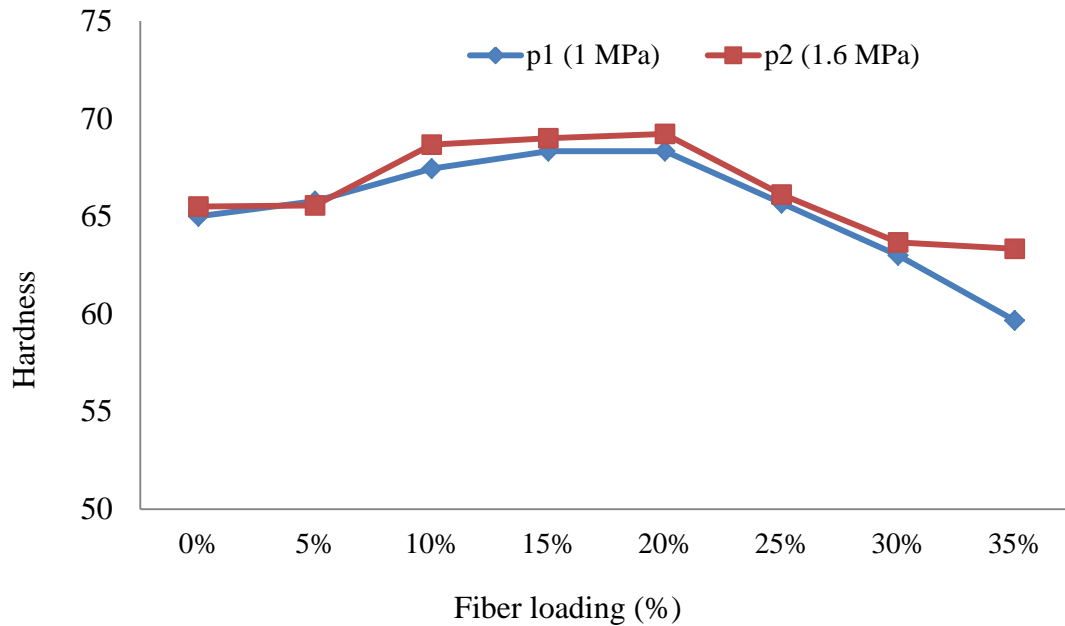


Figure 5.9 Hardness of different samples manufactured at pressure p1 (1 MPa) and p2 (1.6 MPa) with respect to different fiber loading %.

Furthermore, 5% fiber slightly increases the hardness. and At this point, – the 1.0 MPa and 1.6 MPa samples were on a par with each other. However with increase in the fiber amount, the effect of pressure really started to show with increased hardness at 1.6 MPa. Again this was indicative of the domain data and further validates the data trend.

5.1.4 Impact

Due to the nature of this experiment, there were significant variations in the different data that was received from the tests. Sample specimens created with pressures of 1 MPa had impact test results ranging from 40 to 75 kJ/m². For pressures of 1.6 MPa, the impact results ranged from 43 to 92 kJ/m². The faults in the 3-D plane data graph shows that there were some cases where the biocomposite samples would simply break during impact.

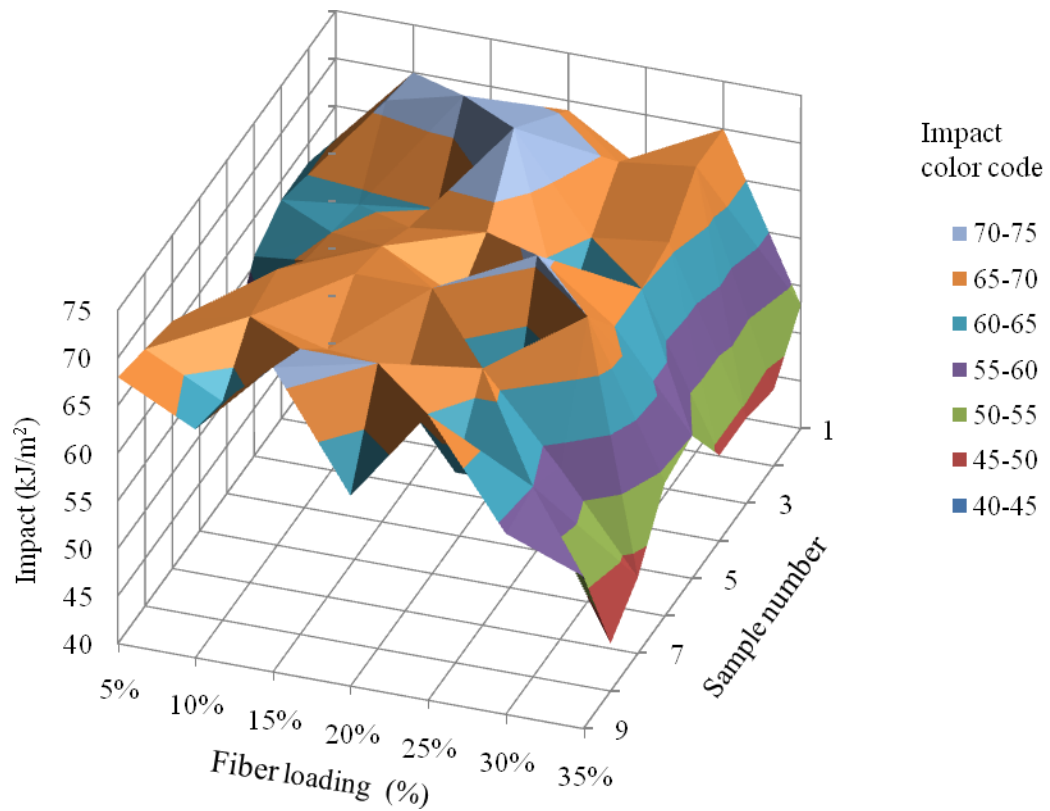


Figure 5.10 3-D graph presenting surface image of impact strength vs. fiber loading with regards to sample number. The samples were created at 1 MPa pressure.

However, when the average data was considered, again, the results corresponded to the biocomposites domain. As expected, an increase in fiber content increased the impact strength of the biocomposite material up to a content of 20%. However, after 20% fiber,

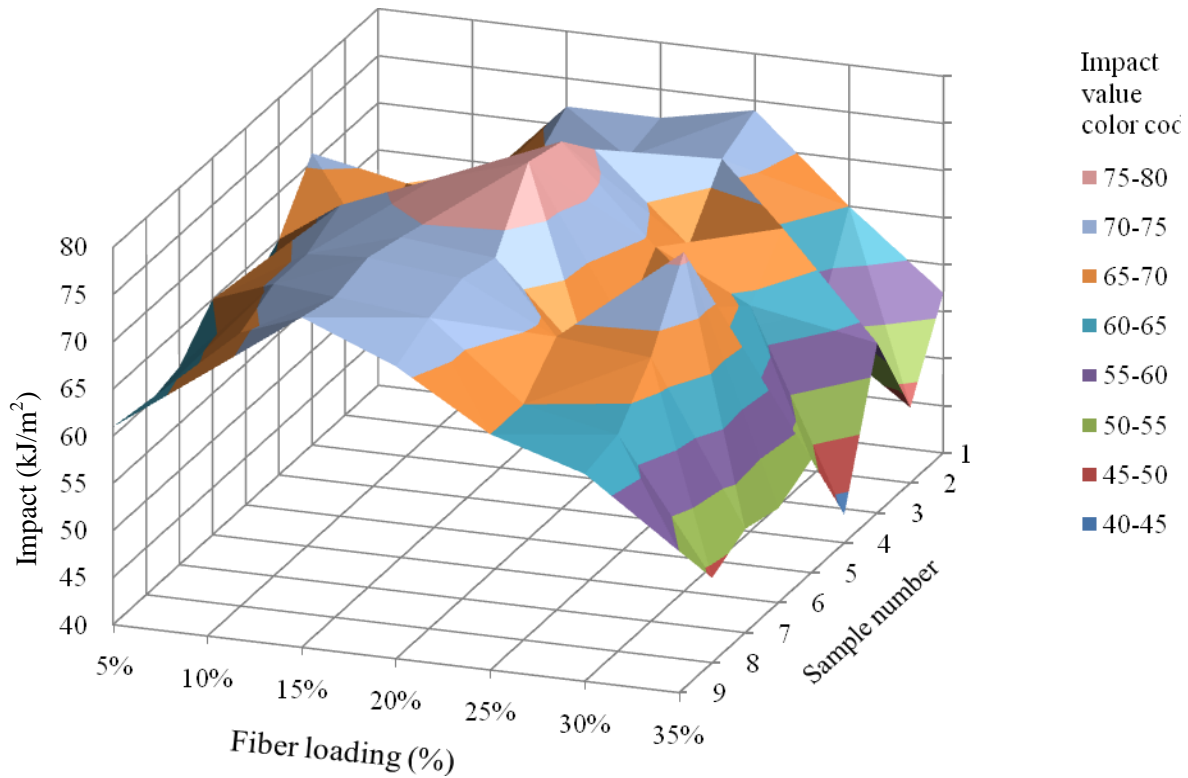


Figure 5.11 3-D graph presenting surface image of sample impact strength vs. fiber loading (%) with regards to sample number. The samples were created at 1.6 MPa pressure.

the impact strength decreases. This could be associated with the decrease in elasticity. It could be seen that with the increase of the fiber there was an increase in the impact strength of the biocomposite sample. However, at the same time, with the increased pressure there was a change in the impact results. It can be seen that the increased pressure results in increased impact strength. Results from the bending strength also showed that it was dependent on pressure. The average impact strengths are presented in Figure 5.12. For a processing pressure of 1 MPa, the highest value for impact strength was obtained

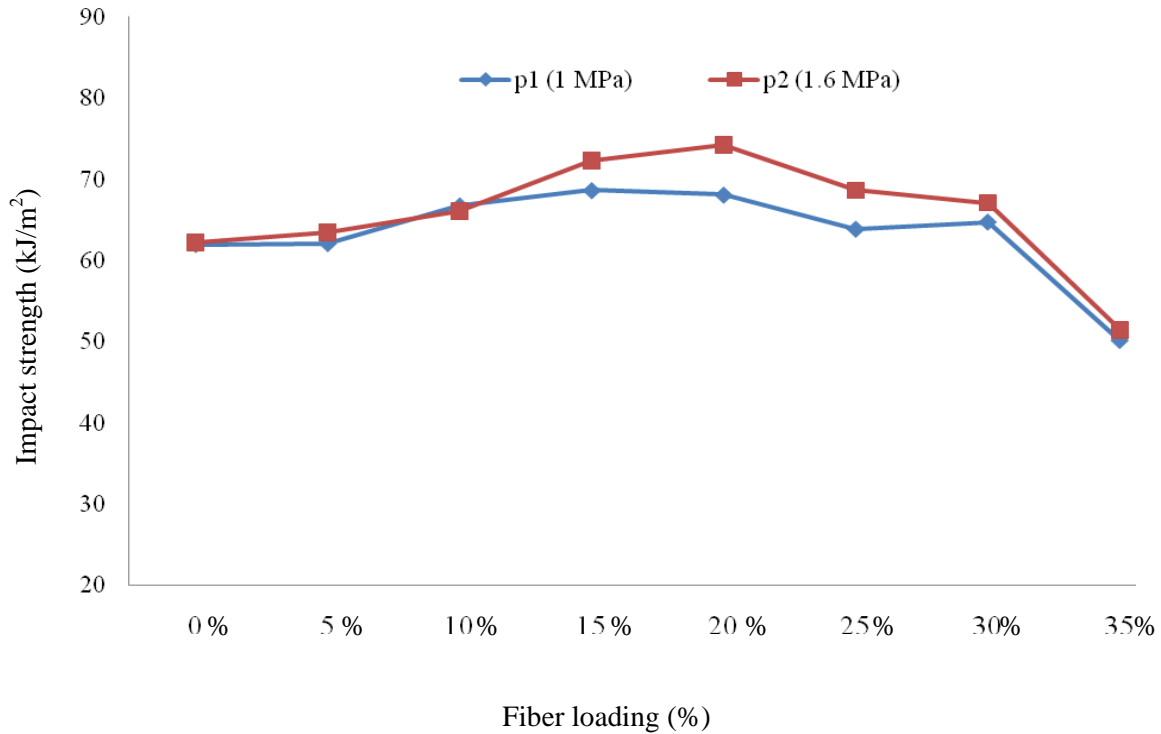


Figure 5.12 Impact strength of different samples manufactured at pressure p1 (1MPa) and p2 (1.6MPa) with respect to different fiber loading (%).

at 15% fiber loading. The highest value for 1.6 MPa occurred at 20% fiber. With increased pressure, further interfacial bonding between fiber and polymer matrix was created. This resulted in the capacity to increase the fiber percentage as well as increase the impact strength. When comparing the biocomposites to 100% HDPE, the line graph for 100% HDPE had lower impact strength than biocomposites.

5.1.5 Density

The density varied from 0.947 gm/cm³ to 1.097 g/cm³ for samples compressed at 1 MPa and varied from 0.95 gm/cm³ to 1.096 gm/cm³ for samples compressed at 1.6 MPa. If all processing parameters were kept at a constant, the change of pressure and fiber amount in the HDPE

polymer effects flax biocomposites density. In all of the treatments we can see that as there were increases in fiber – there were also increase in the density provided that there was higher pressure (1.6 MPa) involved. Increased amount of fiber means fiber loading would significantly increase. This would result in several air pockets and loss of overall material strength. However

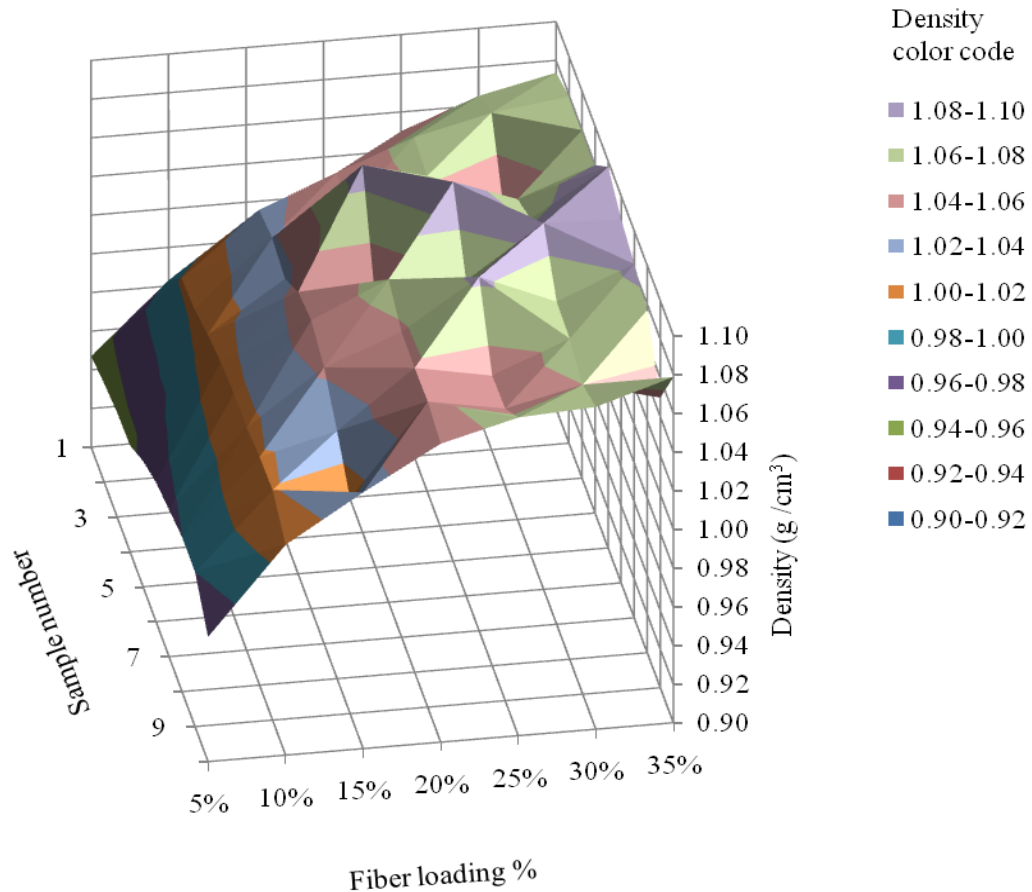


Figure 5.13 3-D graph presenting surface image of density vs. fiber loading % with regards to sample number. The samples were created at 1 MPa pressure.

with the pressure and heat – there was compaction of the fiber and polymer – in the creation of novel composition. But as we found that with further increase the – the density of the fiber would fall after a certain point. This is due to the loss of structural integrity in the biocomposite material.

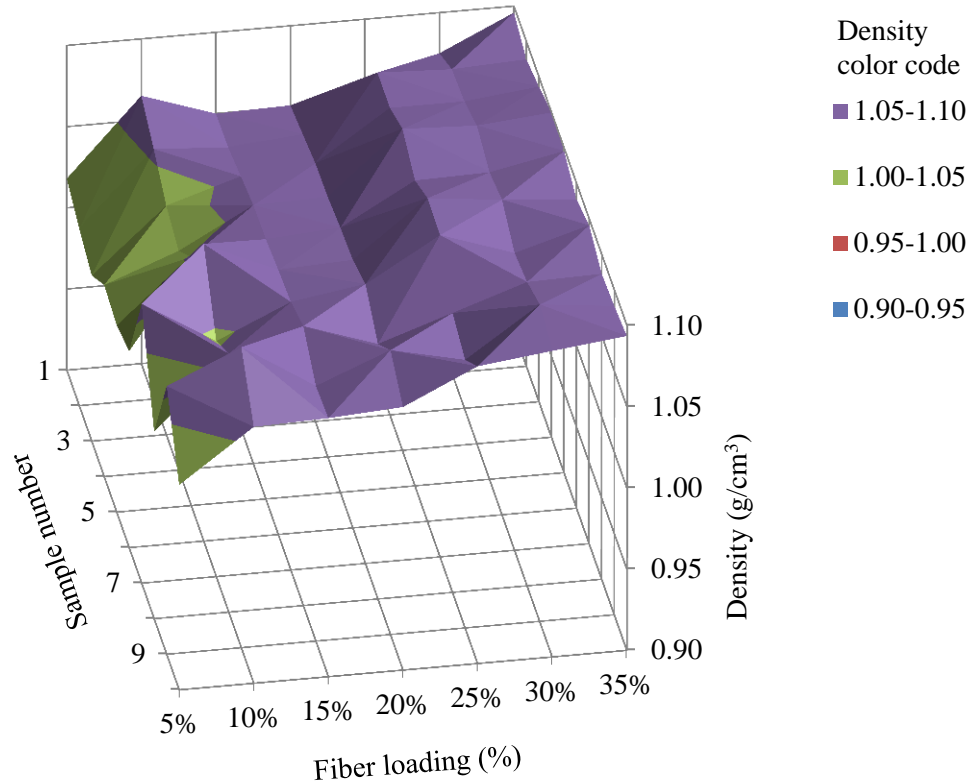


Figure 5.14 3-D graph presenting surface image of density vs. fiber loading % with regards to sample number. The samples were created at 1.6 MPa pressure.

