



**REPUBLIC OF TURKEY  
ADANA ALPARSLAN TÜRKEŞ SCIENCE AND TECHNOLOGY  
UNIVERSITY**

**GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES  
DEPARTMENT OF MECHANICAL ENGINEERING**

**AN EXPERIMENTAL AND NUMERICAL STUDY ON THE EFFECTS  
OF NANOADDITIVES AND MATERIAL EXTRUSION PARAMETERS  
ON THE MECHANICAL AND FLEXURAL CHARACTERISTICS OF  
ABS/PVC BLEND POLYMER CORE SANDWICH PANELS**

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MASTER OF SCIENCE**



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**ADANA 2023**

I hereby declare that all information in this thesis has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all information that is not original to this work.

[Signature]

Deniz GÜRAY GENÇAY



# **ABSTRACT**

## **AN EXPERIMENTAL AND NUMERICAL STUDY ON THE EFFECTS OF NANOADDITIVES AND MATERIAL EXTRUSION PARAMETERS ON THE MECHANICAL AND FLEXURAL CHARACTERISTICS OF ABS/PVC BLEND POLYMER CORE SANDWICH PANELS**

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This thesis investigates the effects of different core structures on the flexural response of composite core shell structures fabricated using fused deposition modeling (FDM). The study explores the influence of various FDM parameters and the composition of the base matrix material on the mechanical properties of the structures. Regression modeling with artificial neural networks (ANN) is employed to predict the mechanical variables of the 3D printed samples, such as in-plane and out-of-plane modulus of elasticity and ultimate strength. Optimization techniques using ant colony optimization (ACO) are applied to optimize the FDM parameters and material composition, resulting in improved mechanical performance. The obtained regression models are used to analyze variations in mechanical properties, visualized through bar-charts and surface responses, and optimization algorithms determine the material extrusion parameters that maximize the response variables individually and cumulatively.

Insights are provided into the influence of material extrusion parameters and the compatibility of additives, such as PVC and carbon nanofibers (CNFs), on the mechanical characteristics of 3D printed samples and composite core shell sandwich panel (CCSSP) specimens. The study highlights the potential for tailoring the mechanical properties of 3D printed materials for specific applications through careful selection and optimization of material extrusion parameters. Furthermore, the research demonstrates the potential of FDM as a viable manufacturing technique for producing composite core shell structures with tailored mechanical properties. By optimizing the core structures and FDM parameters, the flexural

response and overall performance of the fabricated structures can be enhanced. The outcomes of this research contribute to the advancement of additive manufacturing, particularly in the context of composite core shell structures. The findings offer valuable knowledge for engineers and researchers in optimizing FDM processes and material compositions to achieve desired mechanical properties for specific applications.

Key findings of this study include the analysis of mechanical properties of 3D printed samples fabricated at different orientations of principal axes, with the addition of PVC improving in-plane stiffness, particularly at lower extrusion rates and printing orientations. The presence of CNFs has a limited effect on stiffness at different printing orientations. Investigation of ultimate strength reveals that PVC alone does not effectively enhance it, but the inclusion of CNFs counteracts the reduction caused by increased extrusion rates, particularly for samples with a raster orientation of  $[0/90^\circ]$ . The addition of CNFs creates a load-carrying network through mechanical interlocking, improving the compatibility between ABS and PVC molecules and the ultimate strength of the samples.

The response surface analysis of CCSSPs with hybrid circular/triangular corrugated cores (HCTC) elucidates the influence of material extrusion parameters and polymer composition on the flexural response. PVC addition improves flexural stiffness, while CNF presence can reduce stiffness, especially at higher extrusion rates. The optimization process indicates that optimal parameter combinations often involve samples without CNF in the matrix, although the addition of CNF can positively influence the mechanical and flexural response of 3D printed samples for compositions with higher PVC concentrations. Considering CNF concentration, PVC ratio, and extrusion parameters is crucial for achieving desired mechanical properties and tailoring the performance of 3D printed structures.

**Keywords:** material extrusion, extrusion rate, raster orientation, blend polymer ratio, concentration of nanoadditives, acrylonitrile butadiene styrene (ABS), polyvinyl chloride (PVC), carbon nanofiber (CNF), mechanical properties, flexural characteristics, composite core shell sandwich panels, finite element analysis, ANN/Bayesian hybrid regression modeling, ant colony optimization.

# ÖZET

## **ABS/PVC KARIŞIK POLİMER ÇEKİRDEKLİ SANDVIÇ PANELLERİN MEKANİK VE EĞİLME KARAKTERİSTİKLERİ ÜZERİNE NANO KATKI MADDELERİ VE MALZEME EKSTRÜZYON PARAMETRELERİNİN DENEYSEL VE SAYISAL İNCELEMESİ**

Deniz GÜRAY GENÇAY

Makine Mühendisliği Anabilim Dalı

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Bu tez, erimiş biriktirme modellemesi (EBM) kullanılarak üretilen kompozit çekirdek kabuk yapıların eğilme tepkisi üzerinde farklı çekirdek yapılarının etkilerini araştırmaktadır. Çalışma, çeşitli EBM parametrelerinin ve temel matris malzemesinin kompozit yapıların mekanik özellikleri üzerindeki etkisini keşfetmektedir. Yapay sinir ağları (YSA) ile regresyon modelleme kullanılarak 3D baskı örneklerinin düzlem içi ve düzlem dışı elastiklik modülü ve maksimum çekme mukavemeti gibi mekanik değişkenleri tahmin etmektedir. Karınca kolonisi optimizasyonu (KKO) kullanarak EBM parametrelerini ve malzeme bileşimini optimize etmek için optimizasyon teknikleri uygulanarak mekanik performansı artırılmaktadır. Elde edilen regresyon modelleri mekanik özelliklerdeki değişimleri analiz etmek için çubuk grafikleri ve yüzey tepkileri ile görselleştirilmekte ve optimizasyon algoritmaları, yanıt değişkenlerini bireysel ve toplu olarak maksimize eden malzeme ekstrüzyon parametrelerini belirlemektedir. Çalışmada, PVC ve karbon nanofiber (CNF) gibi katkı maddelerinin, 3D baskı örneklerinin ve kompozit çekirdek kabuk sandviç panel (KÇKSP) numunelerinin mekanik özellikleri üzerindeki etkisi hakkında bilgiler sunulmaktadır. Çalışma, malzeme ekstrüzyon parametrelerinin ve katkı maddelerinin uyumluluğunun, özellikle malzeme ekstrüzyon parametrelerinin dikkatli seçimi ve optimize edilmesiyle 3D baskı malzemelerinin mekanik özelliklerinin belirli uygulamalara uygun şekilde şekillendirilebileceğini vurgulamaktadır. Ayrıca, araştırma, EBM'nin özelleştirilmiş mekanik özelliklere sahip kompozit çekirdek kabuk yapıların üretimi için geçerli bir üretim tekniği olarak potansiyelini göstermektedir. Çekirdek

yapılarının ve EBM parametrelerinin optimize edilmesiyle, üretilen yapıların eğilme tepkisi ve genel performansı artırılabilir. Bu araştırmanın sonuçları, özellikle kompozit çekirdek kabuk yapılarının bağlamında, eklemeli imalatın ilerlemesine katkıda bulunmaktadır. Bulgular, EBM süreçlerini ve malzeme bileşimlerini optimize etme konusunda mühendisler ve araştırmacılar için değerli bir bilgi sunmaktadır.

Bu çalışmanın temel bulguları şunları içermektedir: Ana eksenlerin farklı yönelimlerinde üretilen 3D baskı örneklerinin mekanik özelliklerinin analizi, PVC katkısının özellikle daha düşük ekstrüzyon hızlarında ve baskı yönelimlerinde düzlem içi sertliği iyileştirdiğini göstermektedir. CNF varlığının ise farklı baskı yönelimlerinde sertliğe sınırlı etkisi vardır. Nihai mukavemetin incelenmesi, PVC'nin tek başına etkili bir şekilde artırmadığını, ancak CNF katkısının artan ekstrüzyon hızlarına bağlı olarak azalmayı engellediğini özellikle  $[0/90^\circ]$  raster yönelimli örneklerde göstermektedir. CNF'nin katılması, ABS ve PVC molekülleri arasındaki mekanik bağlantılarla birlikte bir yük taşıma ağı oluşturarak numunelerin nihai mukavemetini artırmaktadır.