Figure 5.15 shows a line graph comparing the average densities for the processing pressures of 1 and 1.6 MPa. this line graph shows that the change in pressure does not have any impact on the density of 100% HDPE. However, there was a difference in density between pressures of 1 and 1.6 MPa. This was due to the fact that although the 100% HDPE was produced with different operating pressures, in essence they were the same materials. During the production process, care was taken to ensure that there were no air pockets within the sample biocomposites boards. Air pockets within the board will greatly decrease the density value of the biocomposite.

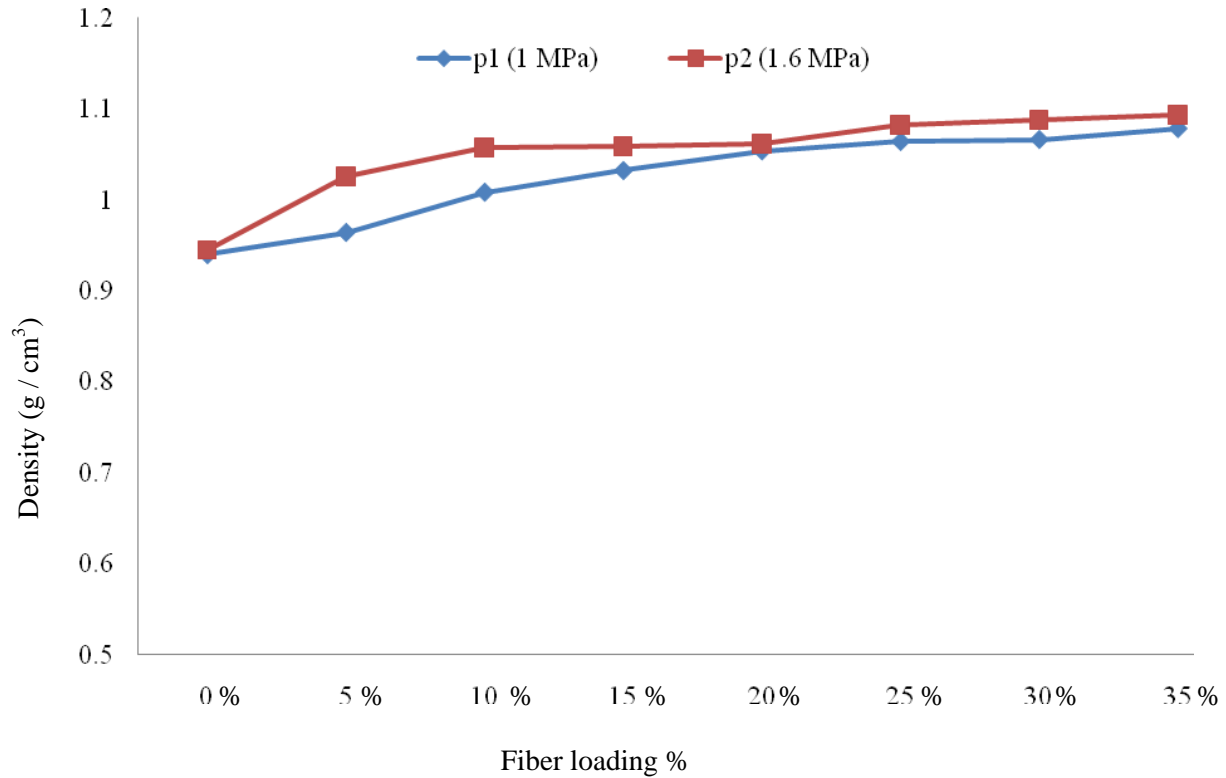


Figure 5.15 Density of different samples manufactured at pressure p1 (1 MPa) and p2 (1.6 MPa) with respect to different fiber loading %.

However, this was also common for the biocomposite materials. The grid line graph in Figure 5.15 shows the a gradual increase of density. It was expected that after 35% fiber loading, the density will fall due to lack of bonding and effective mixture of polymer and fiber. The values of 0.94 and 0.945 g/cm³ were representative values of density for 100% HDPE. Appendix C provides, a graph of density vs. fiber % curve assuming uniform mixing. Based on this we can see that the empirically obtained trend line approximately correlates to the mathematically obtained trend line.

5.2 Neural networks design

The performance of a neural network mostly depends on the neural architecture and the neural network settings. For this research work, the application Matlab TM has been used. A number of different types of neural networks were investigated to determine their suitability.

For this work, the supervised feed forward neural network with backpropagation learning algorithm was found to be the most suitable. The inputs to the neural network were experimentally obtained mechanical characteristics of the biocomposite material. The output was the composition and processing parameter (pressure) of the biocomposites.

Four other neural networks namely, cascade forward backpropagation, feedforward time delay, neural unit and NARX were also used for selection of the neural network. This section provides the results and reasoning behind the selection of the feedforward NN with backpropagation learning as well as the reasoning behind excluding other NNs. All data corresponding to the NN is provided in Appendix D.

5.2.1 Optimal neural network selection

In order to create the optimal neural net, – the first step was to observe the different neural networks that can favorably model the biocomposites property and provide a suitable output. The performance evaluation was carried out based on the time mean square error (MSE) and shortest time required to reach an acceptable performance. Four NN architectures had been selected with the same number of neurons. The first layer had 5 neurons, the second layer had 5 neurons and the third layer had 2 neurons. Three layers for the NN were selected since feed forward neural

networks with more than one hidden layer have been defined to be universal approximators (Kolmogorov, 1957; Kortik et al., 1989). The first two hidden layers used the tansigmoidal transfer function. The third hidden layer used the purelin transfer function.

Table 5.1 Layers description – FFBPNN, NARX, cascade forward BPNN, FF time delay.

| Layer number | Number of neurons | Transfer function |
|---------------------|--------------------------|--------------------------|
| 1 | 5 | TANSIG |
| 2 | 5 | TANSIG |
| 3 | 2 | PURELIN |

This was common for all NN's except for the neural unit, (i.e., Perceptron in Matlab terminology). The LOGSIG transfer function was not selected, since during normalization, it would decrease the input variables value. PURELIN was used in the third and final layer, – since this would be the output and a value within the range of 1 – 1.6 MPa and 5 – 35% was required as output. The first layer had five neurons since there were five inputs to the possible NN. The second layer had five neurons again, to be parallel with the 1st layer and for computational speed.

The fifth neural network selected was the “neural unit”. Its layers are described in Table 5.2.

Table 5.2 Layers description – neural unit

| Layer number | Number of neurons | Transfer function |
|---------------------|--------------------------|--------------------------|
| 1 | 2 | HARDLIM |

In this case, only 2 neurons were used in the first and only layer. The training function, adaptation learning function, performance function and the input ranges were also the same for the first four NNs'. Refer to Table 5.3.

Table 5.3 Functions and input ranges – FFBPNN, NARX, cascade forward BPNN, FF time delay.

| Training function | Adaptation learning function | Performance function | Input ranges |
|--------------------------|-------------------------------------|-----------------------------|---|
| TRAINLM | LEARNGDM | MSE | [10.7 9.2; 21.813 9.319; 40 92; 54 71; 0.947 1.1] |

For the neural unit, Table 5.4 provides the functions and input ranges as used during the simulation of the neural net.

Table 5.4 Functions and input ranges – neural unit

| Transfer function | Learning function | Number of neurons | Input ranges |
|--------------------------|--------------------------|--------------------------|---|
| HARDLIM | LEARNPN | 2 | [10.7 9.2; 21.813 9.319; 40 92; 54 71; 0.947 1.1] |

All of the neural networks were provided with a constant number of training parameters. The common training parameters were the following: maximum number of iterations, goals, maximum number of fails – before the process would truncate, and the value of Mu (Appendix E).

Table 5.5 Common training parameters as used for the different NN training

| | |
|----------------------------|---------|
| Iterations / Epochs | 1000000 |
| Goal | 1 |
| Max fail | 25 |
| Mu | 0.00001 |

The following is a list of the neural networks that were used towards the NN architecture selection process, in the order in which they were investigated:

- a) Cascade forward backpropagation neural network,
- b) Feedforward backpropagation neural network,
- c) Feed forward time delay neural network,
- d) Neural unit, and
- e) Nonlinear autoregressive network with exogenous inputs (NARX).

5.2.1.1 Cascade forward backpropagation neural networks:

The cascade forward backpropagation neural network was trained with 41,950 iterations. After 16 min and 36 s, the NN showed a performance of 5.70599. This is shown in Table 5.6. Figure 5.16 shows that the desired performance or goal of 1 was not reached by the cascade forward back propagation neural network after 250 epochs / iterations.

Table 5.6 Initial training results – cascade forward BPNN

| | |
|------------------------|-------------|
| Total iteration | 41950 |
| Performance | 5.70599 |
| Total time | 16 min 36 s |

After 250 epochs, – the performance (MSE) gradually normalizes to a value that was above 1. In this case, after 16 min and 36 s of running and training with all 126 of the input and output data sets, the NN performance reached 5.70599.

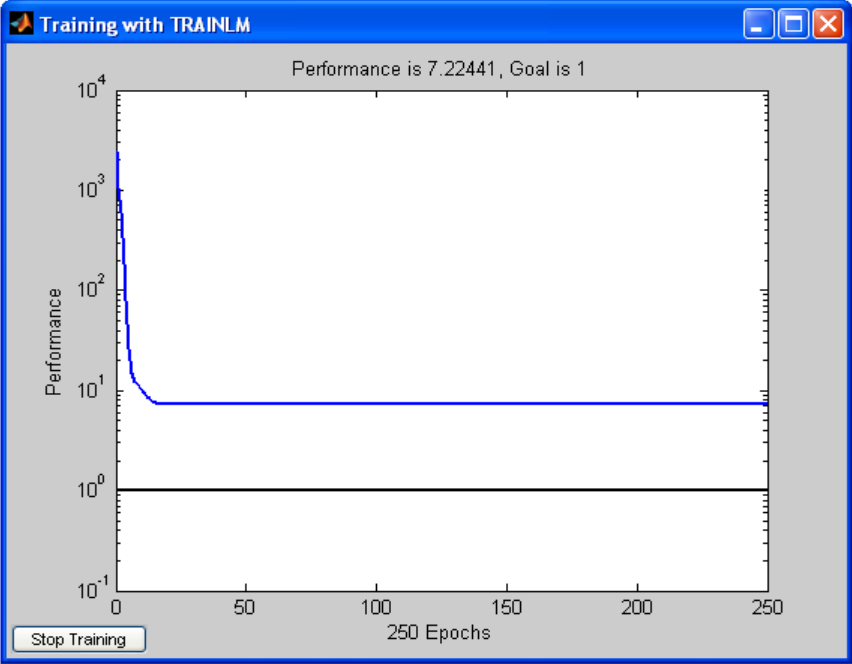


Fig 5.16 Performance vs. epoch graph for cascade forward BPNN

5.2.1.2 Feedforward backpropagation neural network:

For the feed forward backpropagation NN, after 3400 epochs, the performance was better than the cascade forward backpropagations terminal performance of 5.70599. However, after the simulation for the feed forward BPNN was stopped at 9150 iterations,

Table 5.7 Initial training results feed forward BPNN

| | |
|------------------------|------------|
| Total iteration | 10275 |
| Performance | 1.76267 |
| Total time | 6 min 43 s |

(Results and Graphs presented in Appendix D)

the performance was 2.75541. This was better than all of the NN that went through the trial runs. Figure 5.17 shows that the desired performance or goal of one was not reached by the FFBP neural network within the initial few iterations. However, its performance was significantly better than the cascade forward BP NN within the first 500 iterations.

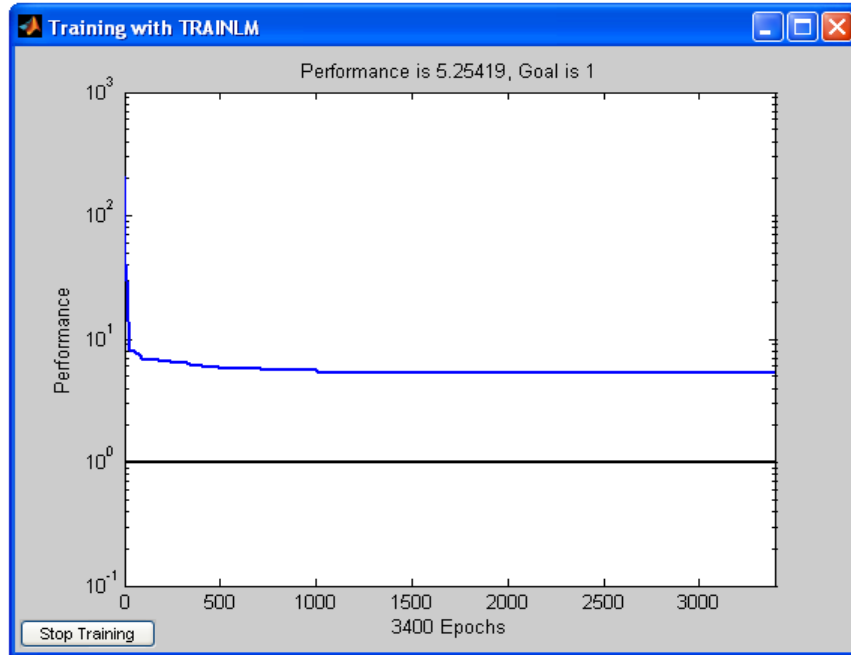


Fig 5.17 Performance vs. epoch graph for feed forward BPNN

5.2.1.3 Feed forward time delay:

Figure 5.18 shows that the desired performance or goal of 1 was not reached by the feed forward time delay neural network. At the same time, it was observed that the NN was considerably slower in training as compared to C – BPNN and FF - BPNN. The FFTD neural net training description and corresponding result is provided in Table 5.8

Table 5.8 Training results feed forward time delay NN

| | |
|------------------------|-------------|
| Total iteration | 47025 |
| Performance | 2.35769 |
| Total time | 18 min 47 s |

(Results and Graphs presented in Appendix E)

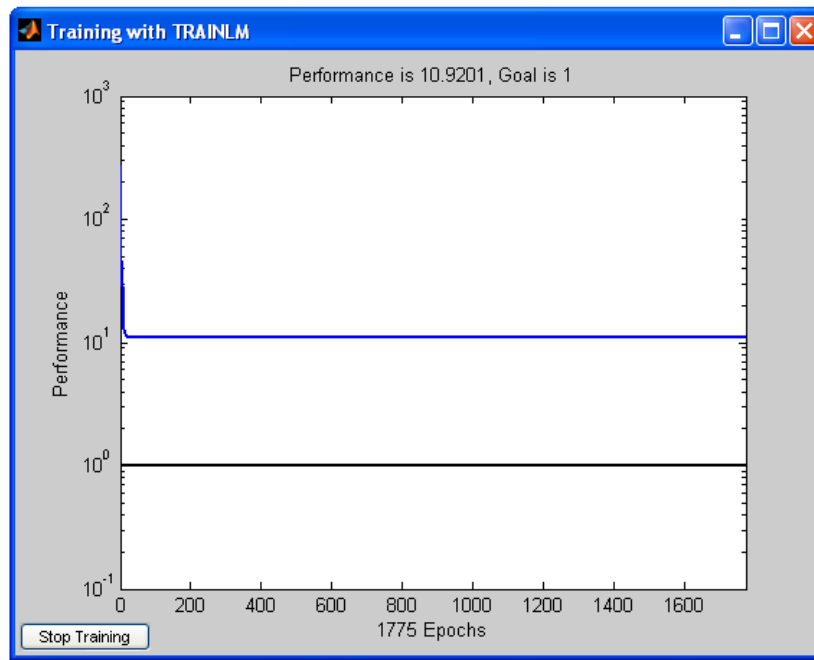


Fig 5.18 Performance vs. epoch graph for feedforward time delay NN

This was due to the time delay in the NN. The delay with computation continued to be observed even as the NNs' time delay was initiated to 0. Even after considerable time and 47025 epochs, the NN did not have any significant performance improvement. This was shown in Appendix D.

5.2.1.4 Neural unit

The neural units training description and corresponding results are provided in table 5.9. Figure 5.19 shows that the desired performance or goal of 1 was not reached by the neural unit (Perceptron) neural network. The line showing performance versus epoch was simply parallel to the x axis, since the NN was not able to fully generalize the problem. This neural network was one of the early neural networks. As a result, it has failed to emancipate the biocomposite data domain.

Table 5.9 Training results for neural unit

| | |
|------------------------|------------|
| Total iteration | 2625 |
| Performance | 9.625 |
| Total time | 5 min 12 s |

(Results and graphs presented in Appendix E)

Also, since the output had 2 neurons, – the time to train also took considerably long. The total time 5 min 12 s represents the time at which this neural networks training was terminated. For small clusters of data and simple function approximation, this may be a good choice. However, for more complicated systems such as the one in this research, the perceptron neural network did not appear to be an ideal candidate. Although the neural unit use has been performed in this research, however, it has not contributed to any significant insight.