Hibrit dairesel/üçgen dalgalı çekirdekler ile KÇKSP'lerin yanıt yüzeyi analizi, malzeme ekstrüzyon parametrelerinin ve polimer bileşiminin eğilme tepkisine olan etkisini açıklamaktadır. PVC katkısı eğilme sertliği artırırken, CNF varlığı özellikle daha yüksek ekstrüzyon hızlarında sertliği azaltabilmektedir. Optimizasyon süreci, optimal parametre kombinasyonlarının genellikle matris içinde CNF olmadığı örnekleri içerdiğini, ancak PVC konsantrasyonu daha yüksek bileşimlerde CNF katkısının mekanik ve eğilme tepkisine olumlu etkisi olabileceğini göstermektedir. CNF konsantrasyonu, PVC oranı ve ekstrüzyon parametrelerinin istenen mekanik özelliklerin elde edilmesi ve 3D baskı yapılarının performansının şekillendirilmesi açısından önemlidir.

**Anahtar Kelimeler:** malzeme ekstrüzyonu, ekstrüzyon hızı, raster yönelimi, karışım polimer oranı, nano katkı maddesi konsantrasyonu, akrilonitril butadien stiren (ABS), polivinil klorür (PVC), karbon nanofiber (CNF), mekanik özellikler, fleksural karakteristikler, kompozit çekirdek kabuk sandviç paneller, sonlu eleman analizi, ANN/Bayesian hibrit regresyon modellemesi, ant koloni optimizasyonu.

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## NOMENCLATURE

|                   |                                         |
|-------------------|-----------------------------------------|
| ABS               | : Acrylonitrile Butadiene Styrene       |
| ACO               | : Ant colony optimization               |
| AI                | : Artificial intelligence               |
| AM                | : Additive Manufacturing                |
| ANN               | : Artificial neural network             |
| ANOVA             | : Analysis of variance                  |
| CNT               | : Carbon nanotube                       |
| CaCO <sub>3</sub> | : Calcium Carbonate                     |
| CAD               | : Computer-Aided Design                 |
| CCSSP             | : Composite core shell sandwich panel   |
| CCVD              | : Catalytical chemical vapor deposition |
| CFRP              | : Carbon fiber reinforced panel         |
| CNF               | : Carbon nanofiber                      |
| CNN               | : Convolutional neural network          |
| CVD               | : Chemical vapor deposition             |
| DMTA              | : Dynamic mechanical thermal analysis   |
| FDM               | : Fused Deposition Modeling             |
| FE                | : Finite element                        |
| FEM               | : Finite element model                  |
| GA                | : Generic algorithm                     |
| HCTC              | : Hybrid circular/triangular corrugated |
| HNT               | : Halloysite nanotubes                  |
| HPF               | : Hard polyurethane foam                |
| LTSP              | : Lattice truss sandwich panel          |
| LWSP              | : Light weight sandwich panels          |
| MWCNT             | : Multi-wall carbon nanotube            |
| NPR               | : Negative Poisson's ratio              |
| PC                | : Polycarbonate                         |
| PEI               | : Polyethyleneimine                     |
| PETG              | : Poly (Ethylene Terephthalate)-Glycol  |

|                        |                                               |
|------------------------|-----------------------------------------------|
| PLA                    | : Polylactic Acid                             |
| PP                     | : Polypropylene                               |
| PVC                    | : Polyvinyl Chloride                          |
| RF                     | : Reference point                             |
| RMSE                   | : Root mean square error                      |
| SBR                    | : CaCO <sub>3</sub> / Styrene butadiene latex |
| SEM                    | : Scanning electron microscope                |
| SLM                    | : Selective laser melting                     |
| SPF                    | : Soft polyurethane foam                      |
| SWCNT                  | : Single-wall carbon nanotube                 |
| TEM                    | : Transmission electron microscope            |
| THF                    | : Tetrahydrofuran                             |
| TPU                    | : Thermoplastic polyurethane                  |
| VCM                    | : Vinyl chloride monomer                      |
| 3D                     | : Three dimensional                           |
| <i>ER</i>              | : Extrusion rate                              |
| <i>PO</i>              | : Printing orientation (raster orientation)   |
| <i>PR</i>              | : Polymer ratio (PVC ratio in ABS)            |
| <i>NP</i>              | : Nanoadditive concentration                  |
| <i>S<sub>ul</sub></i>  | : In-plane ultimate strength                  |
| <i>E<sub>1</sub></i>   | : In-plane modulus of elasticity              |
| <i>F<sub>max</sub></i> | : Maximum flexural loading                    |

# 1. INTRODUCTION AND STATE OF ART

## 1.1. Aspects of this study

Polymeric lightweight sandwich panels are composed of two face-sheets made of fiber/resin composites, with a lightweight cellular polymeric core of unique architecture in between. This core, referred to as the lightweight sandwich panel (LWSP) core, plays a crucial role in enhancing the bending stiffness, shear stiffness, and energy absorption capabilities of the panels. By manipulating the composition and carefully selecting the optimal architecture for the cellular core, the mechanical properties and flexural performance of these sandwich panels can be significantly improved (Schaedler et al., 2016), (Ajdari et al., 2015).

In addition, the material extrusion process, also known as fused deposition modeling (FDM) or 3D printing technique, has emerged as a rapidly growing method for producing polymeric core structures for LWSPs (Sarvestani et al., 2018), (Niknam et al., 2020), (Altan & Kovan, 2016), (Turner, 2017). This technique offers several advantages over traditional manufacturing processes, particularly in its ability to directly fabricate intricate and customized geometries based on CAD models. However, the flexibility of this process is mainly limited by the availability of compatible polymers used as raw materials for filament production during the fabrication stage. The lack of a wide variety of suitable materials hampers the applicability of FDM-fabricated parts and restricts the overall progress of this technology (Rocha et al., 2014).

Therefore, one of the main objectives of this research is to introduce a blend of polyvinyl chloride (PVC) and acrylonitrile butadiene styrene (ABS) polymers in varying proportions as the base material for the filaments used in manufacturing the polymeric core of CCSSPs (composite core shell sandwich panels). ABS is a commonly employed thermoplastic polymer in the FDM process due to its hardness, excellent chemical resistance, favorable mechanical properties, recyclability, and ease of processing, making it widely used for prototyping in 3D printing (Sarvestani et al., 2018). Conversely, rigid PVC is a chemically inert polymer that can enhance the dimensional stability and surface finish of products. It is anticipated that the durability of this polymer will enhance the resilience and toughness of 3D printed samples composed of PVC/ABS blend polymers, compared to those made solely from ABS (McKeen, 2017).

Moreover, the addition of nanosized tubes and particles in concentrations lower than those of micro-sized short fibers and particles has demonstrated a significant enhancement in the mechanical properties of 3D printed samples. For instance, the incorporation of 5wt% nanotitanium oxide (TiO<sub>2</sub>) (Torrado Perez et al., 2014) and 10wt% carbon nanofibers (Shofner et al., 2003) in ABS resulted in a remarkable increase of 13.2% and 39% in the tensile strength of the printed composites, respectively. This phenomenon holds the potential to enhance the strength and stiffness of samples produced using such composites in the FDM process. Carbon nanofibers (CNFs) are particularly noteworthy among the nanoadditives widely employed as reinforcing and surface-enhancing agents in numerous polymer composites.

Therefore, in this research the performance of 3D printed cellular architecture of the polymeric core of composite core shell sandwich panels (CCSSPs) under 3-point bending loading have been investigated through engineering the composition of core structure and addition of reinforcing nanoparticles in the matrix of base filaments. The incorporated ingredients into the composite core were in the form of polyvinyl chloride granules and CNFs nanoadditives in varying concentrations in the extrusion process of acrylonitrile butadiene styrene (ABS) filaments. Such filaments have been subsequently used in the material extrusion process of the core structure of CCSSPs of different configurations.

Fabric-based carbon fibers incorporated in the phenolic resin have been employed to fabricate cover shell of the 3D printed cores using vacuum infusion technique. Three different types of core architectures, namely hexagonal, triangular, and a hybrid circular/triangular corrugated design, have been used in printing process of the core structures of CCSSPs to distinguish between the structural and compositional effects on the flexural performance of the LWSPs. Furthermore, uniaxial tensile tests of polymer samples printed with different grades of composite filaments have been used to characterize the mechanical properties of the fabricated samples. The tensile tests of 3D printed dog-bone samples of composite filaments and 3-point bending of the CCSSPs have been conducted with the different compositions of the base material and the FDM parameters as input variables.

By conducting these experiments and finite element analyses, this research aims to provide insights into the effects of composition, architecture, and FDM parameters on the mechanical properties and flexural performance of CCSSPs, ultimately contributing to the optimization of their design and manufacturing processes.

## **1.2. Sandwich structures**

### **1.2.1. History of sandwich structures**

The concept of using two cooperating faces separated by a distance in a sandwich panel can be traced back to the 1820s when visionaries like Frenchman Duleau and later Fairbair discussed this idea. However, it took several years for the concept to find practical applications. The use of sandwich panels with asbestos faces and a fiberboard core emerged during World War One. A significant milestone in the history of sandwich panels was the mass production of the Mosquito aircraft in England during World War Two. This aircraft utilized veneer faces and a balsa wood core, marking a significant advancement in sandwich panel technology (Zenkert, 1995). Another exceptional achievement involving sandwich construction occurred on 20 July 1969, with the successful landing of a spacecraft on the moon. This monumental event highlighted the crucial role played by the sandwich construction method, among other factors, in accomplishing this remarkable feat (Davies, 2001).

During World War Two, the initial theoretical analysis of sandwich construction gained significant attention. Subsequently, between 1945 and 1955, several publications emerged that focused on the strength and stability of sandwich beams, columns, and plates. However, practical challenges hindered frequent publications until around 1980. These challenges included difficulties in bonding the face sheets to the core, ensuring sufficient stiffness, and establishing reliable repair and inspection procedures (Zenkert, 1995).

From 1980 onwards, the theoretical analysis of sandwich panels shifted towards the optimization of laminates using finite element (FE) analyses. The utilization of FE analysis allows for a more precise solution to derive and solve the complex differential equations governing the deflection of sandwich panels compared to traditional analytical calculations. This shift opened up new avenues for exploring the design and performance of sandwich panels in various applications.

### **1.2.2. The main principle of sandwich structure**

A sandwich panel is a structural construction composed of two outer plates, referred to as facings or skins, which are adhered to a thick core material positioned in the middle, as depicted

in Fig. 1.1. The facings are characterized by their thinness, high stiffness, and strength, while the core material is comparatively thicker and lighter in weight.

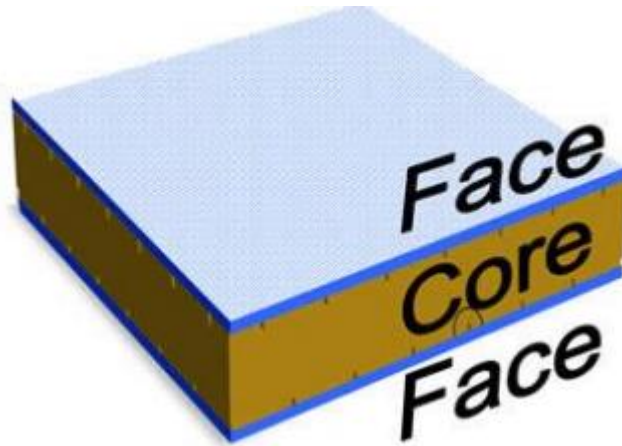


**Figure 1.1.** A schematic view of a typical sandwich panel.

### **1.2.3. Sandwich panel core geometries**

There are numerous designs of core structures available for sandwich panels, with three commonly discussed architectural designs being hexagonal, trapezoidal, and triangular. As an introduction, the key characteristics of these architectures are presented here, while more comprehensive details regarding various designs and their specific characteristics are covered in Chapter 3.

#### **Hexagonal structures**

The conventional hexagonal-core sandwich structures, commonly known as honeycomb sandwich structures, exhibit a remarkable resemblance to the honeycombs found in nature (Fig. 1.2). This resemblance finds support in the classical hexagonal honeycomb conjecture, which was proven by Hales (Hales, 2001). According to this conjecture, the hexagonal unit cell configuration represents the most efficient structure in nature. Additionally, the honeycomb possesses a periodic structure characterized by two-dimensional arrays of unit cells in the in-plane direction and parallel stacks in the out-of-plane direction. As a result, it exhibits tailorable anisotropic properties (Khan et al., 2012). This unique feature empowers the hexagonal honeycomb core to exert greater control over its mechanical and crashworthiness characteristics compared to randomly-structured, disordered, and heterogeneous cores such as foam (Laurin et al., 2005), Voronoi lattice (Zhu et al., 2006), and stochastic lattice (Alkhader & Vural, 2008).

Hexagonal sandwich structures, commonly referred to as honeycomb sandwich structures, offer a multitude of advantages stemming from their exceptional properties, which include high stiffness, strength, and low density (McGregor et al., 2019). Furthermore, they exhibit superior energy absorption capabilities, remarkable stiffness-to-weight ratios, excellent ballistic resistance performance, and notable thermal and acoustic isolation properties (Feng et al., 2020). These highly desirable characteristics make honeycomb sandwich structures extremely well-suited for a wide range of applications, encompassing satellites, aircraft, ships, automobiles, rail cars, wind energy systems, and bridge construction (Vinson, 2005).

The outstanding properties of honeycomb sandwich structures, such as their lightweight nature, high strength, and stiffness, contribute to their widespread use in various applications. They play a vital role in the aerospace industry, serving as essential components in satellites, aircraft, and spacecraft. Additionally, honeycomb sandwich structures find application in diverse fields, including shipbuilding, automotive manufacturing, rail transportation, wind energy systems, and bridge construction. Moreover, they have even found their way into packaging materials, such as paper-based honeycomb cardboard, as well as sporting goods like skis and snowboards. The versatility and adaptability of honeycomb sandwich structures make them invaluable in fulfilling the diverse needs of different industries (Han et al., 2021).

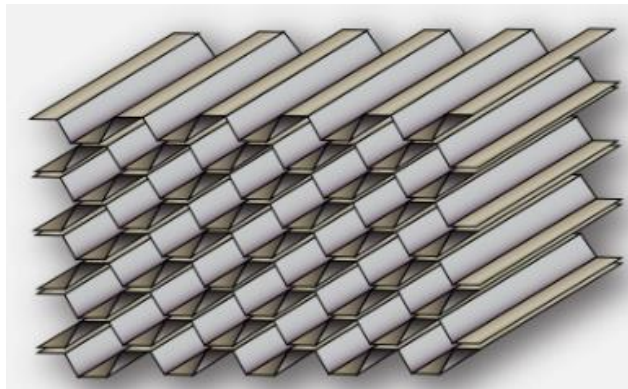


**Figure 1.2.** Hexagonal honeycomb structure (Han et al., 2021).

### **Trapezoidal structures**

Trapezoidal sandwich structures are composite sandwich structures that feature trapezoidal latticed webs for reinforcement. These webs can have angles of  $45^\circ$ ,  $60^\circ$ , and  $75^\circ$ . It has been demonstrated that trapezoidal sandwich structures exhibit exceptional energy absorption capabilities, particularly those with  $45^\circ$  trapezoidal latticed webs, which can absorb about 2.5

times more energy than structures with vertical latticed webs. Additionally, trapezoidal sandwich structures offer high specific strength and stiffness, excellent corrosion resistance, and robust design flexibility (Han et al., 2021).

The applications of trapezoidal sandwich structures are diverse. For instance, they are used as composite bumper devices for bridge pier protection against ship collisions. Moreover, they are increasingly employed in the transportation and aerospace industries due to their ability to enhance damage resistance (Zaid, 2017). A review of sandwich structures indicates that corrugated sandwich structures, which fall within the trapezoidal sandwich structure category, demonstrate higher shear strengths in the longitudinal direction compared to square honeycombs and foam cores (Feng et al., 2020).

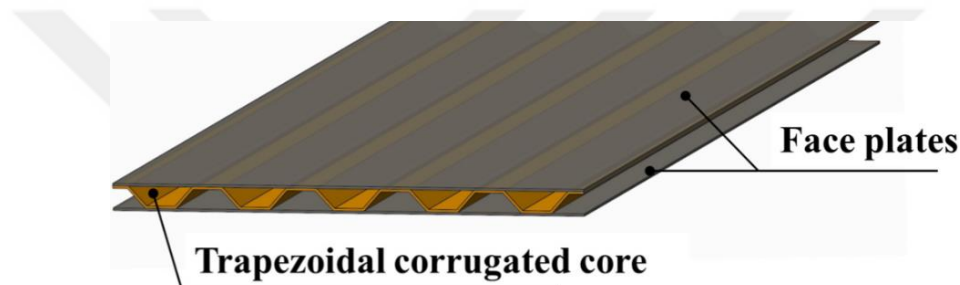


**Figure 1.3.** Trapezoidal corrugated sandwich structure (Feng et al., 2020).

### **Triangular structures**

The corrugated core shell structure refers to a type of sandwich structure where the core layer is composed of a corrugated or wavy material. This structure comprises two outer face sheets or panels that are bonded to the corrugated core, creating a composite system. The corrugated core is characterized by repetitive patterns of ridges and valleys, which contribute to the overall strength, stiffness, and energy absorption capabilities of the structure. Various geometries, including rectangular, triangular, trapezoidal, arc-tangent, or sinusoidal shapes, can be employed for the corrugated core, depending on the desired structural properties and intended applications (Atar et al., 2021).