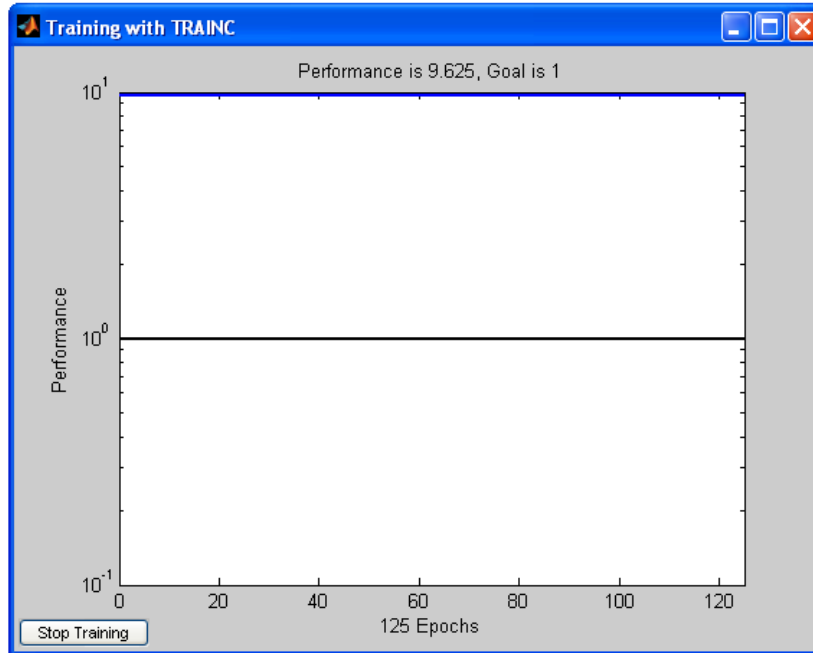


Fig 5.19 Performance vs. epoch graph for neural unit (Perceptron) NN

5.2.1.5 Nonlinear autoregressive network with exogenous inputs (NARX):

The performance of the NARX NN was not acceptable for further training. Due to the its recurrent dynamic nature – instead of feedback connections at the input and the output layer, the

Table 5.10 Initial Training Results for NARX

| | |
|------------------------|-------------|
| Total iteration | 64350 |
| Performance | 17.208 |
| Total time | 20 min 41 s |

(Results and graphs presented in Appendix E)

NN has feedback mechanisms in different layers of the NN. This increases the overall NN training time. The NARX was slower than its counterparts. It took almost 20 minutes ~ to reach to the performance of 17.208 with a goal of 1. This is displayed in figure 5.20.

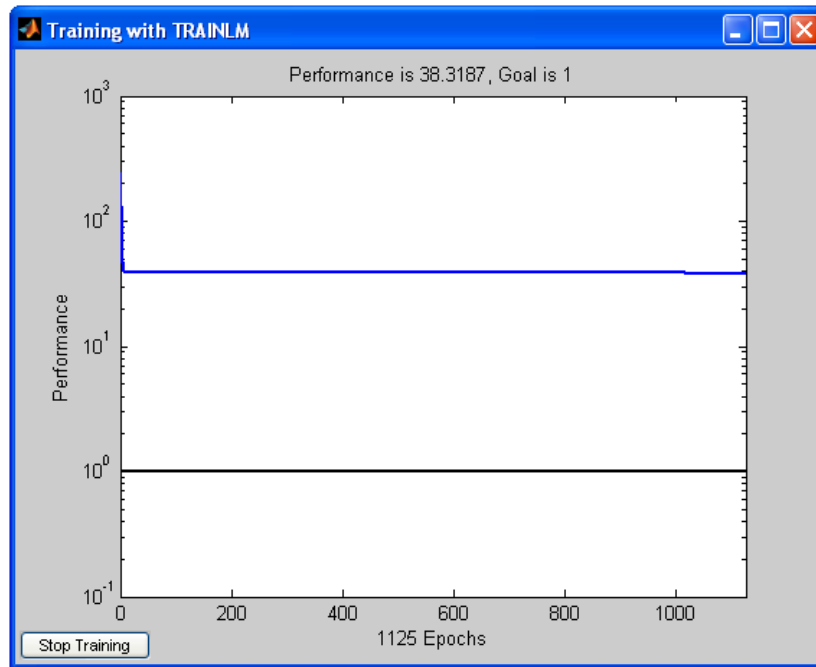


Fig 5.20 Performance vs. epoch graph for NARX

At the same time, – it was only able to complete 64350 epochs, – whereas the feed forward back propagation NN would complete a significantly more epochs within this time frame.

5.2.2 Performance matrix for selection of optimal neural architecture

Table 5.11 provides the results for the five neural networks that were initially studied to find the neural network best-suited for this research. Both the NARX and Neural Unit NN required a large amount of time towards for the training phase. The NARX training time requirement was due to the feedback mechanism within individual layers. However due to failure to reach comparable performance with respect to the feed forward back propagation NN – the NARX NN, Neural unit and feed forward time delay was not further investigated for this research work.

Table 5.11 Comparison of neural networks used in research

| Number | Name of neural network | Performance (MSE) | Time required (min) | Epochs |
|--------|----------------------------|-------------------|---------------------|--------|
| 1 | Cascade forward NN | 5.70599 | 16 min 36 s | 41950 |
| 2 | Feed forward BPNN | 2.35769 | 18 min 47 s | 47025 |
| 3 | Feed forward time delay NN | 3.98453 | 38 min 19 s | 70875 |
| 4 | Neural unit | 9.625 | 5 min 12 s | 2625 |
| 5 | NARX | 17.208 | 20 min 41 s | 64350 |

Overall, the feed forward back propagation NN showed the best performance and lowest time requirement. Based on these two considerations, the FF BPNN was selected as the neural network of choice for this experiment.

5.2.3 Training algorithm selection for FF BP neural networks

The feed forward neural network described above was further trained with six different training algorithms. Similar to the evaluation technique used for the different neural networks, – the training algorithms were evaluated for time required and performance recorded for the same weights and biases in the different layers of the FFBPNN.

5.2.3.1 Learning algorithms

Figure 5.21 shows the different backpropagation training algorithms that were investigated in the NN training. These were used to find the most efficient training algorithm that can effectively predict the composition and pressure of the biocomposite materials. The training

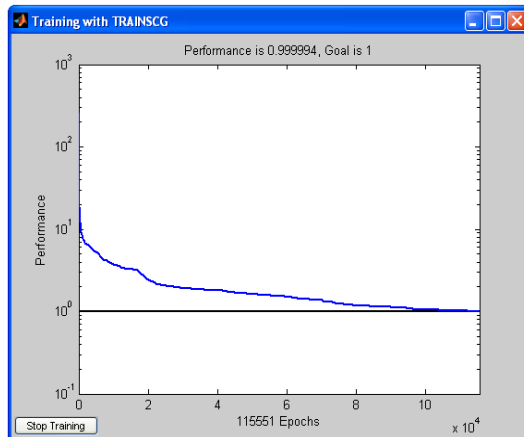
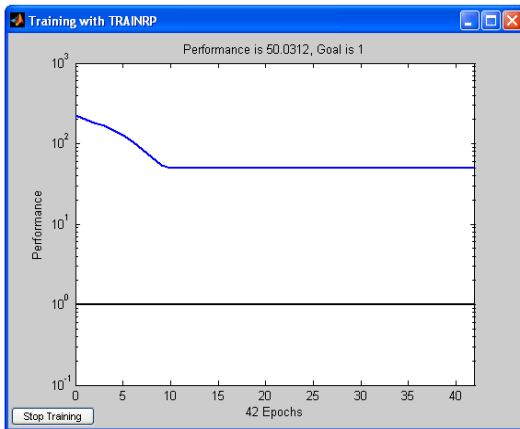
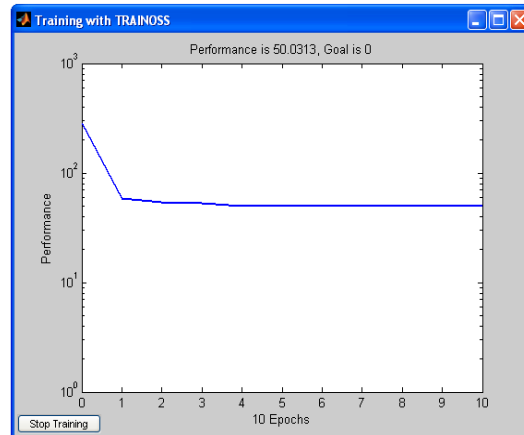
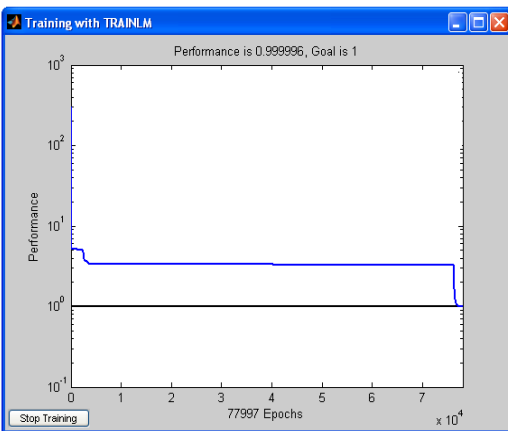
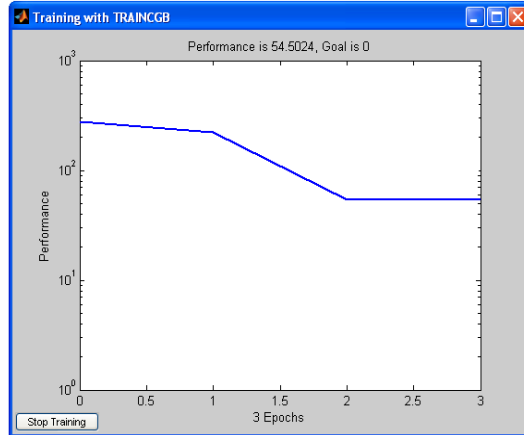
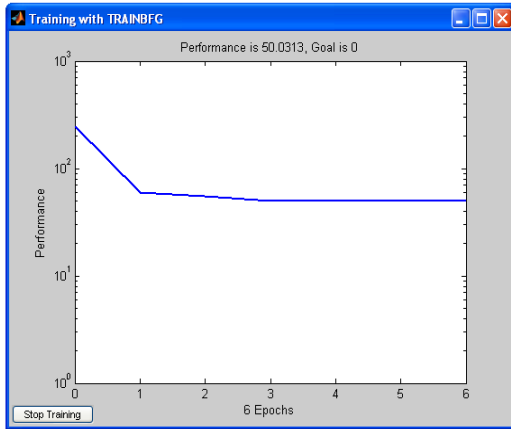


Figure 5.21 Performance vs. Epoch graph for Feedforward back propagation neural network with 6 different types of training algorithms – TRAINBFG, TRAINCGB, TRAINLM, TRAINOSS, TRAINRP, TRAINSCG. Only TRAINSCG and TARINLM were successful to reach goals of 1

algorithms that were investigated: are 1. TRAINBFG, 2. TRAINCGB, 3. TRAINLM, 4. TRAINOSS, 5. TRAINRP, 6. TRAINSCG. This selection was based on research by Vladimir Vacic (www.cs.ucr.edu, 2009) where enhanced performance was based on training, validation, testing and time. For this experiment, – the neural architecture was changed to have 10 neurons, in the first hidden layer, 10 neurons in the second hidden layer and 2 neurons in the third hidden layer. All of the neurons were exposed to the same amount of weight and bias.

Table 5.12 Training algorithms with required time, epochs and performance

| Number | Function name | Algorithm | Time required | Epochs | Performance |
|--------|---------------|--|---------------|--------|-------------|
| 1 | TRAINBFG | BFGS quasi-Newton backpropagation | 6 s | 6 | 50.0313 |
| 2 | TRAINCGB | Powell –Beale conjugate gradient backpropagation | 4 s | 3 | 54.5024 |
| 3 | TRAINLM | Levenberg-Marquardt backpropagation | 38 min 22 s | 77997 | 0.999996 |
| 4 | TRAINOSS | One step secant backpropagation | 10 s | 10 | 50.0313 |
| 5 | TRAINRP | Resilient backpropagation (Rprop) | 8 s | 42 | 50.0312 |
| 6 | TRAINSCG | Scaled conjugate gradient backpropagation | 29 min 12 s | 115551 | 0.999994 |

5.2.3.2 Learning algorithm selection

The TRAINLM (Levenberg – Marquardt) algorithm was found to be optimal for the Feed forward back propagation neural network in the biocomposites domain. It showed a performance of 0.981245 after 578 iterations or epochs were complete. The TRAINBFG, TRAINCGB and TRAINOSS training algorithms were not suitable for the FF BPNN, because all three of the algorithms failed to provide any output and exited upon training. TRAINSCG showed good performance but it was inferior to the TRAINLM algorithm. Hence, – the TRAINLM training algorithm was accepted as the most suitable training algorithm for the FF BPNN. The different weights and biases used are provided in Appendix D. For all training algorithms, the weights and biases were the same.

5.2.4 Optimized neural network

From over all research it is finally concluded that an optimal neural network can be designed for the biocomposites domain. The feed forward back propagation neural network came out as the decisive optimal neural network. Although commonly used it has the capacity to model multiple domains and was flexible and easy in use. Finally the TRAINLM training algorithm was used to in the optimal neural network. A 10 neuron 1st hidden layer, 10 neuron 2nd hidden layer, and 2 neuron 3rd hidden layer was selected as the architecture for the NN. The first hidden layers learning algorithm was tansigmoidal. The 2nd hidden layers learning algorithm was purelin function. The figure representing the neural network is presented in figure 5.22. The higher numbers of neurons were seen as an improvement from an architecture that contained fewer neurons (5 neurons, 1st hidden layer, 5 neurons 2nd hidden layer and 2 neurons 3rd hidden layers).

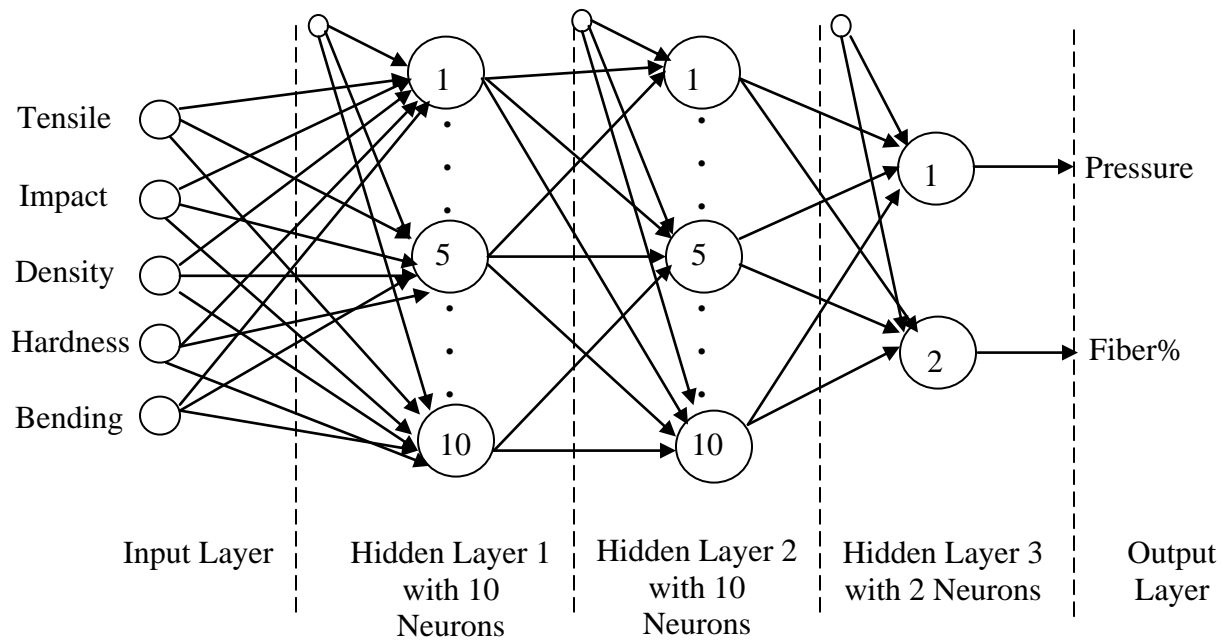


Fig 5.22 Feedforward backpropagation neural network with TRAINSCG

5.3 Neural network results

For the neural network, a multi-layer feed-forward neural network with back propagation learning algorithm and TRAINLM training algorithm was used. The LOO technique was used to test and train the neural network. All of the data sets contained five different mechanical properties that corresponded to specific processing pressures and fiber contents.

5.3.1 Training and testing results

For the first run, – there were 125 datasets used for training, and the 126th dataset was used for testing. In this case, the performance was 0.419. So, next the 1st – 124th dataset and the 126th dataset was used for training and the 125th dataset was used for testing. This process of LOO was continued until the 104th dataset was used for testing. For this dataset, – it was realized that the

NN was optimally trained, since the performance reached the goal of 0.05. Hence, the training and testing regimen was terminated. Results are given in Table 5.13.

Table 5.13 Training and Testing Performance Results using LOO technique

| Test number | Testing data | Performance (MSE) |
|--------------------|---------------------|--------------------------|
| 1 | 126 | 0. 82 |
| 2 | 125 | 0. 13913763 |
| 3 | 124 | 0. 248 |
| 4 | 123 | 0.3157273 |
| 5 | 122 | 0.6673 |
| 6 | 121 | 0.860526 |
| 7 | 120 | 0.3303 |
| 8 | 119 | 0.070409 |
| 9 | 118 | 0.224 |
| 10 | 117 | 0.556446 |
| 11 | 116 | 0.567149 |
| 12 | 115 | 0.2307 |
| 13 | 114 | 0.085 |
| 14 | 113 | 0.89143 |
| 15 | 112 | 0.718905 |
| 16 | 111 | 0.09065 |
| 17 | 110 | 0.46682 |
| 18 | 109 | 0.79297 |
| 19 | 108 | 0.24286 |
| 20 | 107 | 0.48149 |
| 21 | 106 | 0.66197 |
| 22 | 105 | 0.49162 |
| 23 | 104 | 0.0465501 |

5.3.2 Biocomposites prediction results

Fourteen sets of experimentally derived data were selected for testing the NN for its prediction capability. The data was randomly selected using a two-dimensional array in Microsoft Excel. The first array was for the data type and the second array was for the data cluster.

For the unknown dataset, the different averages from the individual data clusters were selected. The neural network was not trained with this dataset. However, they both represent the same data domain and collected with efforts in the same research. The error percentage indicates the ability of the neural network to generalize.

Table 5.14 shows actual input data and actual output data as obtained from lab research results on biocomposites. Table 5.15 shows the output data as predicted by the neural network. The data provided in Table 5.16 shows the data that was not used in the initial training of the neural network. These are the unknown training data. From the unknown training data or the experimentally derived training data, table 5.17 provides the NN trained results. The difference between the different types of predicted data for the NN is provided in table 5.18. In some of the iterations, the error level was extremely high. For example, one case reported a fiber %percentage of 325. instead of reporting 35 % which is the maximum in the designed data domain, results showed 325. Since the desired maximum in the designed data domain was 35%, cases such as this was considered to be errors non-representative of the data domain. In this event these results were simply excluded from the results table and further simulation was performed to retrieve data that is representative of the data domain.