Corrugated core shell structures find wide usage across industries such as aerospace, automotive, construction, and marine due to their exceptional load-bearing capacity, lightweight nature, and efficient energy absorption. These structures are highly suitable for absorbing and dissipating energy. The specific design of a corrugated core shell structure is tailored to the intended application and performance requirements. By adjusting parameters

such as geometry, material properties, and bonding techniques, the mechanical properties of the structure can be customized to meet specific needs, including enhanced strength, stiffness, or impact resistance (Atar et al., 2021).

Corrugated triangular sandwich cores represent a specific type of sandwich structure frequently employed in lightweight applications, such as aircraft fuselages and marine hulls. In comparison to honeycomb cores, corrugated cores can exhibit higher bending strength, stiffness, and resistance to twisting along the longitudinal axis. Corrugated triangular sheet structures are renowned for their exceptional shear strength, energy absorption capabilities, and load-bearing capacity, making them suitable as cores for panel constructions. Another advantage of corrugated cores lies in the presence of open channels, which allow for venting to avoid moisture accumulation. This feature can be particularly advantageous in aircraft construction where moisture accumulation is a concern with honeycomb sandwich panels (Zaid et al., 2016).

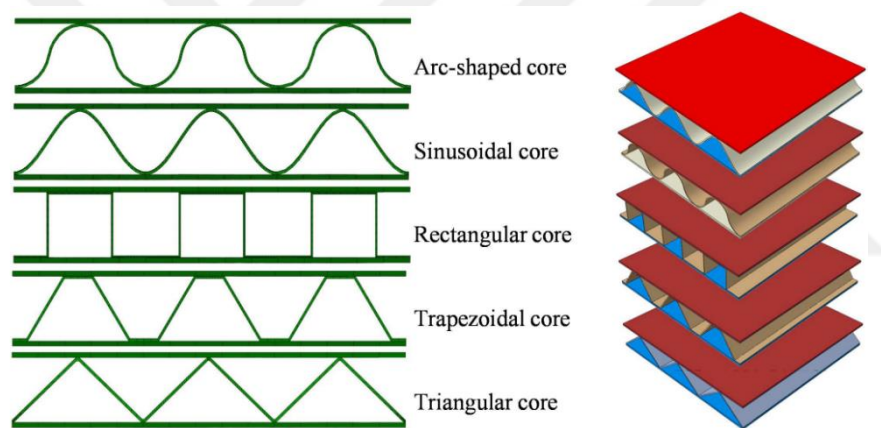


**Figure 1.4.** Sandwich panels featuring corrugated cores with distinctive geometric configurations: (a) cross-sections and (b) axonometric drawing (Rong et al., 2018).

#### 1.2.4. Light-weight sandwich panels (LWSP)

Lightweight sandwich panels have gained significant popularity across various industries, including aerospace, marine, automotive, wind energy, and construction, due to their exceptional properties such as a high flexural stiffness-to-weight ratio, excellent thermal insulation, and remarkable energy absorption capability (Schaedler & Carter, 2016). These panels consist of two thin but rigid face sheets positioned at the top and bottom, with a lightweight and relatively thick core material in between. The core material plays a critical role

in connecting the face sheets, adding minimal weight while significantly enhancing the overall performance of the sandwich panels.

One of the key advantages of a lightweight core is its ability to provide high bending stiffness and resistance to buckling (Gibson & Ashby, 1999). By incorporating a core material with suitable mechanical properties, sandwich panels can effectively distribute and withstand external loads, ensuring structural integrity and stability. The core's resistance to bending forces is particularly crucial in applications where the panels may experience bending or flexural loads, such as aerospace structures or wind turbine blades.

Moreover, sandwich panels with a lightweight core offer excellent shear stiffness, referring to their capacity to resist deformation under shear stress (Allen & Neal, 2013). This property is vital in scenarios where the panels are subjected to shear forces, as in marine applications or structures exposed to wind loads. The shear stiffness of the core material helps maintain the structural integrity of the sandwich panels and prevents excessive deformation or failure.

In addition to their mechanical advantages, sandwich panels with a lightweight core exhibit exceptional energy absorption capability. The core material absorbs and dissipates energy during impacts or dynamic loading, reducing the transmitted forces to the face sheets and protecting the overall structure from damage. This energy absorption capability is particularly valuable in applications where impact resistance and crashworthiness are critical, such as automotive safety components or marine structures.

Continuous advancements in core materials and manufacturing techniques have led to the development of innovative lightweight cores, including honeycomb structures, foam cores, and lattice trusses. Figure 1.5 illustrates a typical example of such structures. These advancements contribute to further improvements in the mechanical properties and overall performance of sandwich panels, making them increasingly sought after in various industries.

Overall, lightweight sandwich panels with their combination of high stiffness, thermal insulation, energy absorption, and weight reduction benefits have become indispensable in

modern engineering applications. They offer a versatile solution for achieving optimal structural performance and efficiency, meeting the diverse needs of different industries.

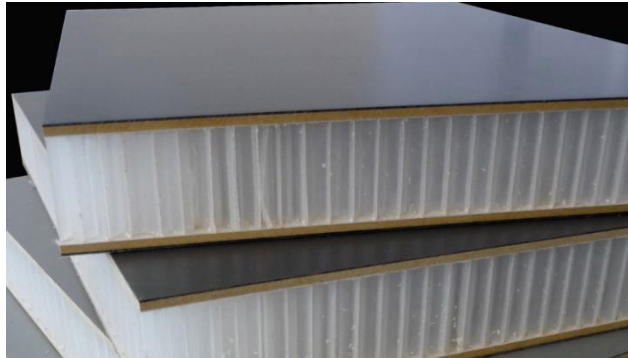


**Figure 1.5.** Examples of LWSP with Honeycomb core structure (Allen & Neal, 2013).

### **1.3. Additive manufacturing Technology**

Additive manufacturing (AM), commonly referred to as three-dimensional printing (3D printing), is a rapidly emerging disruptive technology that is currently revolutionizing design, engineering, materials, and manufacturing processes. It is reshaping various industries by driving cost reduction, waste minimization, and overall operational efficiency improvements. With its transformative potential, AM is expected to have profound industrial, economic, and societal impacts. The roots of AM can be traced back to the 1980s when it was initially utilized for small-scale product manufacturing and prototyping. Figure 1.6 presents a timeline showcasing key discoveries and milestones in the field of AM from the 1980s to the present day (Alghamdi et al., 2021). Despite its historical development, AM remains a dynamic and evolving technology, continuously progressing to enable the production of high-quality, intricate components with exceptional precision and performance. It has expanded its capabilities to encompass a wide range of materials, including multimaterials, further enhancing its versatility and potential applications.

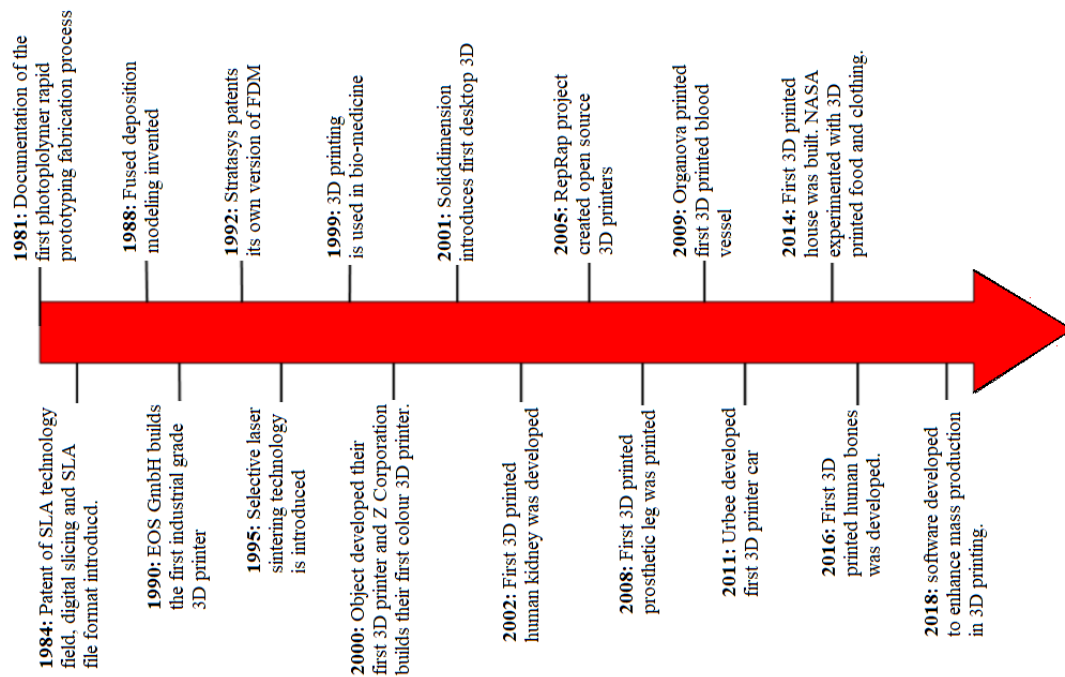


**Figure 1.6.** Evolution and milestones in the timeline of 3D printing technology from the 1980s to the present day (Alghamdi et al., 2021).

### 1.3.1. Additive Manufacturing Applications

In the present day, additive manufacturing (AM) technologies have gained widespread acceptance globally, with their usage experiencing exponential growth due to their numerous advantages over traditional manufacturing methods. AM offers remarkable flexibility in creating lightweight and intricate structures with high precision, while also significantly reducing production time. Unlike conventional manufacturing processes, AM eliminates the need for additional tools such as molds, as it operates based on layer-by-layer fabrication of the desired geometry. The data representing the object is sliced into layers, enabling the production of complex shapes without encountering any constraints. Consequently, detailed analysis of part geometry, determination of production sequences, selection of specific equipment and processes, or the use of additional fixtures becomes unnecessary. This automation and simplification of the production process result in reduced production costs, rendering AM technologies highly valuable in various industries, including aerospace, automotive, healthcare, and food (Bayraktar, 2018), (Gibson et al., 2015), (Mosleh et al., 2022).

While various types of additive manufacturing (AM) technologies exist, they are all grounded in similar principles. The distinctions between them arise from the selection of materials, the

process of layer formation, and the methods employed to connect these layers. These differences can have an impact on factors such as the precision of the final part, as well as its material and mechanical properties. Additionally, these variations influence process-related aspects such as lead time, the necessity for post-processing, the extent of post-processing required, the size of the AM machine utilized, and the overall production and machine costs. It is crucial to dispel common misconceptions about AM, as it extends beyond the creation of mere prototypes. When seamlessly integrated into comprehensive process chains, AM holds the potential to significantly reduce product development time and costs, leading to improved efficiency (Gibson et al., 2015).

### **1.3.2. Fused Deposition Modeling (FDM)**

The material extrusion process, also known as fused deposition modeling (FDM) or 3D printing, is a widely utilized additive manufacturing technique that employs a continuous filament of thermoplastic material. In this process, the filament is fed from a large spool through a heated printer extruder head, which moves in a controlled manner to deposit the material onto the work being built (Hamzah et al., 2018a). The deposition occurs layer by layer, with the print head typically moving in two dimensions to create each horizontal plane or layer. After completing a layer, the work or print head is incrementally raised vertically to initiate the next layer. This precise movement allows for the creation of intricate shapes and structures. Figure 1.7 illustrates the working principle and fabrication process in a typical FDM system.

One advantage of FDM is the ability to control the speed of the extruder head, allowing for the initiation and interruption of deposition as needed. This capability enables the creation of interrupted planes without the occurrence of unwanted stringing or dribbling between different sections. The filament is carefully melted by the heated print head, and upon deposition, it rapidly solidifies, forming a robust bond with the previous layers and resulting in a solid object. The term "fused deposition modeling" was coined by the members of the RepRap project to provide an unrestricted acronym (FDM) that could be freely used without legal limitations (Jones et al., 2011). This process has gained popularity due to its accessibility, versatility, and cost-effectiveness, making it widely adopted across various industries and applications.

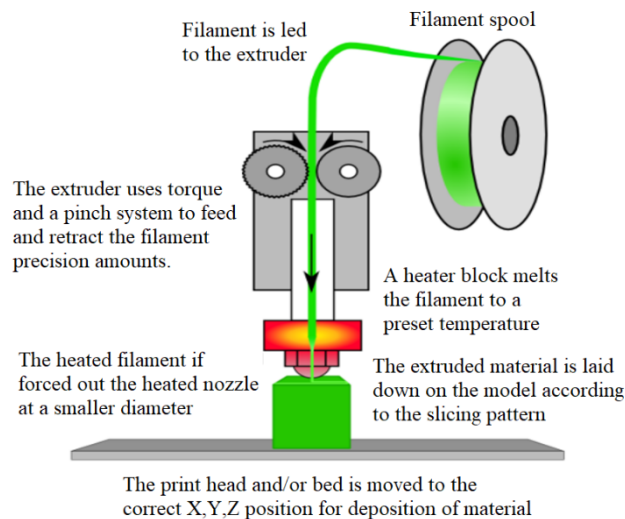


**Figure 1.7.** A schematic representation of the mechanism of material extrusion in a fused deposition modeling 3D printing system (Hamzah et al., 2018a).

### 1.3.3. Material extrusion variables and state of art

The properties of deposited layers and the bonding energy between them in the FDM process are significantly influenced by various process parameters (Chua & Leong, 2017). These parameters, in conjunction with the base material composition, play a critical role in determining the mechanical characteristics of the fabricated samples (Zou et al., 2016; Alaimo et al., 2017). Key FDM parameters that impact the response variables of printed specimens include the extrusion rate (*printing speed*), thickness of layer, filling ratio, and deposition pattern (filling architecture and raster orientation) of the samples. Material deposition in FDM occurs as thin beads placed side-by-side, with fusion taking place based on a defined internal architecture as the part grows (Hamzah et al., 2018b). It is essential to optimize these process parameters carefully to achieve the desired mechanical properties and overall quality of the printed samples.

The material extrusion process offers a wide range of filament options consisting of thermoplastic materials, each with distinct properties and applications. Examples of such filaments include polylactic acid (PLA), acrylonitrile butadiene styrene (ABS), polycarbonate (PC), polyethylene terephthalate glycol (PETG), polyethyleneimine (PEI), and Thermoplastic Polyurethane (TPU). Among the various choice of filament materials in FDM, PLA (Polylactic Acid) stands out as one of the most popular choices. PLA is a biodegradable thermoplastic

polymer derived from lactic acid  $(C(CH_3)(OH)HCOOH)_n$ , known for its ease of production due to low melting and print bed temperatures (Zhou et al., 2018).

Following PLA, ABS (Acrylonitrile Butadiene Styrene) ranks among the most widely used materials in FDM printing. This thermoplastic polymer is renowned for its strength, durability, and versatility. ABS filament finds applications across various industries, including prototyping, manufacturing, engineering, and consumer goods. It offers several advantages for FDM printing. With good mechanical properties, ABS is suitable for functional parts and prototypes that require strength and impact resistance. Moreover, ABS exhibits excellent temperature resistance, enabling printed objects to withstand moderate heat without deformation. ABS also boasts favorable post-processing capabilities, making it easily sandable, glueable, and paintable.

However, it is essential to note that successful printing with ABS requires careful consideration. ABS has a tendency for higher shrinkage and may be prone to warping if not properly controlled during the printing process. To mitigate these issues and improve overall print quality, the use of a heated bed and an enclosed print chamber are recommended. These measures help maintain optimal printing conditions and minimize the impact of shrinkage and warping, ensuring better outcomes.

Extensive research has been conducted, encompassing both experimental and numerical analyses, with the aim of addressing defects in FDM-printed samples and optimizing printing parameters to enhance the mechanical and physical properties of fabricated components. Ahn et al. (2016) conducted a study specifically focused on investigating the impact of deposition layer thickness, extrusion temperature, raster angle, and color pigments in ABS filaments on the porosity between beads and the mechanical properties of the printed components. Their findings highlighted that the raster angle, or printing orientation, exerted the most significant influence, affecting the density of air gaps between layers and the overall strength of the printed samples. In another notable study, Bellini and Güseri (2003) utilized the linear elastic theory of orthogonally isotropic components to assess the mechanical properties of ABS samples fabricated using FDM. Through their research, they effectively demonstrated the dependence of these properties on both the printing orientation and the architecture of the deposition layers.

Alaimo et al. (2017) focused on examining the influence of deposition bead diameter and raster orientation on the mechanical properties. They found that the bonding between fibers significantly impacted the yield strength and strain at failure of the 3D printed samples.

Bayraktar et al. (2017) took a different approach by utilizing tensile tests on PLA samples with varying extruder temperature, layer thickness, and printing orientation settings. They used an artificial neural network (ANN) model to predict the ultimate strength of the printed samples, showcasing the potential of ANN models for accurately estimating strength based on different process parameters. In a separate study, Abouelmajd et al. (2021) focused on the effects of printing velocity, orientation, and extrusion temperature using a Taguchi L9 orthogonal array. They examined the flexural strength and stiffness of PLA printed samples and employed variance analysis (ANOVA) along with an arbitrary desirability function to identify the optimal levels of process parameters for achieving the best response variables.