Table 5.14 Experiment derived real world input data and corresponding real world output data

| | | | | | | | | | | | | | | |
|------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 15.93 | 14.13 | 14.75 | 14.70 | 15.2 | 16.29 | 15.8 | 15 | 17.67 | 17.9 | 11.13 | 17.5 | 10.78 | 14.19 |
| Bending (MPa) | 24.09 | 22.67 | 25.73 | 22.89 | 27.82 | 25.92 | 24.73 | 25.09 | 26.41 | 27.36 | 25.08 | 28.11 | 25.84 | 23.48 |
| Hardness | 67 | 61 | 67 | 63 | 70 | 66 | 64 | 66 | 68 | 67 | 64 | 69 | 69 | 63 |
| Impact (kJ/m ²) | 75 | 40 | 63 | 59 | 69 | 64 | 60 | 62 | 63 | 60 | 67 | 71 | 76 | 51 |
| Density (g/cm ³) | 1.096 | 1.083 | 1.018 | 1.06 | 1.021 | 1.009 | 0.947 | 1.015 | 1.055 | 1.098 | 1.089 | 1.055 | 1.083 | 1.096 |
| Fiber % | 25 | 35 | 10 | 30 | 20 | 15 | 5 | 5 | 15 | 25 | 30 | 20 | 10 | 35 |
| Pressure (MPa) | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |

Table 5.15 Output data predicted by NN (for experiment derived real world input data)

| Sample# | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|-------------------|-------|-------|-------|-------|-------|-------|------|------|-------|-------|-------|-------|-------|-------|
| NN Fiber % | 24.65 | 35.63 | 11.64 | 32.88 | 20.06 | 15.51 | 5.86 | 4.91 | 15.47 | 22.92 | 32.88 | 20.06 | 10.09 | 36.76 |
| NN Pressure (MPa) | 1.01 | 1.04 | 1.14 | 1.20 | 1.37 | 1.24 | 1.19 | 1.31 | 1.38 | 1.27 | 1.40 | 1.28 | 1.26 | 1.34 |

Table 5.16 Experiment relevant input data and corresponding output data (Unknown by NN)

| | | | | | | | | | | | | | | |
|------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 15.07 | 15.26 | 16.25 | 15.14 | 15.19 | 13.19 | 12.98 | 15.33 | 14.66 | 16.59 | 17.20 | 14.74 | 14.52 | 14.29 |
| Bending (MPa) | 24.36 | 25.00 | 26.47 | 27.40 | 24.15 | 23.21 | 22.43 | 24.83 | 25.30 | 26.36 | 28.59 | 27.54 | 24.30 | 24.22 |
| Hardness | 66 | 67 | 67 | 68 | 66 | 63 | 60 | 66 | 69 | 69 | 69 | 66 | 64 | 63 |
| Impact (kJ/m ²) | 62 | 67 | 68 | 68 | 65 | 65 | 51 | 63 | 68 | 72 | 74 | 67 | 65 | 51 |
| Density (g/cm ³) | 0.964 | 1.009 | 1.032 | 1.054 | 1.064 | 1.067 | 1.079 | 1.026 | 1.058 | 1.059 | 1.062 | 1.083 | 1.088 | 1.093 |
| Fiber % | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 5 | 10 | 15 | 20 | 25 | 30 | 35 |
| Pressure (MPa) | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |

Table 5.17 Output data predicted by NN (for experiment relevant input data, data normalized to 3 decimal points)

| Sample# | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|-------------------|-------|-------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| NN Fiber % | 6.016 | 7.696 | 13.11 8 | 20.83 3 | 24.71 2 | 29.16 2 | 34.99 6 | 10.33 1 | 12.11 6 | 14.15 0 | 21.96 8 | 22.12 3 | 28.98 5 | 37.37 8 |
| NN Pressure (MPa) | 1.078 | 1.128 | 1.272 | 1.384 | 1.232 | 1.143 | 1.231 | 1.251 | 1.287 | 1.395 | 1.395 | 1.367 | 1.187 | 1.194 |

Error Calculation for known Experimentally derived (ED) data and Experiment relevant (ER) data are provided as follows:

Table 5.18 Error Calculation for ED and ER data (Data Normalized to 4 Decimal points).

| Error | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | | |
|-------------|-------|--------|--------|-------|-------|--------|--------|--------|-------|-------|--------|-------|-------|-------|-------|-------|
| ED Pressure | 1.407 | -1.80 | -16.43 | -9.59 | -0.27 | -3.41 | -17.14 | 1.77 | -3.11 | 8.32 | -9.59 | -0.27 | -0.93 | -5.04 | | |
| ED Fiber % | -0.88 | -4.07 | -13.87 | - | 19.86 | -37.37 | -23.59 | -19.2 | 18.36 | 13.76 | 20.79 | 12.75 | 20.15 | 21.37 | 16.33 | |
| ER Pressure | - | 16.89 | 29.93 | 14.34 | -4 | 1.16 | 2.87 | 0.010 | - | 51.60 | -17.46 | 6 | -8.95 | 13 | 3.5 | -6.36 |
| ER Fiber % | -7.84 | -12.75 | -27.18 | - | 38.39 | -23.24 | -14.29 | -23.11 | 21.83 | 19.56 | 12.8 | 12.83 | 14.56 | 25.83 | 25.37 | |

5.3.3 Summary of the results

Pressure average error calculated for known data types from table 5.14 was: -4.%, Fiber % average error calculated for known data types from table 5.14 was: 0.33%, Pressure average error calculated for relevant data types from table 5.17 was: -2.45%, Fiber % average error calculated for relevant data types from table 5.17 was: -0.99%

The error percentile formula that was used for the calculation of error on every value is:

$$\text{Error \%} = \frac{(\text{Empirical data} - \text{NN Result})}{\text{Empirical data}} \times 100$$

The average MSE for the pressure prediction was $(26/10) \% = 2.6\%$ (samples with invalid values were not used). Individual error percentages are provided in Appendix F.

The variability of error in this case was simply due to the close proximity of the values of 1 MPa and 1.6 MPa. Hence, the neural network that has been generated for the biocomposite domain has been clearly trained and tested. It also provides good predictions based on the provided input.

In all of the mechanical tests, we see that the processing pressure of 1.6 MPa was clearly better for materials quality. The tensile strength for 1.6 MPa varied from 10 MPa to 19.24559 MPa. The higher pressure material had better tensile strength. For a biocomposite with fiber content of 20%, the maximum bending strengths were 28.1 MPa and 29.3 MPa for the processing pressures of 1 and 1.6 MPa, respectively. The maximum hardness result was found for the samples with 20% fiber and pressure of 1.6 MPa. Sample specimens created with the pressure 1 MPa had impact strength results ranging from, 40 to 75 kJ/m². For 1.6 MPa, the impact strength results ranged from, 43 to 92 kJ/m². With the increased pressure, the density also increased. The density varied from 0.947 to 1.097 g/cm³ for 1 MPa and from 0.95 to 1.096 g/cm³ for 1.6 MPa. From all of these experimental results, an increase in pressure will create a better mechanical property even with increased fiber content.

CHAPTER VI

CONCLUSIONS

6.1 Summary of the research project

For this research project, the mixtures of flax fiber and HDPE went through a series of processing steps. The mixtures were extruded using a laboratory single-screw extruder. The extrudates were ground and compressed to make biocomposite boards. The biocomposite boards were subjected to five mechanical tests. Once the data was collected from the experiments, the first section of this research, the data acquisition was complete.

Data collected from the experimental domain was used to train a feedforward backpropagation neural network. Once the training was complete, the NN was subjected to rigorous testing to ensure reliability and fidelity of the data. The results were found to be representative for the particular domain.

The research shows that through the use of a NN, it is possible to create a model which can predict biocomposites composition and processing parameter; and successfully aid in its design. The study sets a precedent towards furthering this research by involving various other processing and operating parameters to ensure a complete model capable of successfully describing the entire biocomposite domain and include all possible variables towards this domain description.

6.2 Research finding: Neural network – a potential tool for biocomposites design

The trained neural network has shown an ability to generate outputs when presented with input data that have not been used before. Therefore, the model has been able to adapt to new information and has also gained sufficient capacity to generalize.

Without huge amounts of human expertise, the NN system produces satisfactory results. It has shortened the research and development life cycle. The prospect of rapid design of biocomposites has been realized. The prototype development life cycle has also been significantly decreased.

In relation to Wu et al. (1990), we predict that through further research, all mechanical properties of biocomposites can be represented within the unified environment of the NN. The experimental NN tool created here is a far from a complete NN tool that describes all aspects of biocomposites. With the aid of further continuous research and increased attention to biocomposites, we can achieve the true potential of NN as a complete design tool.

In compression-molded flax fiber and HDPE polymer biocomposites, the processing pressure has a significant influence on the mechanical properties of the biocomposites. Fiber content can be increased by increasing the pressure in the compression mold. After fiber contents of 25 to 30%, values of the mechanical properties sharply declines.

6.3 Objectives achieved

1. An effective process of creating neural networks for biocomposites has been established. A complete step by step process has been provided in the materials and methods chapter. Chapter V provided the different results as they were achieved through Matlab.
2. The appropriate neural network structure found for the biocomposite domain is a three layer Feedforward Backpropagation neural network that is trained with the TRAINSCG – training algorithm. The first two hidden layers have 10 neurons each. The third hidden layer has 2 neurons. The transfer function for the first two hidden layers is sigmoidal. The transfer function for the third hidden layer is linear.
3. A complete neural network has been developed in Matlab. It uses five inputs: – tensile strength, impact strength, hardness, bending strength and density. Once these inputs have been provided, – the neural network provides the composition and processing pressure of the biocomposite boards, with acceptable performance.

6.4 Future work

The data domain where fiber content varies from 5 to 35% is the area of concern for this research work. For fiber contents greater than 25%, the mechanical properties of the biocomposites decrease, therefore the datasets that have been created are sufficient for this experiment. However, more data are required for enhanced and improved prediction. The domain knowledge for the expert system will continue to grow when new results are added to the existing knowledge base. The neural system will continue to learn directly by receiving further data. Ultimately, it will be robust and predict information not presently known by human experts.

In the case of biocomposite materials, it is difficult to find a mathematical model that encompasses all properties for the biocomposites. There are individual properties that can describe a particular feature such as tensile, shear, hardness, flexural, tension, heat absorption, moisture absorption, etc. However, there is currently no model that is capable of describing all features of biocomposites and generating the desired outputs for the user. Future work should aim towards creating a complete model that successfully describes all aspects of the biocomposites domain and aids in intelligent information retrieval.

6.5 Concluding remarks

Through this research, an effective process of creating neural networks for the biocomposites domain has been completed. This NN can now be further developed for creating a complete knowledge base that can be migrated to an application to support biocomposites design and processing. With increasing automation and smart applications being used in different fields, - this research hopes to open a similar venue for the biocomposite field.

A significant volume of work is required to create a complete expert system in the area of biocomposite materials. Henceforth there is ample opportunity to extend this study and forward it through further research, towards a true and complete expert system. This is an introductory work conducted within a M.Sc. thesis project time scale. Future work based on this research can contribute to a complete knowledge base that can describe the biocomposites complete knowledge domain.

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APPENDICES

APPENDIX A: Number of samples required for each test

The number of specimens as required by each test was based on the following considerations.

The study used research practices as used by Patil and coworkers (1995).

The sample size was calculated with the following equation:

$$N = (tv)^2 / A^2$$

Here we have:

N = sample size

t = 1.96, (value of students t used for 95% probability and infinite degrees of freedom)

v = estimate of coefficient of variation CV

A = 15%, the value of allowable variation.

| CV | t ² (t = 1.96) | A ² (A = 15) | v ² | Number of Samples |
|----|------------------------------|----------------------------|----------------|----------------------|
| 1 | 3.8416 | 225 | 1 | 864.36 |
| 2 | 3.8416 | 225 | 4 | 216.09 |
| 3 | 3.8416 | 225 | 9 | 96.04 |
| 4 | 3.8416 | 225 | 16 | 54.0225 |
| 5 | 3.8416 | 225 | 25 | 34.5744 |
| 6 | 3.8416 | 225 | 36 | 24.01 |
| 7 | 3.8416 | 225 | 49 | 17.64 |
| 8 | 3.8416 | 225 | 64 | 13.50563 |
| 9 | 3.8416 | 225 | 81 | 10.67111 |
| 10 | 3.8416 | 225 | 100 | 8.6436 |
| 11 | 3.8416 | 225 | 121 | 7.143471 |
| 12 | 3.8416 | 225 | 144 | 6.0025 |
| 13 | 3.8416 | 225 | 169 | 5.114556 |
| 14 | 3.8416 | 225 | 196 | 4.41 |
| 15 | 3.8416 | 225 | 225 | 3.8416 |
| 16 | 3.8416 | 225 | 256 | 3.376406 |
| 17 | 3.8416 | 225 | 289 | 2.990865 |
| 18 | 3.8416 | 225 | 324 | 2.667778 |
| 19 | 3.8416 | 225 | 361 | 2.394349 |
| 20 | 3.8416 | 225 | 400 | 2.1609 |

From an acceptable CV = 10 and Number of samples = 8.6436, the number of samples for every test was decided to be 9.

APPENDIX B: Biocomposite Materials Property

1. Tensile strength

Table 1. At 1 MPa pressure following data was acquired for biocomposite specimens Tensile Test. Tensile Strength in MPa (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 15.80 | 15.33 | 16.29 | 15.20 | 15.20 | 13.30 | 12.90 |
| 2 | 15.34 | 15.34 | 15.80 | 14.83 | 15.39 | 13.76 | 13.50 |
| 3 | 15.05 | 15.29 | 16.05 | 14.50 | 15.29 | 13.82 | 12.02 |
| 4 | 13.79 | 14.79 | 16.20 | 15.34 | 16.10 | 13.01 | 13.63 |
| 5 | 15.90 | 16.49 | 16.50 | 15.67 | 15.93 | 12.13 | 12.43 |
| 6 | 14.78 | 14.78 | 16.02 | 15.39 | 14.87 | 13.20 | 13.73 |
| 7 | 15.75 | 16.05 | 16.20 | 14.69 | 14.08 | 13.30 | 12.20 |
| 8 | 14.75 | 14.75 | 16.78 | 15.10 | 14.28 | 12.90 | 13.10 |
| 9 | 14.50 | 14.50 | 16.40 | 15.49 | 15.53 | 13.30 | 13.30 |
| Avg / Mean | 15.07 | 15.26 | 16.25 | 15.14 | 15.19 | 13.19 | 12.98 |
| Stdev | 0.70 | 0.66 | 0.29 | 0.39 | 0.68 | 0.50 | 0.64 |
| Coeff of Variance | 4.64 | 4.29 | 1.78 | 2.58 | 4.47 | 3.78 | 4.90 |

Table 2. At 1 MPa pressure following data was acquired for biocomposite specimens Tensile Test. Tensile Strength in MPa (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 16.50 | 14.80 | 16.87 | 18.20 | 15.35 | 13.57 | 14.17 |
| 2 | 16.10 | 15.10 | 17.32 | 17.50 | 15.00 | 14.83 | 13.01 |
| 3 | 14.92 | 14.70 | 17.68 | 16.20 | 15.20 | 14.63 | 14.78 |
| 4 | 15.80 | 14.60 | 17.10 | 16.20 | 15.00 | 13.96 | 14.39 |
| 5 | 15.00 | 14.63 | 16.10 | 17.25 | 15.00 | 14.81 | 14.51 |
| 6 | 14.78 | 15.78 | 16.45 | 17.68 | 14.50 | 14.35 | 15.72 |
| 7 | 14.27 | 16.05 | 15.78 | 16.87 | 15.20 | 14.85 | 14.14 |
| 8 | 14.80 | 13.75 | 16.20 | 17.61 | 13.40 | 15.02 | 13.78 |
| 9 | 15.75 | 12.50 | 15.78 | 17.32 | 14.00 | 14.70 | 14.08 |
| Avg / Mean | 15.33 | 14.66 | 16.59 | 17.20 | 14.74 | 14.52 | 14.29 |
| Stdev | 0.74 | 1.06 | 0.69 | 0.67 | 0.65 | 0.48 | 0.74 |
| Coeff of Variance | 4.80 | 7.21 | 4.15 | 3.90 | 4.42 | 3.29 | 5.15 |

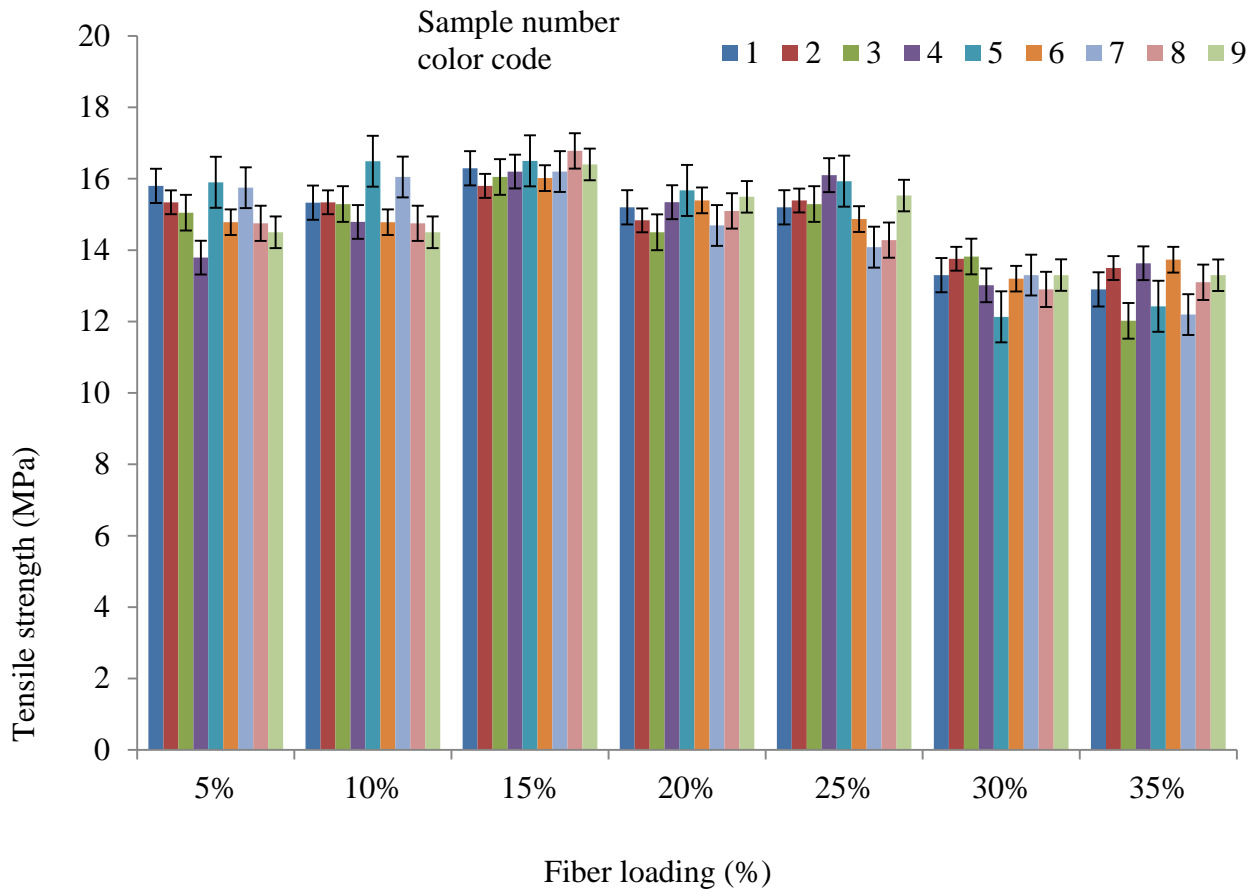


Figure 1. Individual samples tensile strength at 1 MPa pressure. Samples with the same fiber loading are grouped together.