Yadav et al. (2021) employed a hybrid approach that combined an artificial neural network (ANN) and a genetic algorithm (GA) to optimize FDM process parameters for achieving the highest tensile strength in ABS/PETG multi-material 3D printed samples. Their results demonstrated a low average error, approximately 2.6%, between the predicted strength using the ANN function and the experimental value under the optimized material extrusion parameters.

Zhang et al. (2020) focused on investigating the dynamic performance of Nylon 618 spur gears fabricated using FDM. They performed wear and fatigue tests and developed a multi-regression function using the experimental data. Furthermore, they employed an artificial neural network/genetic algorithm (ANN/GA) hybrid optimization technique to fine-tune the process parameters for improved performance. In a separate study, Zhou et al. (2018) developed a meso-structure numerical model coupled with an artificial neural network (ANN) algorithm. Their goal was to determine the internal architecture and filling ratio that would result in the maximum ultimate strength-to-weight ratio and modulus of elasticity for FDM-printed samples. Their model achieved an error of 14.8% in predicting the mechanical properties of 3D printed PLA samples.

In summary, the studies discussed in this section, along with numerous others in the field, highlight the significance of specific FDM (Fused Deposition Modeling) process parameters, such as printing speed, layer thickness, internal architecture, and filling pattern, in determining the mechanical properties of synthesized components. These parameters are interconnected and have a profound influence on the final characteristics of the printed parts.

Furthermore, the incorporation of fibers and nanoparticles to enhance the mechanical and physical properties of polymeric components has been widely explored in various industries.

Investigations conducted on samples produced by the mold injection technique have shown substantial improvements in the tensile strength of printed composites through the addition of 5wt% nanotitanium oxide ( $\text{TiO}_2$ ) (Torrado Perez et al., 2014) and 10wt% carbon nanofiber (Shofner et al., 2003), resulting in increases of 13.2% and 39%, respectively.

The effects of incorporating  $\text{CaCO}_3$  nanofillers into polypropylene (PP) have also been studied. Chan et al. (2002) observed that the addition of  $\text{CaCO}_3$  nanoparticles did not alter the crystallinity or melting temperature ( $T_m$ ) of the material but increased the crystallization temperature ( $T_c$ ) by  $10^\circ\text{C}$ , indicating a nucleating effect. This resulted in a 300% improvement in impact strength and a 100% increase in modulus of elasticity due to decreased spherulite size and enhanced interaction between the nanoparticles and PP.

Other researchers have reported similar findings with the addition of  $\text{CaCO}_3$  nanofillers to polyurethane (PU), polyamide, and styrene butadiene (SBR) latex composites. The inclusion of  $\text{CaCO}_3$  nanoparticles led to changes in crystallization behavior, mechanical properties, thermal stability, and viscoelastic response of the nanocomposites, resulting in improved performance in terms of modulus of elasticity, hardness, storage modulus ( $E'$ ), and glass transition temperature ( $T_g$ ).

Overall, these studies demonstrate the positive impact of incorporating nanofillers into polymer matrices, showing enhancements in mechanical strength, thermal properties, and crystallinity, which can be leveraged to tailor the properties of the nanocomposites for specific applications.

However, the incorporation of nanoparticles in the FDM process has received limited attention in research. Among the available studies, Dul et al. (2018) employed a melt-blending technique to produce nanocomposite filaments with varying weight fractions (up to 8wt%) of carbon nanotubes (CNT). They observed that as the weight fraction of CNTs in the matrix increased, the printed nanocomposites exhibited higher modulus of elasticity and yield strength, while experiencing a decrease in elongation at break. Another study by Venkatesh et al. (2019) focused on fabricating PLA filaments with the inclusion of up to 5wt% Halloysite nanotubes (HNT) using a melt blending technique. The addition of HNT resulted in notable enhancements, including a 12.2% increase in tensile strength, a 13.4% increase in modulus of elasticity, and a 13.3% decrease in elongation at break of the printed samples. Spinelli et al. (2020) developed PLA nanocomposites by incorporating up to 6wt% multi-walled carbon nanotubes (MWCNT) and graphene nanoplatelets (GNP) through a melt blending process. At a concentration level of 3wt%, a uniform distribution of MWCNT/GNP within the matrix was achieved, leading to

significant improvements in tensile strength (60% increase), modulus of elasticity (19.4% increase), and elongation at break (9.7% increase).

Furthermore, Zarybnicka et al. (2022) investigated the effects of three crystalline polymorphs of micro-sized  $\text{CaCO}_3$  particles (calcite, vaterite, and aragonite) as additives in polypropylene filaments produced via melt blending. The results revealed that the PP/calcite composite filament displayed the lowest surface roughness and highest density among the different compositions of PP. This composite demonstrated good load-carrying capacity and maximum elongation at break, although its strength did not surpass the PP polymers containing other  $\text{CaCO}_3$  morphologies.

Christian et al. (2016) conducted an investigation on the impact of FDM parameters on the strength of 3D printed composites made from ABS/hydrous magnesium silicate. Kovan et al. (2018) found that the addition of short carbon fibers in the PLA matrix reduced the anisotropy of samples caused by the additive nature of FDM fabrication. Patanwala et al. (2018) examined the microstructure and mechanical properties of 3D printed specimens with the inclusion of carbon nanotubes (CNTs) mixed at weight ratios of 0.5, 2.5, and 5wt% in the PLA matrix. They observed that the distribution of 5wt% CNT in PLA led to a 30% enhancement in elastic modulus but resulted in a reduction in the ultimate strength of the specimens. Papon et al. (2018) noted that the addition of carbon nanofibers (CNFs) in the PLA polymer reduced the melted polymer contact angle and increased the fraction of voids in the structure compared to pure PLA. The fracture surfaces of PLA/CNF nanocomposites exhibited a coarse topography with fibers being pulled out of the matrix, which contributed to higher fracture energy in FDM samples compared to neat specimens. Tambrallimath et al. (2019) explored the influence of FDM parameters and the addition of short glass fibers (GFs) at a weight fraction of 30% on the mechanical properties of polyethylene (PE) polymer. They reported that the samples containing GFs, fabricated with a printing orientation of  $0^\circ$  and high layer thickness, exhibited the highest yield strength and elastic modulus.

#### **1.4. Modeling Based on Artificial Intelligence Techniques**

Artificial intelligence (AI) techniques have been widely used in modeling and predicting the response of various engineering processes, including desalination systems, water treatment, power generation plants, solar systems, heat generators, material processing, metal cutting, friction stir welding (FSW), and laser welding and cutting of metals and polymers, among

others. For instance, Elsheikh et al. (2023) developed a neural network (NN) model based on the random vector functional link (RVFL) network integrated with the Runge Kutta optimizer (RUN) to predict the efficiency parameters of a vertical water distillation tower operated by solar stills. The RVFL-RUN model achieved a coefficient of correlation ( $R$ ) value of 0.91 and 0.97 for predicting the water productivity and temperature, respectively. In another study, Moustafa and Elsheikh (2023) proposed a coupled Multi-Layer Perceptron (MLP) model integrated with different internal optimizers, including Archimeder optimizer (AO), conventional Gradient Descent technique (GD), and Particle Swarm optimizer (PSO), to predict the response variables of dissimilar polymethyl methacrylate/polycarbonate (PMMA/PC) joints. The MLP models demonstrated promising accuracy with root mean square error (RMSE) values of 39.798, 19.909, and 2.283 for MLP-GD, MLP-PSO, and MLP-AO, respectively, in predicting shear strength and seam width of laser transmission-welded joints. Similarly, Elsheikh et al. (2022a) employed the RVFL model integrated with a Gradient-Based optimizer (GBO) to predict the average temperature and joint strength in ultrasonic welding of dissimilar acrylonitrile butadiene styrene (ABS) and PC blend polymers. The RVFL-GBO model outperformed other models, achieving coefficient of determination ( $R^2$ ) values between 0.9898 and 0.9992 and the lowest RMSE values ranging from 0.385 to 4.028 for testing. Elsheikh (2022b) developed a mathematical model using AI techniques to study the dynamic behavior of bistable morphing composites in response to different actuators. Elsheikh et al. (2021a) implemented an AI model combining the RVFL network and parasitism predation optimization algorithm (PPA) to predict the temperature and damage factor in drilling of glass-fiber reinforced composites. The hybrid RVFL-PPA model exhibited superior performance in terms of  $R$  and RMSE criteria compared to other models. Furthermore, Khoshaim et al. (2021) introduced a hybrid MLP model integrated with the metaheuristic Gray Wolf optimizer (GWO) to compute the response variables of friction stir process in the fabrication of Aluminum-based nanocomposites. The proposed model achieved higher  $R^2$  values ranging from 0.915 to 0.971 compared to the standalone MLP model. Lastly, Elsheikh et al. (2021b) utilized a fine-tuned ANN model integrated with pigeon optimization algorithm (POA) and PSO to predict the effects of cutting conditions on residual stresses in Inconel 718 alloy samples during metal cutting. The fine-tuned ANN models exhibited high correlation ( $R^2$ ) values of 0.991 and 0.938 for ANN-POA and ANN-PSO, respectively, when compared to the standalone ANN model ( $R^2 = 0.585$ ) and experimental measurements.