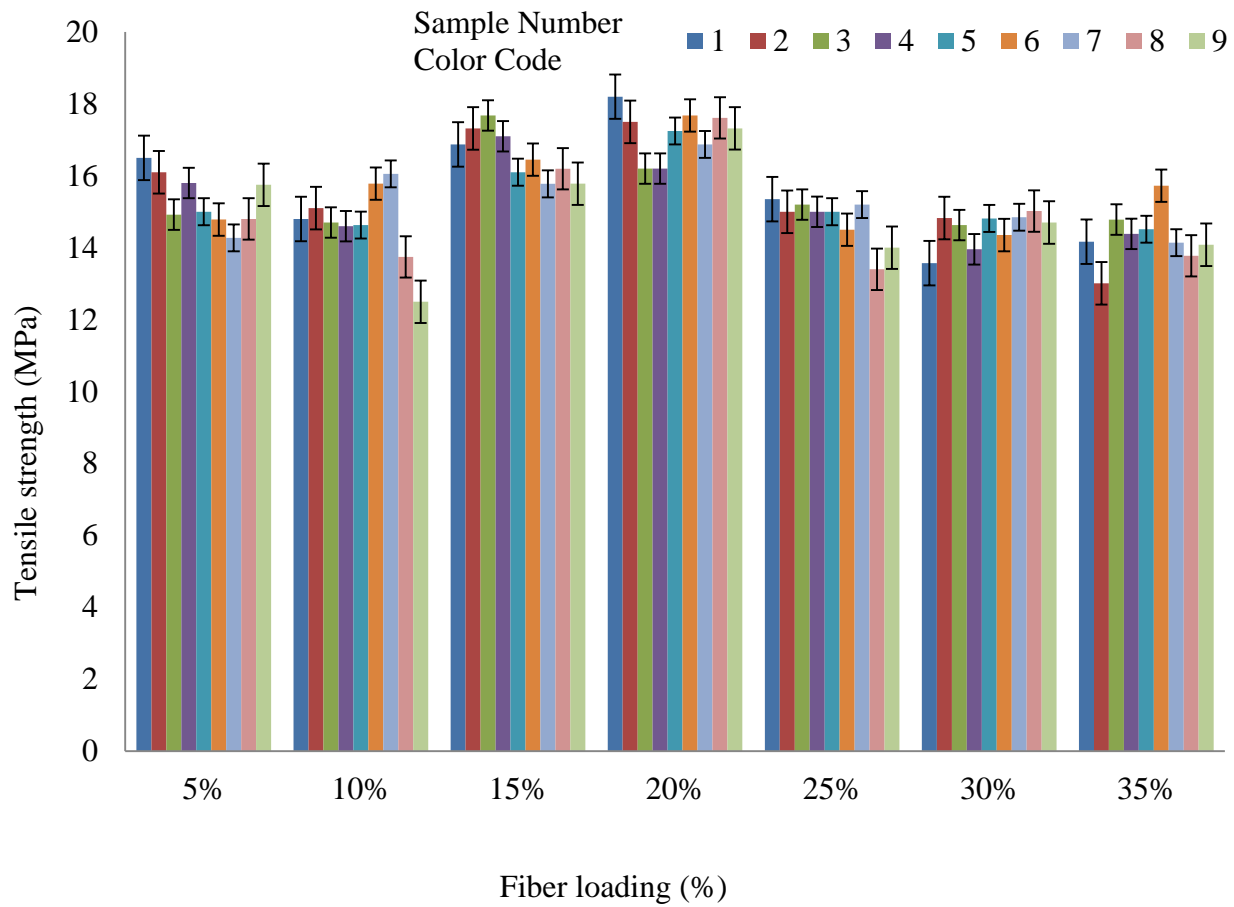


Figure 2. Individual samples tensile strength at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

2. Bending strength

Table 3. At 1 MPa pressure following data was acquired for biocomposite specimens bending strength. Bending strength in MPa (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 24.73 | 24.33 | 25.93 | 27.83 | 24.93 | 23.14 | 23.21 |
| 2 | 24.21 | 25.01 | 26.37 | 27.23 | 23.81 | 23.40 | 22.08 |
| 3 | 23.93 | 24.40 | 26.02 | 27.39 | 23.49 | 23.09 | 22.00 |
| 4 | 24.22 | 25.18 | 27.01 | 27.86 | 24.58 | 22.36 | 21.81 |
| 5 | 24.21 | 25.74 | 26.86 | 28.11 | 24.09 | 23.49 | 22.65 |
| 6 | 24.95 | 25.29 | 26.14 | 27.33 | 24.08 | 23.77 | 22.08 |
| 7 | 24.33 | 24.18 | 26.71 | 27.02 | 24.39 | 23.39 | 22.68 |
| 8 | 24.18 | 25.74 | 26.86 | 26.99 | 23.92 | 23.35 | 22.96 |
| 9 | 24.47 | 25.18 | 26.28 | 26.83 | 24.03 | 22.90 | 22.36 |
| Avg / Mean | 24.36 | 25.00 | 26.47 | 27.40 | 24.15 | 23.21 | 22.43 |
| Stdev | 0.31 | 0.58 | 0.40 | 0.44 | 0.43 | 0.41 | 0.47 |
| Coeff of Variance | 1.29 | 2.33 | 1.53 | 1.62 | 1.78 | 1.75 | 2.12 |

Table 4. At 1.6 MPa pressure following data was acquired for biocomposite specimens bending strength. Bending strength in MPa (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 24.98 | 25.08 | 26.00 | 28.83 | 27.42 | 24.08 | 24.33 |
| 2 | 24.49 | 25.71 | 26.18 | 28.11 | 28.29 | 23.83 | 24.87 |
| 3 | 25.16 | 24.91 | 26.42 | 28.11 | 27.27 | 24.76 | 24.29 |
| 4 | 24.38 | 25.17 | 26.58 | 29.32 | 27.36 | 24.70 | 24.05 |
| 5 | 25.10 | 25.35 | 26.86 | 28.95 | 27.18 | 25.09 | 24.71 |
| 6 | 25.20 | 25.84 | 26.89 | 28.44 | 27.70 | 23.97 | 23.43 |
| 7 | 24.83 | 24.98 | 26.38 | 28.99 | 27.38 | 24.22 | 23.49 |
| 8 | 24.38 | 25.77 | 25.55 | 28.46 | 27.14 | 24.13 | 24.58 |
| 9 | 24.94 | 24.89 | 26.42 | 28.11 | 28.11 | 23.96 | 24.25 |
| Avg / Mean | 24.83 | 25.30 | 26.36 | 28.59 | 27.54 | 24.30 | 24.22 |
| Stdev | 0.33 | 0.38 | 0.42 | 0.45 | 0.41 | 0.44 | 0.50 |
| Coeff of Variance | 1.32 | 1.51 | 1.59 | 1.57 | 1.49 | 1.80 | 2.06 |

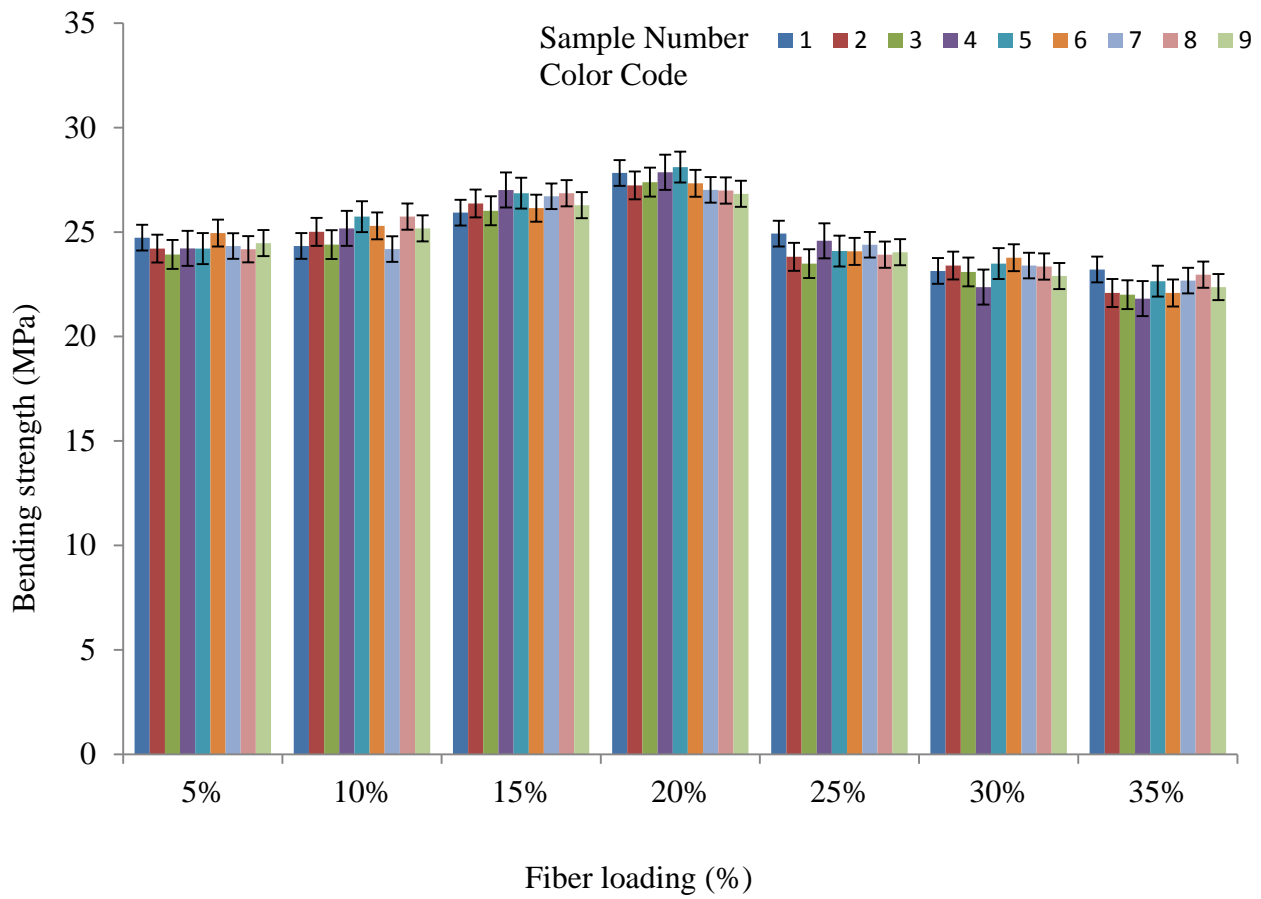


Figure 3. Individual samples bending strength at 1 MPa pressure. Samples with the same fiber loading are grouped together.

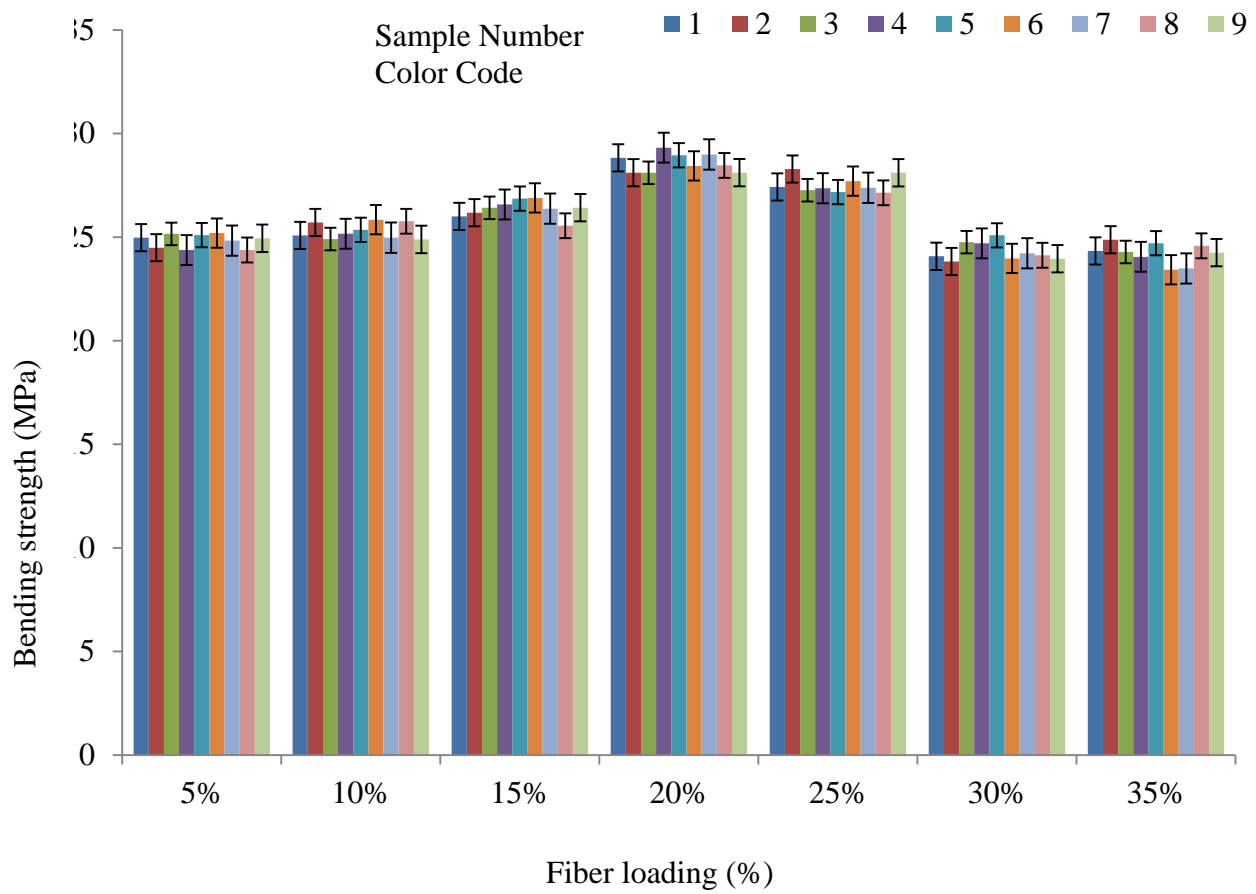


Figure 4. Individual samples bending strength at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

3. Hardness

Table 5. At 1 MPa pressure following data was acquired for specimens hardness Test. (data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 64 | 68 | 66 | 70 | 67 | 64 | 54 |
| 2 | 64 | 69 | 69 | 71 | 65 | 62 | 64 |
| 3 | 65 | 66 | 69 | 68 | 66 | 66 | 55 |
| 4 | 68 | 69 | 69 | 67 | 64 | 63 | 62 |
| 5 | 63 | 68 | 70 | 69 | 67 | 64 | 61 |
| 6 | 64 | 65 | 68 | 68 | 69 | 63 | 60 |
| 7 | 66 | 66 | 58 | 66 | 65 | 61 | 61 |
| 8 | 69 | 67 | 67 | 67 | 64 | 61 | 60 |
| 9 | 69 | 69 | 69 | 69 | 64 | 63 | 60 |
| Avg / Mean | 65.78 | 67.44 | 67.22 | 68.33 | 65.67 | 63.00 | 59.67 |
| stdev | 2.33 | 1.51 | 3.67 | 1.58 | 1.73 | 1.58 | 3.20 |
| Coeff of Variance | 3.55 | 2.24 | 5.45 | 2.31 | 2.64 | 2.51 | 5.37 |

Table 6. At 1.6 MPa pressure following data was acquired for specimens hardness test. (data corrected to 2 decimal points)

| | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 66 | 70 | 65 | 68 | 68 | 64 | 64 |
| 2 | 65 | 70 | 68 | 69 | 66 | 64 | 64 |
| 3 | 66 | 69 | 68 | 69 | 65 | 64 | 63 |
| 4 | 65 | 67 | 70 | 69 | 67 | 64 | 63 |
| 5 | 66 | 69 | 70 | 70 | 65 | 64 | 63 |
| 6 | 62 | 69 | 70 | 69 | 65 | 63 | 64 |
| 7 | 66 | 69 | 70 | 70 | 65 | 63 | 63 |
| 8 | 67 | 67 | 69 | 70 | 69 | 64 | 63 |
| 9 | 67 | 68 | 71 | 69 | 65 | 63 | 59 |
| Avg/Mean | 65.56 | 68.67 | 69.00 | 69.22 | 66.11 | 63.67 | 62.89 |
| stdev | 1.51 | 1.12 | 1.80 | 0.67 | 1.54 | 0.50 | 1.54 |
| Coeff of Variance | 2.30 | 1.63 | 2.61 | 0.96 | 2.32 | 0.79 | 2.44 |