Moreover, the utilization of AI techniques holds promise in developing models that can capture the intricate relationship between input parameters and response variables in additive manufacturing (AM) processes. Understanding this relationship is crucial for ensuring design reliability and the quality of final AM products. However, due to the inherent complexity of these techniques, both numerical simulation-based and analytical modeling-based approaches often lack the required accuracy to predict the performance parameters of AM processes. To address this challenge, modern machine learning approaches, such as transfer learning-based Artificial Neural Network (TL-ANN), can be employed. TL-ANN has the ability to accurately model the complex relationship between input parameters and output variables, even when the dataset is limited.

The application of machine learning techniques in AM processes has been explored in various studies. For example, Caiazzo and Caggiano (2018) used an ANN to establish the relationship between process parameters in laser direct metal deposition and the geometrical features of deposited metal traces in selective laser melting (SLM). The proposed ANN demonstrated the capability to determine the optimal process parameters required to achieve specific trace geometries accurately. Hong et al. (2021) developed an NN-based geometry compensation model to enhance the printing accuracy of SLM-fabricated truss lattice structures. The multilayer perceptron structure of the NN model enabled the creation of improved free-form lattice cross-sections, resulting in higher dimensional accuracy compared to analytical approaches.

Mehrpouya et al. (2019) proposed an NN-based prediction model to estimate the transformation temperature and strain recovery ratio of NiTi shape memory alloys produced by SLM. The results exhibited a high level of agreement between experimental data and estimated values by the NN, with an  $R^2$  value of 97-99%. Oh et al. (2021) employed a convolutional neural network (CNN) to estimate the build time of AM processes. Due to the limited availability of experimental data, they utilized data obtained through virtual slicing of STL files to create a sufficiently large database for training the CNN. The results demonstrated that CNN-based time prediction was strongly dependent on the size of 3D models, with larger models yielding more accurate network predictions. Gu et al. (2018) developed a machine learning approach for designing bio-inspired hierarchical materials based on a database of various structures obtained through finite element analysis. The optimal designs predicted by machine learning were validated through tensile tests performed on SLM-fabricated parts, showcasing the creation of

high-performance hierarchical composite materials with exceptional tensile strength and toughness.

Zhu et al. (2021) proposed a physics-based NN to predict the melt pool dynamics in AM processes. The NN was trained using conservation laws of mass, energy, and momentum, resulting in accurate predictions of pressure, temperature, and velocity fields of the melt pool, even with limited datasets. Chen et al. (2020) developed a supervised machine learning method to predict the printability of materials in the SLM process. The predictive NN model, trained and tested with surface morphology data, showed the height and width of track cross-sections. By leveraging the intellectual feature-learning capability of NN, a defect-free process parameter window could be identified.

Westphal et al. (2021) employed CNN for automatic classification of powder bed defects in the selective laser sintering process. Powder bed images were accurately classified into two groups (good and bad) with a high accuracy level of 95.8%. Similarly, Xing et al. (2022) utilized CNN for the classification of melt pool images in the pulsed SLM process, achieving a high classification accuracy of 96.6% and demonstrating the reliable and efficient performance of CNN in melt pool monitoring. Ho et al. (2021) implemented a residual RNN to evaluate the melt pool temperature in the SLM process. Based on thermal images of the melt pool, the network could predict the formation of porosities with high classification accuracy and short inference time.

Patpatiya et al. (2022) introduced a predictive modeling and optimization approach to minimize dimensional tolerance in Polyjet Additive Manufacturing (AM). Their research focused on developing an accuracy-based predictive model for thermoplastic structures fabricated using the Polyjet technique. By employing statistical analysis and neural networks, the researchers evaluated the influence of various printing parameters on the dimensional stability of the printed structures. The findings were subsequently optimized using a genetic algorithm. This study sets new benchmarks for additive manufacturing of thermoplastic components and explores potential industrial applications.

In a separate study, Mohamed et al. (2016) conducted a regression analysis of dynamic flexural modulus and complex viscosity in the FDM process. Their developed model incorporated multiple parameters such as layer thickness, air gap, raster angle, build orientation, road width, and number of contours. By employing ANOVA and response surface plots, the effects of these parameters on the dynamic properties were analyzed. Through an optimization process, the

optimal parameter settings were identified to achieve maximum dynamic mechanical properties. The results highlighted that layer thickness, air gap, and number of contours exerted the greatest influence on the dynamic mechanical properties of the fabricated samples. Experimental results confirmed the accuracy of the predicted values.

Meiabadi et al. (2021) conducted a study aimed at enhancing the quality of FDM printed objects using polylactic acid (PLA) with a focus on toughness, part thickness, and production cost. Statistical analysis and modeling were performed using the response surface method (RSM) and the artificial neural network-genetic algorithm (ANN-GA). The ANN-GA approach demonstrated higher accuracy compared to a single ANN method, resulting in improvements of approximately 7.5% in toughness, 11.5% in part thickness, and 4.5% in production cost. The optimization of process parameters led to cost-effective PLA printed parts with improved toughness and desired part thickness. This study showcased the potential of hybrid machine learning techniques in enhancing the quality of 3D printed objects.

### **1.5. What is this study is all about**

In this study, the focus is on investigating the effects of different conventional and hybrid core structures on the flexural response of composite core shell structures. The core structures are developed using a material extrusion process, commonly known as fused deposition modeling (FDM). The study takes into account the influence of various FDM parameters and the composition of the base matrix material.

*Chapter 2* of the study discusses the details of the material extrusion process and the fabrication of specimens. This section covers aspects such as the equipment used for FDM, the selection of materials for the base matrix, and the specific parameters employed during the printing process. It also discusses the preparation of the specimens and any post-processing steps involved.

*Chapter 3* delves into the mechanical characteristics of the different core structures. This section includes review of the state of art, numerical modeling and experimental evaluation on the flexural performance of the developed core shell structures. The selection of core structures for further analysis is discussed in the same chapter. This involves choosing specific core configurations from the range of developed structures based on predetermined criteria. These criteria may include stiffness, load-carrying capacity, or other desired mechanical properties.

This chapter reflects the results of investigations to determine the in-plane and out-of-plane modulus of elasticity and ultimate strength of the printed samples and their application as engineering constants in the FDM. The study mainly is about the variations in the FDM parameters and material composition to evaluate their impact on the mechanical properties of the core structures.

To further analyze and optimize the mechanical properties of the 3D printed samples, the study employs regression modeling using artificial neural networks (ANN) and optimization techniques using ant colony optimization (ACO). ANN models are developed to predict the mechanical variables of the 3D printed samples, such as in-plane and out-of-plane modulus of elasticity and ultimate strength. This approach allows for a better understanding of the relationships between the FDM parameters, material composition, and mechanical properties. The ACO optimization method is then utilized to optimize the FDM parameters and material composition for achieving desired mechanical performance.

Finally, *chapter 4* presents the results and discussions of the study. This section includes the findings from the regression modeling and optimization processes. The performance of the core shell structures under flexural loading conditions is evaluated and compared based on the obtained mechanical properties. The implications and significance of the results are discussed, potentially highlighting the effectiveness of the proposed methodologies and providing insights for future improvements or applications.

## 2. MATERIALS AND METHODS

### 2.1. Materials

#### 2.1.1. Base polymers, characteristics and mixing

Polyvinyl chloride (PVC) is a versatile synthetic polymer derived from the vinyl chloride monomer. With an annual production exceeding 40 million tons, PVC ranks as the third-most widely manufactured synthetic polymer globally, following polyethylene and polypropylene. It is available in two primary forms: rigid and flexible. Rigid PVC finds extensive use in the construction industry for applications such as pipes, profiles (e.g., doors and windows), plastic bottles, non-food packaging, food-covering sheets, and plastic cards like bank or membership cards. By incorporating plasticizers, notably phthalates, PVC can be rendered softer and more flexible. This flexible variant is utilized in various fields, including plumbing, electrical cable insulation, imitation leather, flooring, signage, phonograph records, inflatable products, and as a substitute for rubber in numerous applications (Elgharbawy, 2022).