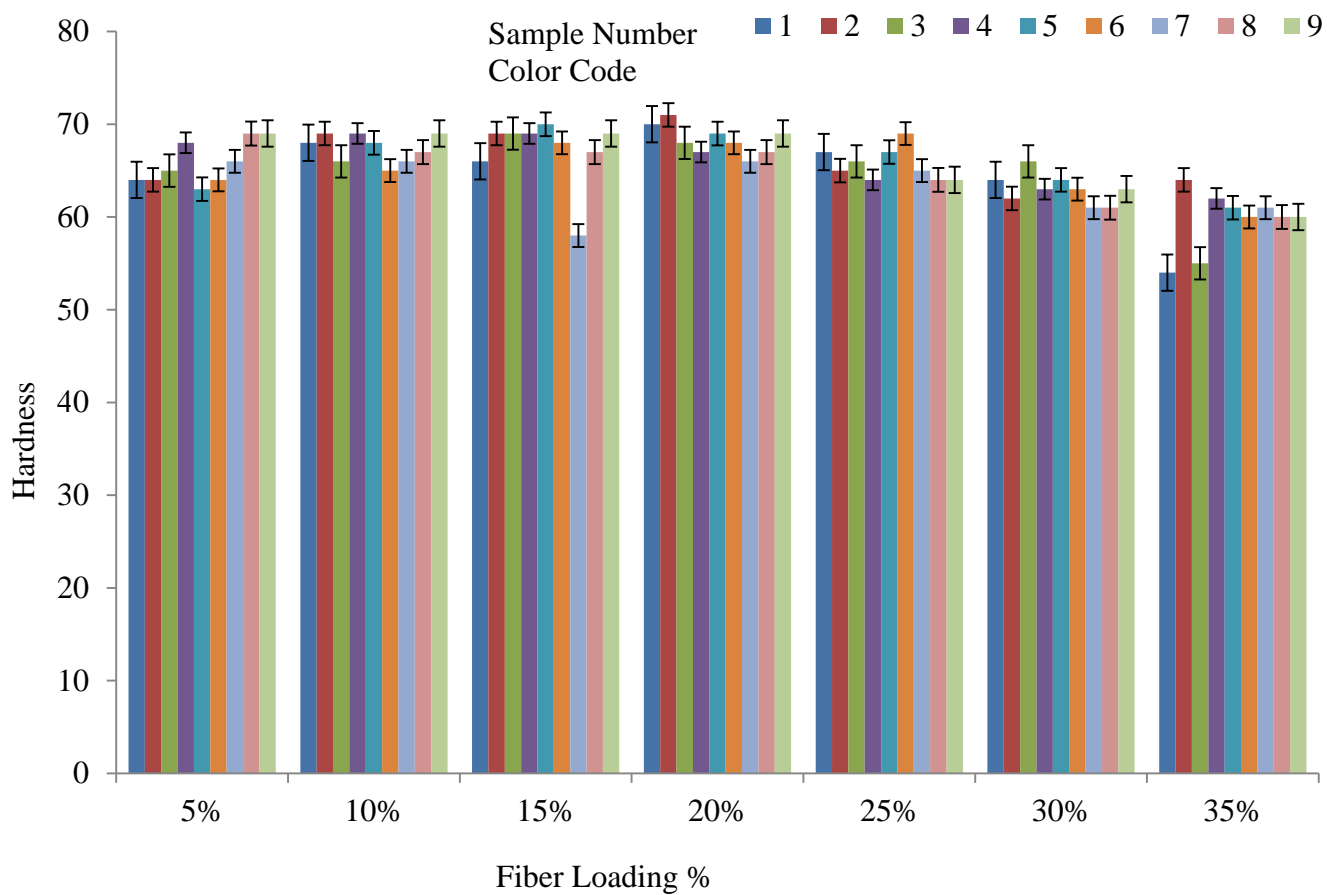


Figure 5. Individual samples hardness at 1 MPa pressure. Samples with the same fiber loading are grouped together.

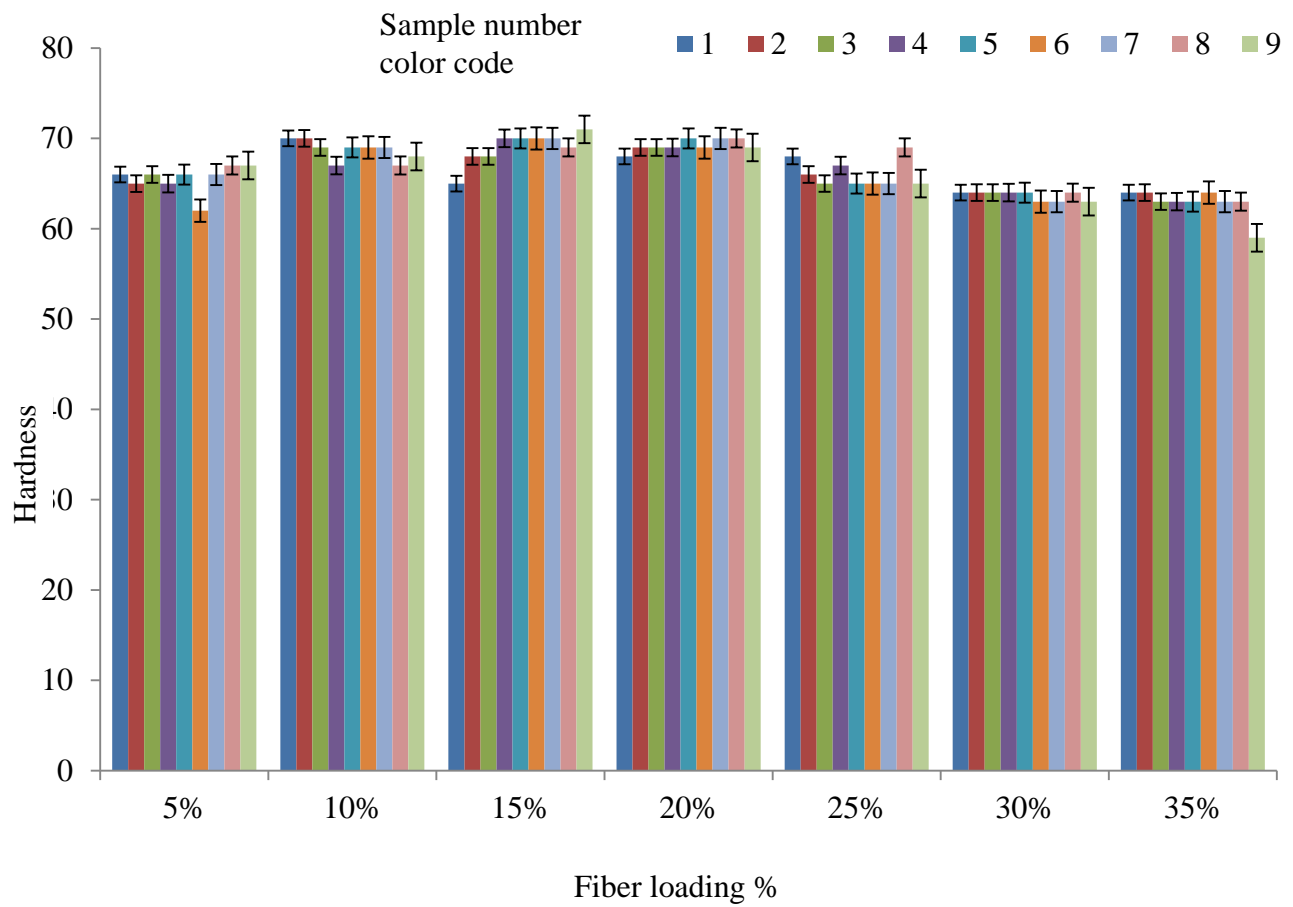


Figure 6. Individual samples hardness at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

4. Impact Strength

Table 7. At 1 MPa pressure following data was acquired for biocomposite specimens Impact Test. Impact Strength in kJ/m² (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 60 | 70 | 64 | 69 | 64 | 70 | 53 |
| 2 | 63 | 71 | 73 | 72 | 69 | 70 | 48 |
| 3 | 63 | 64 | 65 | 75 | 65 | 66 | 49 |
| 4 | 61 | 65 | 67 | 68 | 60 | 65 | 49 |
| 5 | 54 | 66 | 69 | 65 | 71 | 65 | 55 |
| 6 | 57 | 69 | 70 | 70 | 55 | 70 | 54 |
| 7 | 66 | 68 | 66 | 64 | 67 | 58 | 48 |
| 8 | 67 | 63 | 70 | 70 | 60 | 60 | 45 |
| 9 | 68 | 64 | 72 | 60 | 70 | 59 | 56 |
| Avg / Mean | 62.11 | 66.67 | 68.44 | 68.11 | 64.56 | 64.78 | 50.78 |
| stdev | 4.90 | 2.92 | 3.13 | 4.51 | 5.36 | 4.82 | 3.80 |
| Coeff of Variance | 7.88 | 4.37 | 4.57 | 6.62 | 8.31 | 7.43 | 7.48 |

Table 8. At 1.6 MPa pressure following data was acquired for biocomposite specimens Impact Test. Impact Strength in kJ/m² (Data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 59 | 62 | 72 | 72 | 74 | 65 | 57 |
| 2 | 60 | 61 | 69 | 71 | 72 | 55 | 48 |
| 3 | 71 | 69 | 63 | 75 | 66 | 69 | 58 |
| 4 | 65 | 65 | 72 | 79 | 69 | 64 | 43 |
| 5 | 62 | 73 | 77 | 80 | 64 | 67 | 52 |
| 6 | 65 | 71 | 74 | 73 | 63 | 76 | 50 |
| 7 | 61 | 71 | 75 | 74 | 69 | 68 | 51 |
| 8 | 60 | 69 | 74 | 73 | 65 | 63 | 49 |
| 9 | 61 | 68 | 75 | 71 | 65 | 62 | 55 |
| Avg / Mean | 62.67 | 67.67 | 72.33 | 74.22 | 67.44 | 65.44 | 51.44 |
| Stdev | 3.77 | 4.15 | 4.18 | 3.27 | 3.78 | 5.73 | 4.72 |
| Coeff of Variance | 6.02 | 6.14 | 5.78 | 4.41 | 5.60 | 8.75 | 9.17 |

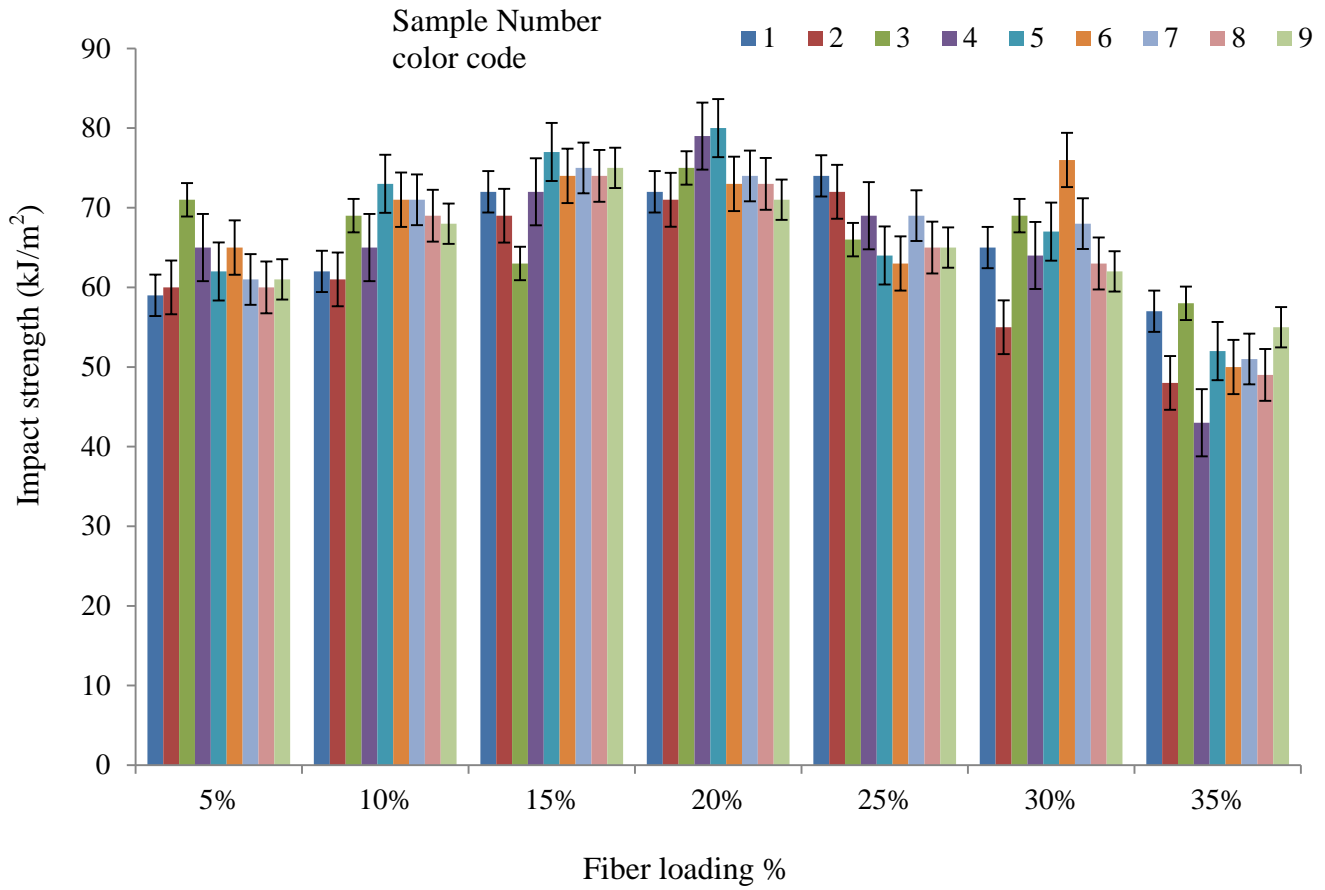


Figure 7. Individual samples impact strength at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

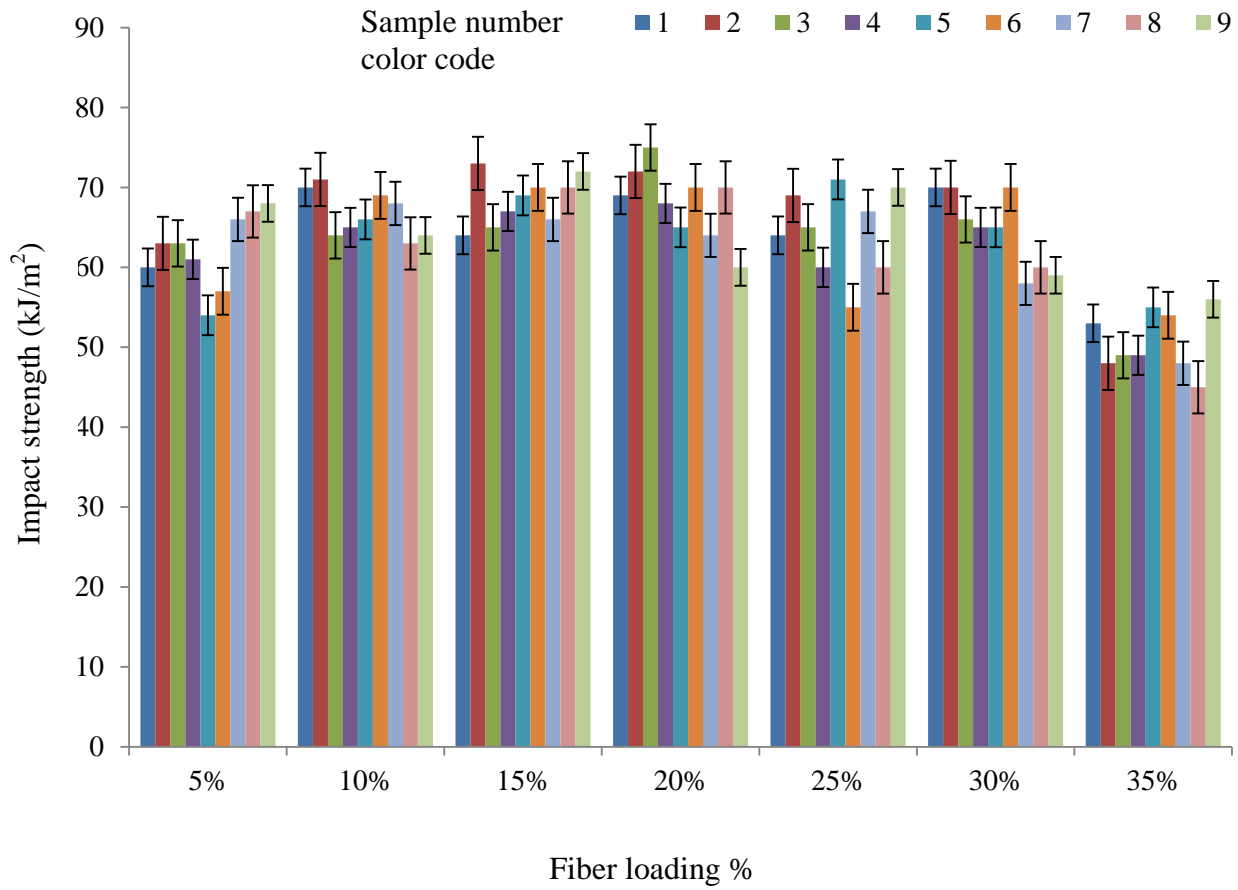


Figure 8. Individual samples tensile strength at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

5. Density

Table 9. At 1 MPa pressure following data was acquired for specimens density. Density in g / cm³ (data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|------|------|------|------|------|------|------|
| 1 | 0.95 | 0.98 | 1.01 | 1.02 | 1.05 | 1.07 | 1.07 |
| 2 | 0.95 | 1.00 | 1.03 | 1.05 | 1.07 | 1.07 | 1.08 |
| 3 | 0.95 | 1.00 | 1.04 | 1.05 | 1.06 | 1.04 | 1.08 |
| 4 | 0.96 | 1.01 | 1.03 | 1.09 | 1.06 | 1.07 | 1.08 |
| 5 | 0.97 | 1.01 | 1.05 | 1.04 | 1.10 | 1.07 | 1.10 |
| 6 | 0.97 | 1.02 | 1.05 | 1.07 | 1.06 | 1.09 | 1.09 |
| 7 | 0.98 | 1.02 | 1.04 | 1.06 | 1.08 | 1.07 | 1.08 |
| 8 | 0.98 | 1.02 | 1.03 | 1.06 | 1.05 | 1.07 | 1.08 |
| 9 | 0.98 | 1.02 | 1.01 | 1.06 | 1.05 | 1.06 | 1.05 |
| Avg / Mean | 0.96 | 1.01 | 1.03 | 1.05 | 1.06 | 1.07 | 1.08 |
| stdev | 0.01 | 0.01 | 0.01 | 0.02 | 0.02 | 0.01 | 0.01 |
| Coeff of Variance | 1.35 | 1.12 | 1.38 | 1.81 | 1.48 | 1.26 | 1.18 |

Table 10. At 1.6 MPa pressure following data was acquired for specimens density. Density in g / cm³ (data corrected to 2 decimal points)

| Number | 5% | 10% | 15% | 20% | 25% | 30% | 35% |
|-------------------|------|------|------|------|------|------|------|
| 1 | 1.02 | 1.07 | 1.05 | 1.05 | 1.05 | 1.08 | 1.10 |
| 2 | 1.01 | 1.05 | 1.05 | 1.06 | 1.09 | 1.09 | 1.09 |
| 3 | 1.00 | 1.04 | 1.06 | 1.06 | 1.09 | 1.09 | 1.09 |
| 4 | 1.02 | 1.04 | 1.06 | 1.06 | 1.10 | 1.10 | 1.10 |
| 5 | 1.02 | 1.05 | 1.06 | 1.06 | 1.09 | 1.09 | 1.10 |
| 6 | 1.02 | 1.08 | 1.06 | 1.07 | 1.10 | 1.09 | 1.09 |
| 7 | 1.07 | 1.05 | 1.07 | 1.07 | 1.10 | 1.08 | 1.10 |
| 8 | 1.02 | 1.06 | 1.07 | 1.06 | 1.07 | 1.09 | 1.09 |
| 9 | 1.07 | 1.09 | 1.06 | 1.08 | 1.07 | 1.10 | 1.09 |
| Avg / Mean | 1.03 | 1.06 | 1.06 | 1.06 | 1.08 | 1.09 | 1.09 |
| stdev | 0.02 | 0.02 | 0.01 | 0.01 | 0.02 | 0.01 | 0.00 |
| Coeff of Variance | 2.41 | 1.65 | 0.66 | 0.73 | 1.62 | 0.60 | 0.40 |

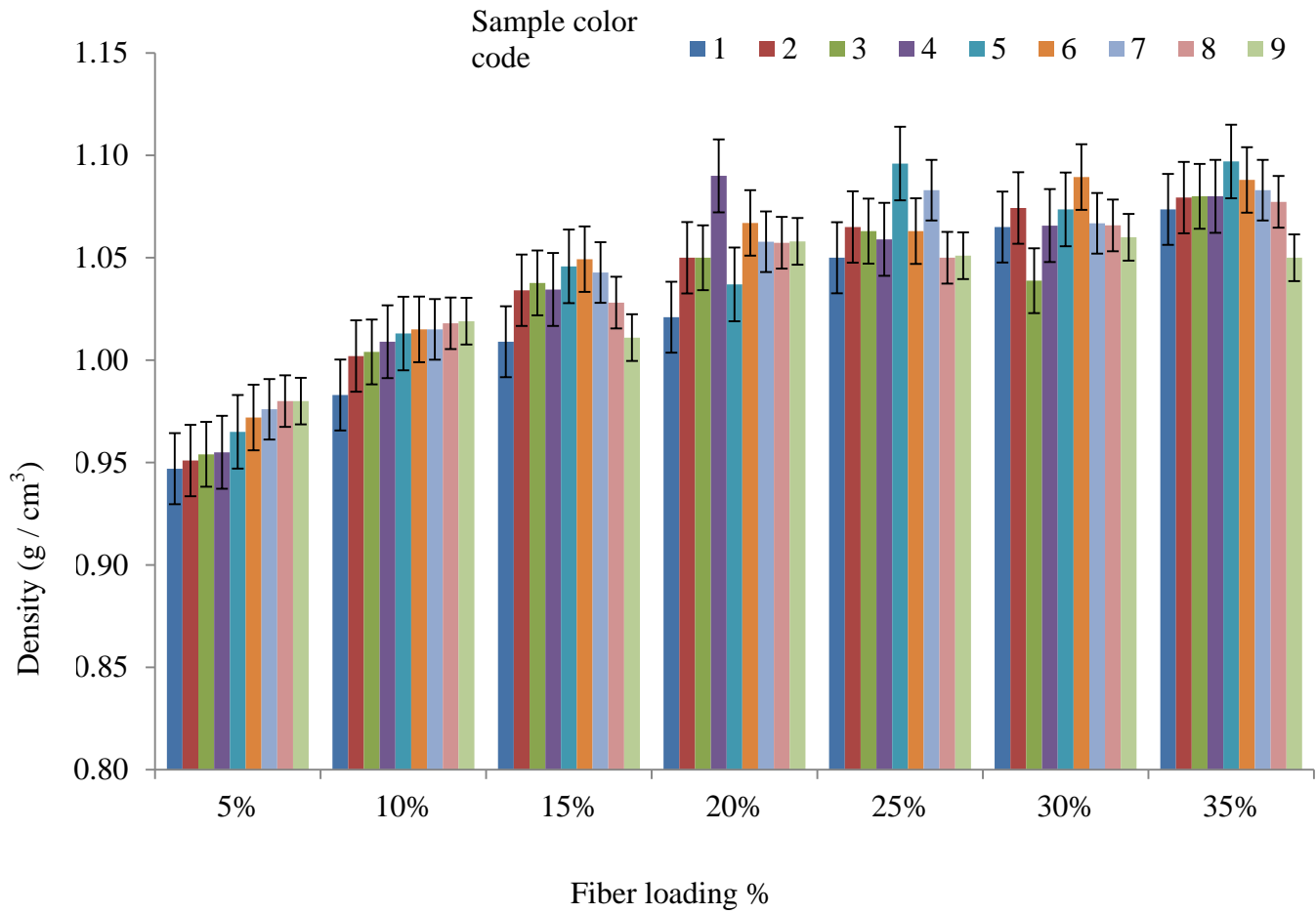


Figure 9. Individual samples density at 1.6 MPa pressure. Samples with the same fiber loading are grouped together

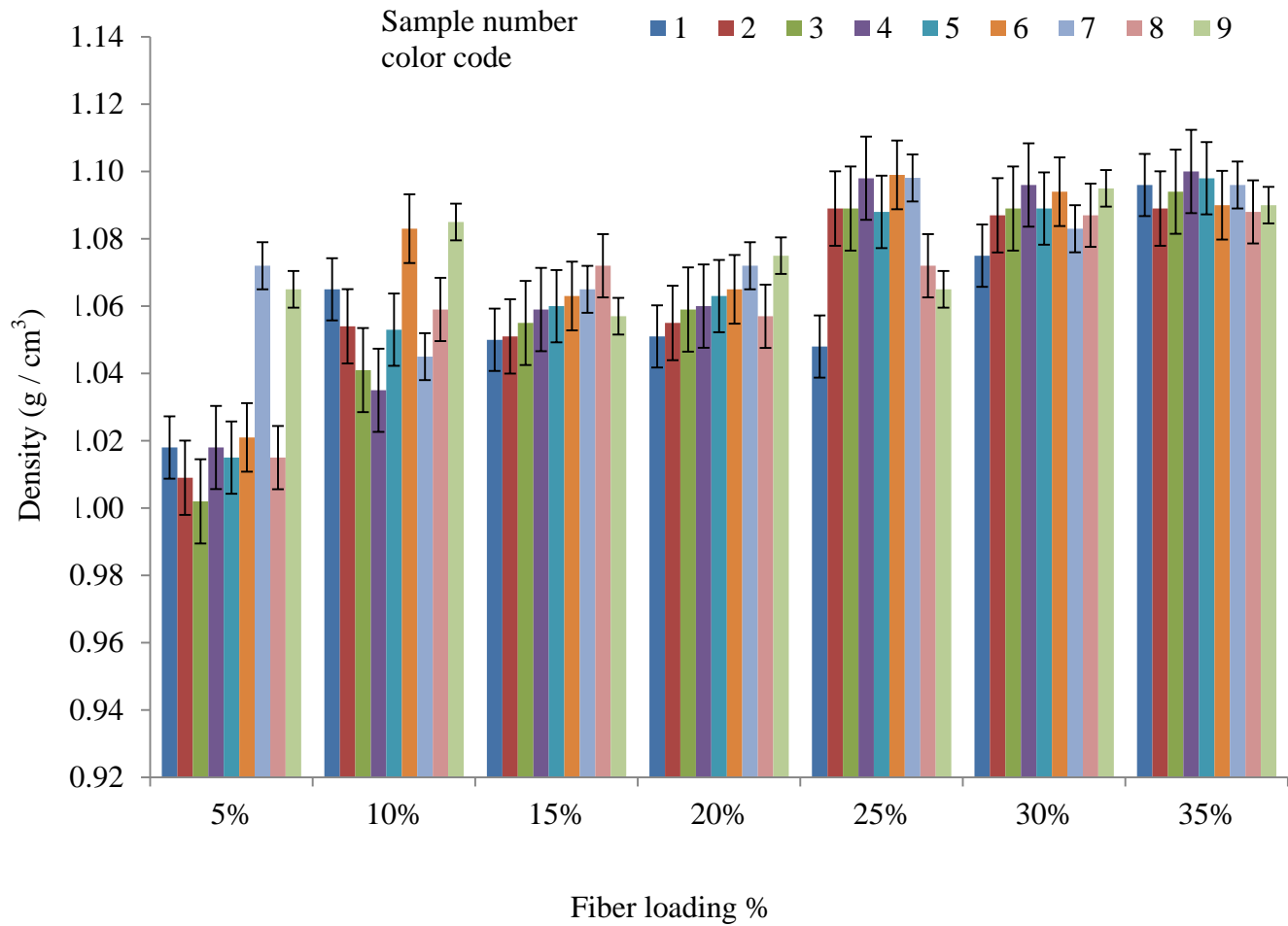


Figure 10. Individual samples density at 1.6 MPa pressure. Samples with the same fiber loading are grouped together.

APPENDIX C: Density Prediction

Data Collected from: Table 3.2 Mechanical properties of natural fibers as compared to conventional reinforcing fibers.

(Li et al., 2007)

Graph Created by: Bill Crerar

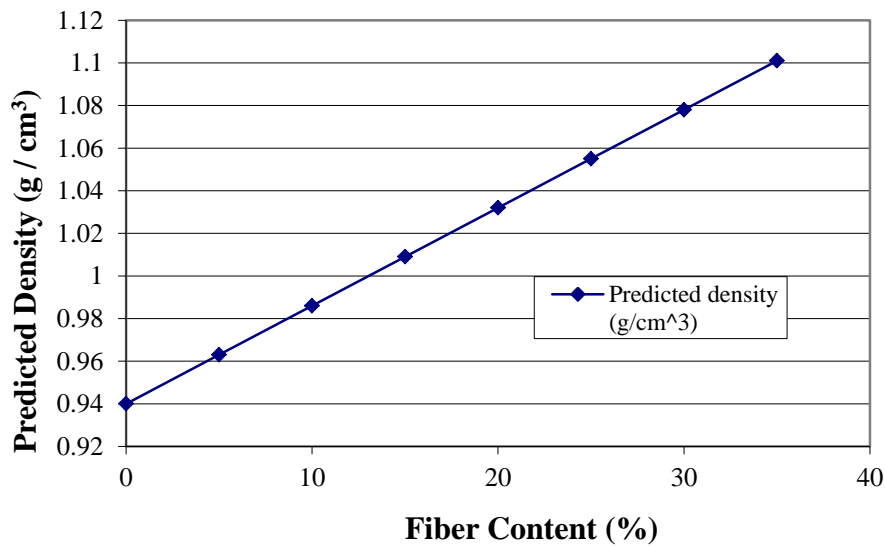
0.94 g/cm³: Plastic density

1.4 g/cm³: Fiber Density

Table 1. Perfect Mixture predicted density

| | | | | | | | | |
|--|------|-------|-------|-------|-------|-------|-------|-------|
| Percent Fibre | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 |
| Percent Plastic | 100 | 95 | 90 | 85 | 80 | 75 | 70 | 65 |
| Fiber contribution g / cm ³ | 0 | 0.07 | 0.14 | 0.21 | 0.28 | 0.35 | 0.42 | 0.49 |
| Plastic contribution g / cm ³ | 0.94 | 0.893 | 0.846 | 0.799 | 0.752 | 0.705 | 0.658 | 0.611 |
| Predicted density g / cm ³ | 0.94 | 0.963 | 0.986 | 1.009 | 1.032 | 1.055 | 1.078 | 1.101 |
| Percent Fibre (%) | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 |
| Predicted density (g / cm ³) | 0.94 | 0.963 | 0.986 | 1.009 | 1.032 | 1.055 | 1.078 | 1.101 |

Fig 1. Effect of Fibre Content on Predicted Density (Perfect Biocomposite mixture)



APPENDIX D: Neural network design

1. Architecture and weights for cascade forward back propagation NN with 3 Layer, -5(h1), 5(h2) and 2(h3)

iw {1,1} - Weight to layer 1 from input 1

[-74.575 25.8385 6.8858 1.7016 -35.1042;
30.4322 45.8454 -12.4418 -5.2679 -318.2534;
-0.10476 0.76466 -0.17406 0.010761 8.6214;
0.060586 0.46721 -0.020792 0.025949 -11.2176;
-116.3762 84.8679 22.4664 -46.7554 95.1977]

iw {2,1} - Weight to layer 2 from input 1

[89.3509 -176.784 51.0752 -7.7686 -30.9525;
-5.1425 -44.7766 22.2478 -0.47532 -49.7102;
30.9809 -30.4512 7.5574 -3.3373 173.6969;
-12.8939 62.7195 -74.3399 45.788 -18.051;
1.5717 0.32517 -0.25522 0.21391 6.1011]

iw {3,1} - Weight to layer 3 from input 1

[4.83 -7.1392 0.57888 -0.31605 49.5008;
-0.12493 0.36043 -0.042538 0.0084795 2.0057]

Iw{2,1} - Weight to layer

[-126.2156 25.9299 -29.7925 10.3042 22.5856;
-10.1114 -18.1037 10.1581 20.0329 53.2972;
27.4038 6.8442 27.3451 27.2088 105.2578;
42.3891 -92.3049 51.0522 -38.955 2.388;
0.41001 0.77038 -1.8743 1.4406 0.44843]

Iw{2,1} - Weight to layer

[-126.2156 25.9299 -29.7925 10.3042 22.5856;
-10.1114 -18.1037 10.1581 20.0329 53.2972;
27.4038 6.8442 27.3451 27.2088 105.2578;
42.3891 -92.3049 51.0522 -38.955 2.388;
0.41001 0.77038 -1.8743 1.4406 0.44843]

Iw{3,1} - Weight to layer

[4.3501 1.2835 21.8543 -8.8483 -25.5457;
-0.16349 -0.071995 -0.47295 -0.25096 0.10549]

Iw{3,2} - Weight to layer

[-2.8999 5.3583 -2.8992 0.097117 19.96;
0.034047 -0.084768 0.11961 0.061958 -4.0441]

b{1} - Bias to layer 1

[21.3013;
-145.4961;
-16.5492;
-0.66323;
116.419]

b{2} - Bias to layer 2

[-34.8218;
-70.6142;
-92.8;
-11.1477;
-2.1719]

2. Architecture and weights for feed forward back propagation NN with 3 Layer, - 5(h1), 5(h2) and 2(h3)

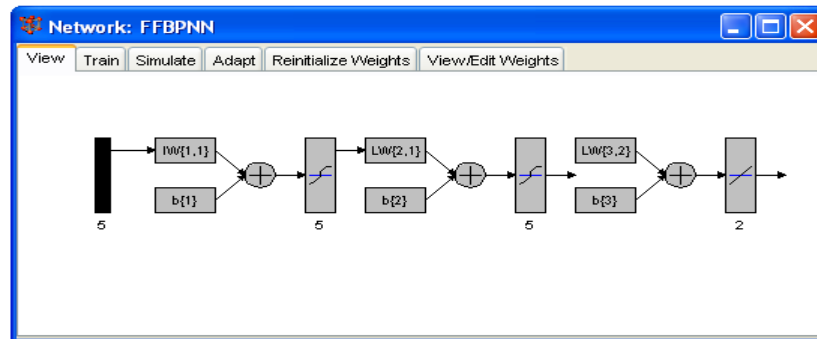


Figure 1. Feedforward backpropagation neural network as represented by Matlab NNTOOL app. There are 5 neurons in the input layer, 5 neurons in the 2 hidden layer and 2 neurons are presented in the output layer

iw {1,1} - Weight to layer 1 from input 1

[-0.7212 -1.2823 -7.2603 5.9629 7.1239;
 -1.826 8.6673 -2.2749 -0.49603 -14.8221;
 0.42744 0.63657 0.094311 -0.00052865 -10.8435;
 1.4027 -1.3538 -1.5332 1.6838 2.7597;
 13.7657 9.1898 -3.8973 -2.2992 -6.0114]

b{2} - Bias to layer 2

[-9.348;
 18.7439;
 -11.4251;
 -0.22339;
 -4.9789]

iw {2,1} - Weight to layer 2 from input 1

[3.8726 21.3161 -4.5029 -33.8075 2.6233;
 -15.4151 -24.3792 25.5511 32.4013 -1.3254;
 5.7496 9.69 27.3048 8.0247 -8.8856;
 -26.4937 -134.5904 147.7569 33.0177 -72.3805;
 -1.1207 4.4242 1.2122 0.31334 -0.045444]

b{3} - Bias to layer 3

[22.6629;
 1.5074]

Iw {3,2} - Weight to layer

[-3.404 -6.7069 5.886 -8.3904 -8.3155;
 -0.01416 -0.14127 0.13488 0.069177 0.018995]

b{1} - Bias to layer 1

[-7.687;
 -2.8443;
 -17.7111;
 -7.3964;
 18.1809]

3. Feedforward time delay NN with 3 Layer, - 5(h1), 5(h2) and 2(h3)

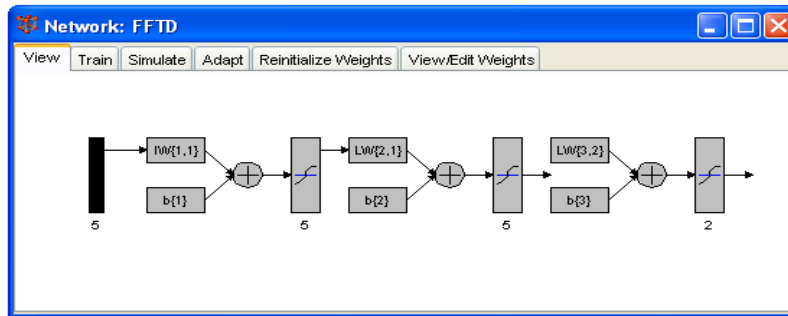


Figure 2. Feedforward time delay neural network as represented by Matlab NNTOOL app. There are 5 neurons in the input layer, 5 neurons in the 2 hidden layer and 2 neurons are presented in the output layer

iw {1,1} - Weight to layer 1 from input 1

```
[-33.2206 -50.3589 -135.3751 -135.1487 8.4999 -33.2794 -50.4196 -135.387 -135.1666
-7.5744 0.065903 -0.19384 0.0072567 0.023779 -3.7294;
-3.6664 -5.955 -15.9818 -13.5879 -7.841 -3.6676 -5.9561 -16.1237
-13.6129 7.2648 -0.10398 0.11377 -0.031877 -0.011435 2.5083;
4.1091 -0.33067 -3.2203 1.0921 6.0975 -0.078859 0.15846
-0.057588 -0.011102 2.4689 -0.15103 -0.1145 -0.020803 0.0035924 6.3899;
-79.4811 -134.3924 -353.3838 -311.5916 -13.6396 -79.2854 -134.5975
-353.366 -311.5551 -10.5189 -0.065808 -0.14654 -0.067404 -0.015414 1.0397;
0.21006 0.2566 0.58185 -0.045649 -16.7822 -0.054972 0.28312 0.5938
-0.041981 -13.4954 -0.14021 0.096861 0.071156 0.0056401 9.7603]
```

Iw {2,1} - Weight to layer 2 from input 1

```
[-0.92626 6.0165 -0.54486 -2.6766 3.216;
-0.47442 -2.0235 -4.2719 -0.59191 -10.314;
-3.5443 -0.54273 -2.8448 -5.2103 13.9421;
-0.97197 0.89229 2.0946 -0.049414 -
22.8777;1.8053 -1.2823 0.47273 -4.0733 -
0.51883]
```

b{3} - Bias to layer 3

```
[9.7456;
1.4]
```

Iw {3,2} - Weight to layer

```
[-6.706 -4.7009 -12.9906 -3.8029 10.9112;
0.90807 -0.13125 0.047191 0.075132 0.92237]
```

b{1} - Bias to layer 1

```
[0.99755;
-2.9659;
-9.1243;
11.1686; -56.6902]
```

b{2} - Bias to layer 2

```
[-7.4369;
3.6404;
0.24525;
-2.0989; 1.5782]
```

4. Architecture and weights for Neural Unit NN with 1 Layer, - 2 neuron - HARDLIM - learning algorithm

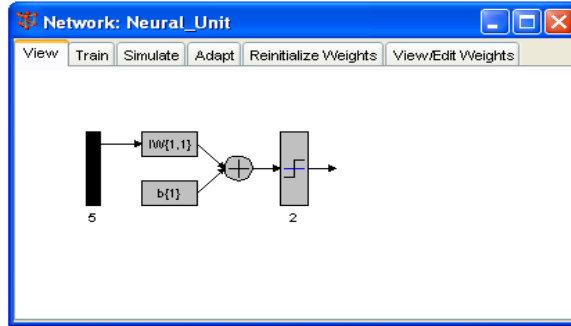


Figure 3. Neural architecture for neural unit with 5 inputs, single input and HARDLIM learning algorithm providing two outputs.

$iw \{1,1\}$ - Weight to layer 1 from input 1

$b(1)$ bias to layer 1

[1439316.9 2466719.55 6286515 6339470 101712.938;
107375794.4001 181119359.9319 457183210 471272266 7732616.192]

[95319;
7244244]

5. Architecture and weights for NARX - NN with 3 Layer, - 5(h1), 5(h2) and 2(h3)

$iw \{1,1\}$ - Weight to layer 1 from input 1

[0.067962 0.1449 0.092475 0.071983 3.6114 -0.036087 0.044791 -0.0022259 0.013904 -8.3556;
-1.8998 -7.3568 2.706 1.5078 -4.4378 0.055654 0.026694 -0.056315 -0.00088134 1.3302;
-0.04769 0.17771 -0.061706 -0.00046086 2.6673 0.1273 0.092476 0.037832 -0.023757 6.7673;
0.0078132 0.0096397 0.20767 -0.006298 -23.5656 -0.044691 0.0044589 0.084015 0.0093804 3.364;
-0.030659 -0.057294 0.013238 -0.010306 -2.1853 -0.028595 0.11975 0.058656 -0.008419 10.6153]
-0.030659 -0.057294 0.013238 -0.010306 -2.1853 -0.028595 0.11975 0.058656 -0.008419 10.6153]

$iw \{2,1\}$ - Weight to layer

[0.64456 -6.1276 0.96079 -48.2893 1.2824;
3.4551 20.8745 -4.9463 -3.0088 -2.3265;
0.54541 -2.1085 -0.22871 -2.6316 0.88312;
-1.3658 0.99677 1.1175 3.4119 0.18827;
3.0384 1.0364 -1.765 18.7931 -2.2842]

$b\{1\}$ - Bias to layer 1

[-4.1197;
-4.2106;
-15.2006;
10.3584;
-14.1644]

$Iw \{3,2\}$ - Weight to layer

[3.0329 3.6177 34.3772 -14.7302 11.065;
0.058963 -1.315 0.071505 -0.89194 0.061888]

$b\{2\}$ - Bias to layer 2

[-2.3699;
2.4442;
-0.2799;
-2.0886;
3.4857]

Iw{1,3} - Weight to layer

[0.81977 0.17286 0.44487 -0.73894;
-0.67228 -0.68689 0.36574 0.67887;
-0.22389 0.11389 -0.10919 0.66665;
0.071771 0.29715 0.19864 0.15088;
-0.38735 0.75165 0.4927 -0.4007]

b{3} - Bias to layer 3

[19.3219;
1.7769]

6. Feed Forward Back Propagation NN with 3 Layer, - 10(h1), 10(h2) and 2(h3)

iw {1,1} - Weight to layer 1 from input 1

[0.10777 0.32181 -0.035907 -0.081651 18.0256;
-0.31813 -0.27688 -0.014689 0.043556 -17.2059;
-0.27091 0.24591 -0.035967 0.14885 -6.8003;
-0.18815 0.42496 0.044804 0.057595 4.9539;
-0.086451 0.10287 0.052629 -0.12012 -17.1656;
-0.026505 -0.5449 -0.0080759 -0.075201 6.8654;
0.26793 0.23154 0.048894 -0.10224 -9.2456;
0.12821 0.16611 -0.07683 -0.0062313 6.4649;
-0.1926 0.25693 0.06809 -0.051079 0.37868;
-0.023144 -0.49016 0.046747 -0.019357 -2.0769]

iw {2,1} - Weight to layer

[0.091236 -0.42688 0.62528 0.48048 0.99072 0.46997 -0.54805 0.13668 0.048707 -0.87762;
0.70581 -0.61886 0.77575 0.1104 0.09245 -0.43396 0.6905 -0.28834 -0.61104 -0.69361;
-0.37128 -0.13306 -0.062545 -0.091959 -1.1397 -0.11815 -0.86582 -0.29352 0.6333 -0.62341;
-0.19049 -0.064476 0.78142 -0.1061 0.18657 -0.63589 0.85513 0.71348 -0.24238 0.84016;
-0.32068 -0.80929 -0.08161 -0.68744 0.52727 0.78176 0.33659 -0.21315 0.53925 -0.72849;
-0.16052 0.29778 0.55274 -0.10259 0.86599 -0.26189 0.63108 -0.77381 -0.82292 -0.42798;
-0.38987 0.40808 0.59896 -0.24351 -0.50648 -0.82131 -0.5295 -0.54668 0.17833 0.90979;
-0.2079 -0.4288 -0.65533 -0.38776 0.39997 0.5014 -0.088185 -0.88464 0.88198 -0.56556;
0.0070206 -0.55471 -0.24709 0.81943 0.051379 0.9195 -0.97566 0.15536 -0.49188 -0.0037035;
0.42313 0.39738 0.039567 0.49461 0.82517 -0.40763 0.6693 -0.72067 0.74118 -0.39936]

Iw {3,2} - Weight to layer

[0.34551 0.5331 -0.73811 -0.97027 0.63346 -0.96527 0.24228 -0.51194 -0.47358 0.31929;
0.91598 0.33225 -0.80917 -0.42361 0.97097 0.63879 0.12044 0.64402 0.50727 -0.57187]

b{1} - Bias to layer 1

[-23.0337;
29.418;
-0.97338;
-18.939;
20.5116;
12.287;
3.4403; -6.0873; -7.1042;

b{2} - Bias to layer 2

[-1.7625;
-1.3708;
0.97916;
0.5875;
0.19583;
-0.19583;
-0.5875;
-0.97916; 1.3708;

b{3} - Bias to layer 3

[0.20423;
0.20987]

APPENDIX E:

Matlab Terminologies

1. Matlab Terminologies as Used in this Project

1.1 Neural Networks Used:

- a) Cascade forward backpropagation, b) Feedforward time delay neural network
- c) Feedforward backpropagation neural network, d) Neural unit.
- e) Nonlinear autoregressive exogenous model (NARX)

1.2 Training Functions:

TRAINSCG: This training function updates weights based on the Scaled conjugate gradient backpropagation method.

1.3 Adaptation and Learning Functions

LEARNGDM: This is a gradient descent with momentum weight and bias learning function (mathworks.com).

1.4 Performance Function

MSE: Mean Square Error is a process to quantify the amount by which the estimated value differs from the true value of the quantity being estimated.

For i number of calculations of actual value A_i and experimentally derived values D_i we have, $E_i = A_i - D_i$

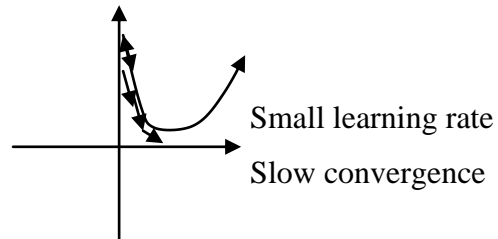
$$\text{Then MSE} = \frac{1}{n} \sum_{i=1}^n e_i^2$$

1.5 Training Parameters

Epochs: A single scan of all cases in the training data is called an epoch. (ocw.mit.edu)

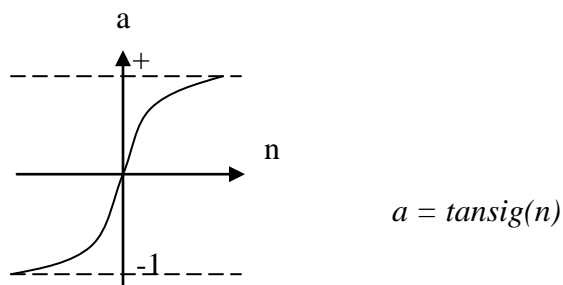
Goal: Desired performance to be reached by a neural network.

1.6 Mu



This is the learning rate. It determines how much weight is changed at each step. Small mu takes longer time to converge. (dspguide.com, 2009)

1.7 Transfer Function

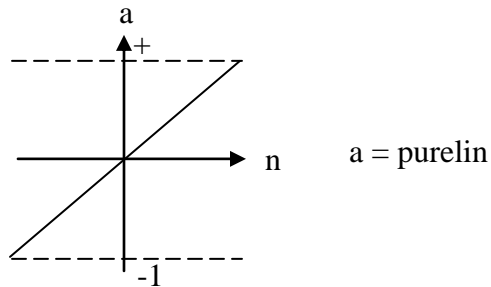


1.8 TANSIG

This is the sigmoidal transfer function. The equation here in concern is:

$a(n) = 1 / (1 + e^{-n})$. It calculates corresponding layers output from the net input that it receives

(mathwork.com)



1.9 PURELIN

This is the Linear Transfer function. The equation in concern for this transfer function is $a = n$.

This transfer function was used for the 3rd hidden layer. It also calculates the layers output from its net input. (mathworks.com)

APPENDIX F: Experimental Data and Experimental Results Error Calculation

Known NN test data (Data already used in Training): ED

| | | | | | | |
|-------------------------------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 15.93 | 14.14 | 14.75 | 14.70 | 15.20 | 16.29 |
| Bending (MPa) | 24.09 | 22.68 | 25.74 | 22.90 | 27.83 | 25.93 |
| Hardness | 67 | 61 | 67 | 63 | 70 | 66 |
| Impact (kJ/m ²) | 75 | 40 | 63 | 59 | 69 | 64 |
| Density (g /cm ³) | 1.096 | 1.083 | 1.018 | 1.06 | 1.021 | 1.009 |
| Fiber % (%) | 25 | 35 | 10 | 30 | 20 | 15 |
| Pressure (MPa) | 1 | 1 | 1 | 1 | 1 | 1 |

Unknown NN test data (Data never used in Training): ER

| | | | | | | |
|-------------------------------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 15.07 | 15.26 | 16.25 | 15.14 | 15.19 | 13.19 |
| Bending (MPa) | 24.36 | 25.00 | 26.47 | 27.40 | 24.15 | 23.21 |
| Hardness | 66 | 67 | 67 | 68 | 66 | 63 |
| Impact (kJ/m ²) | 62 | 67 | 68 | 68 | 65 | 65 |
| Density (g /cm ³) | 0.964 | 1.009 | 1.032 | 1.054 | 1.064 | 1.067 |
| Fiber % (%) | 25 | 35 | 10 | 30 | 20 | 15 |
| Pressure (MPa) | 1 | 1 | 1 | 1 | 1 | 1 |

Output data predicted by NN (for experimental input data): ED

| | | | | | | | |
|-------------------|-----------------------|--------|-----------|---------|-----------|--------|-----------|
| | Sample # | 1 | 2 | 3 | 4 | 5 | 6 |
| Exp Data | Fiber % | 25 | 35 | 10 | 30 | 20 | 15 |
| | Pressure | 1 | 1 | 1 | 1 | 1 | 1 |
| NN Derived Data | NN Fiber % | 24.65 | 35.63 | 11.64 | 32.88 | 20.06 | 15.51 |
| NN Derived Data | NN Pressure | 1.01 | 1.04 | 1.14 | 1.20 | 1.37 | 1.24 |
| Error Calculation | Fiber Data Error % | 1.4076 | -1.804286 | -16.431 | -9.596667 | -0.279 | -3.419333 |
| Error Calculation | Pressure Data Error % | -0.88 | -4.07 | -13.87 | -19.86 | -37.37 | -23.59 |

Avg Error % Fiber % **-4.008874** %

Output data predicted by NN (for experiment relevant input data): ER

| | | | | | | | |
|-------------------|-----------------------|---------|--------|---------|---------|---------|---------|
| | Sample # | 1 | 2 | 3 | 4 | 5 | 6 |
| Exp Relevant Data | Fiber % | 5 | 10 | 15 | 20 | 25 | 30 |
| | Pressure | 1 | 1 | 1 | 1 | 1 | 1 |
| NN Derived Data | NN Fiber % | 6.0164 | 7.696 | 13.1177 | 20.8334 | 24.7117 | 29.1621 |
| NN Derived Data | NN Pressure | 1.0784 | 1.1275 | 1.2718 | 1.3839 | 1.2324 | 1.1429 |
| Error Calculation | Fiber Data Error % | -16.893 | 29.937 | 14.349 | -4 | 1.16 | 2.873 |
| Error Calculation | Pressure Data Error % | -7.84 | -12.75 | -27.18 | -38.39 | -23.24 | -14.29 |

Avg Error % Fiber % **-2.459637** %

| | | | | | | | | |
|---------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 15.80 | 15.00 | 17.68 | 17.90 | 11.13 | 17.50 | 10.78 | 14.20 |
| Bending (MPa) | 24.73 | 25.10 | 26.42 | 27.36 | 25.09 | 28.11 | 25.84 | 23.49 |

| | | | | | | | | |
|------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Hardness | 64 | 66 | 68 | 67 | 64 | 69 | 69 | 63 |
| Impact (kJ/m ²) | 60 | 62 | 63 | 60 | 67 | 71 | 76 | 51 |
| Density (g/cm ³) | 0.947 | 1.015 | 1.055 | 1.098 | 1.089 | 1.055 | 1.083 | 1.096 |
| Fiber % | 5 | 5 | 15 | 25 | 30 | 20 | 10 | 35 |
| Pressure (MPa) | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |

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| | | | | | | | | |
|------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Tensile (MPa) | 12.98 | 15.33 | 14.66 | 16.59 | 17.20 | 14.74 | 14.52 | 14.29 |
| Bending (MPa) | 22.43 | 24.83 | 25.30 | 26.36 | 28.59 | 27.54 | 24.30 | 24.22 |
| Hardness | 60 | 66 | 69 | 69 | 69 | 66 | 64 | 63 |
| Impact (kJ/m ²) | 51 | 63 | 68 | 72 | 74 | 67 | 65 | 51 |
| Density (g/cm ³) | 1.079 | 1.026 | 1.058 | 1.059 | 1.062 | 1.083 | 1.088 | 1.093 |
| Fiber% | 5 | 5 | 15 | 25 | 30 | 20 | 10 | 35 |
| Pressure (MPa) | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |

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| | | | | | | | | |
|-----------------------|--------|---------|----------|----------|--------|----------|--------|----------|
| Sample# | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Fiber% | 5 | 5 | 15 | 25 | 30 | 20 | 10 | 35 |
| Pressure | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| NN Fiber % | 5.86 | 4.91 | 15.47 | 22.92 | 32.88 | 20.06 | 10.09 | 36.76 |
| NN Pressure | 1.19 | 1.31 | 1.38 | 1.27 | 1.40 | 1.28 | 1.26 | 1.34 |
| Fiber Data Error % | -17.14 | 1.774 | -3.106 | 8.3224 | -9.596 | -0.279 | -0.934 | -5.042 |
| Pressure Data Error % | -19.2 | 18.3625 | 13.76875 | 20.79375 | 12.75 | 20.15625 | 21.375 | 16.33125 |

Avg Error % Pressure **0.3** %

Continued from previous page

| | | | | | | | | |
|-----------------------|--------|---------|---------|--------|---------|----------|---------|--------|
| Sample # | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Fiber % | 35 | 5 | 10 | 15 | 20 | 25 | 30 | 35 |
| Pressure | 1 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| NN Fiber % | 34.99 | 10.33 | 12.11 | 14.15 | 21.96 | 22.12 | 28.98 | 37.37 |
| NN Pressure | 1.2311 | 1.2507 | 1.287 | 1.3952 | 1.3946 | 1.3669 | 1.1866 | 1.194 |
| Fiber Data Error % | 0.0105 | -51.603 | -17.46 | 6 | -8.95 | 13 | 3.5 | -6.36 |
| Pressure Data Error % | -23.11 | 21.831 | 19.5625 | 12.8 | 12.8375 | 14.56875 | 25.8375 | 25.375 |

Avg Error % Pressure **-0.9** %

(Empirical Data – NN Result)

Error % = ----- x 100

Emperical Data