The production of polyvinyl chloride involves the polymerization of vinyl chloride monomer (VCM), as depicted in the chemical reaction (Chanda & Roy, 2006).

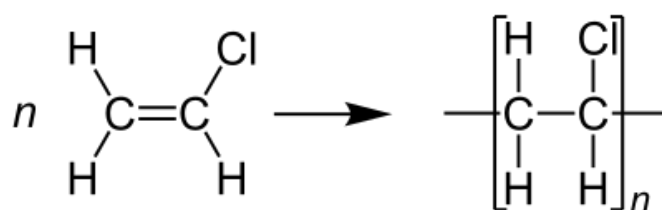


**Figure 2.1.** Vinyl chloride monomer and polymerization of PVC polymer.

Polychloroethene, commonly known as polyvinyl chloride (PVC), is characterized by its linear polymer chains, which exhibit significant strength. The arrangement of monomers predominantly follows a head-to-tail pattern, resulting in alternating carbon centers carrying chloride groups. PVC typically possesses an atactic stereochemistry, where the relative arrangement of chloride centers is random. However, there is a small degree of syndiotacticity present in the chain, contributing to a few percent of crystallinity that greatly influences the material's properties. Notably, approximately 57% of PVC's mass comprises chlorine atoms. This abundance of chloride groups imparts distinct properties to the polymer, distinguishing it from structurally similar materials such as polyethylene (Harper, 2002).

In terms of density, PVC exhibits a value of 1.4 g/cm<sup>3</sup>, which is higher than its structurally related counterparts like polyethylene (0.88–0.96 g/cm<sup>3</sup>) and polymethylmethacrylate (1.18 g/cm<sup>3</sup>). This disparity in density further contributes to the unique characteristics and applications of PVC in various industries.

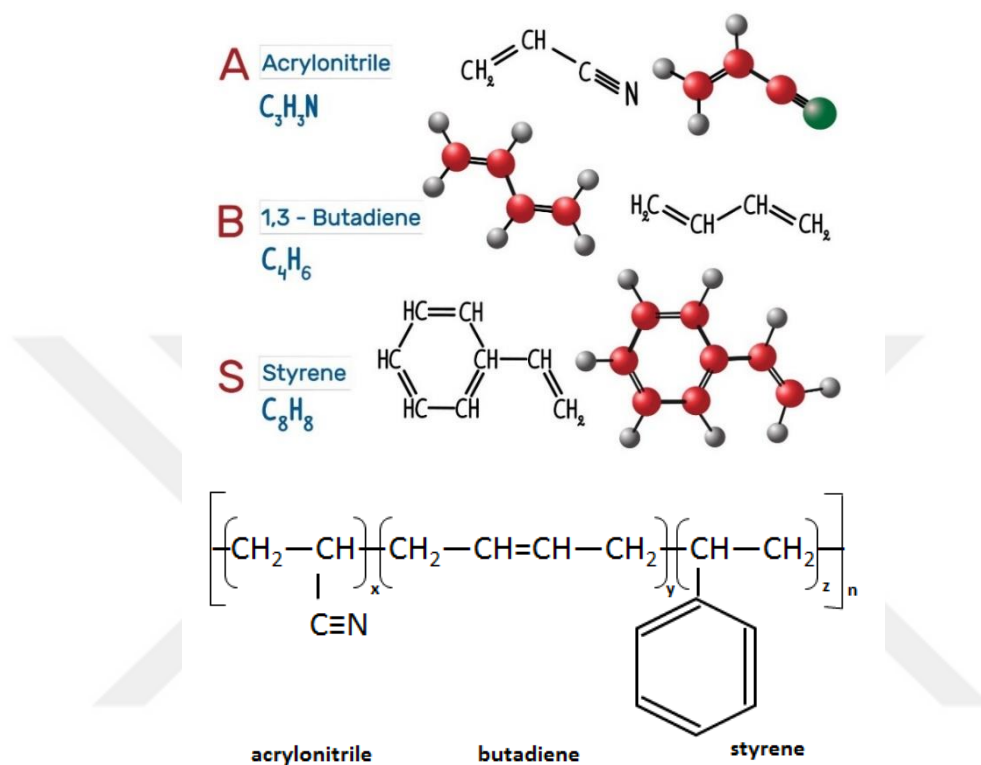


**Figure 2.2.** Polymerization of acrylonitrile butadiene styrene (ABS) polymer; a) base monomers and b) molecular structure of ABS (Gupta et al., 2019).

Acrylonitrile–butadiene–styrene (ABS) is a highly significant engineering copolymer extensively utilized in various industries due to its exceptional mechanical properties, chemical resistance, ease of processing, and recyclability. ABS finds application in building and construction, personal care products, toys, computer and business equipment, medical devices, and automotive interior components (Salamone, 1999). It is a terpolymer formed by polymerizing styrene and acrylonitrile in the presence of polybutadiene. The composition of ABS can vary, typically ranging from 15% to 35% acrylonitrile, 5% to 30% butadiene, and 40% to 60% styrene. This results in a long polybutadiene chain intermingled with shorter chains of poly(styrene-co-acrylonitrile). The polar nitrile groups of neighboring chains attract each other and create bonds, effectively enhancing the overall strength of ABS compared to pure polystyrene (Gupta et al., 2019). Figure 2.2 illustrates the polymerization process of the three

monomers, commonly accomplished through emulsion or suspension polymerization, leading to the formation of the ABS polymer. The resultant polymer is a blend of acrylonitrile, butadiene, and styrene units, delivering a well-balanced combination of strength, impact resistance, heat resistance, and processability.

Mixing PVC (Polyvinyl Chloride) and ABS (Acrylonitrile Butadiene Styrene) can be done to achieve certain desired properties or to modify the characteristics of the resulting material. Here are some common motivations for mixing PVC and ABS:

1. *Improved Mechanical Properties:* PVC and ABS have different mechanical properties. PVC is relatively rigid and has good chemical resistance, while ABS is known for its toughness and impact resistance. By blending PVC and ABS, it is possible to combine their respective strengths and achieve a balance of properties. The resulting material may exhibit improved impact resistance, toughness, and rigidity compared to either PVC or ABS alone.

2. *Enhanced Processing Characteristics:* PVC and ABS also have different processing characteristics. PVC has good melt flow and can be easily processed, while ABS has better dimensional stability (*Mechanically strong and stable over time*) and surface finish. By mixing PVC with ABS, the blend may inherit some of the processing advantages of PVC, such as improved flowability during molding or extrusion, while still benefiting from the improved properties of ABS.

3. *Cost Reduction:* ABS is generally more expensive than PVC. In applications where cost is a significant factor and the specific properties of ABS are not critical, blending PVC with ABS can help reduce material costs. By adjusting the blend ratio, it is possible to strike a balance between cost savings and maintaining acceptable performance for the intended application.

4. *Property Customization:* The blending of PVC and ABS allows for the customization of material properties. By adjusting the blend ratio, it is possible to tailor the resulting material to meet specific requirements. This includes controlling factors such as rigidity, flexibility, impact resistance, heat resistance, chemical resistance, and other desired characteristics.

Blending PVC (Polyvinyl Chloride) and ABS (Acrylonitrile Butadiene Styrene) polymers can be achieved through several methods. Here are a few commonly used techniques for blending PVC and ABS:

1. *Mechanical Blending*: The most straightforward method is to physically mix PVC and ABS pellets or powders using mechanical blending equipment, such as a high-speed mixer or a twin-screw extruder. This method involves combining the PVC and ABS materials and subjecting them to heat and shear forces to achieve intimate mixing. The blend is then cooled and pelletized for further processing.

2. *Melt Blending*: In this method, PVC and ABS are melted together to form a homogeneous blend. The PVC and ABS pellets or powders are introduced into an extruder, where they are heated to their melting temperatures and mixed together as molten materials. The molten blend is then cooled and solidified, either by passing through a cooling system or by pelletizing.

3. *Solution Blending*: In this approach, PVC and ABS are dissolved in a common solvent, such as tetrahydrofuran (THF) or cyclohexanone, to form a solution. The two polymers can be dissolved separately or together, depending on their solubility in the chosen solvent. The solution is then subjected to evaporation or precipitation techniques to remove the solvent and recover the blended PVC-ABS polymer.

4. *In-Situ Polymerization*: This method involves the polymerization of PVC and ABS monomers in the presence of each other. The monomers are mixed together with appropriate initiators and catalysts, and polymerization is carried out under controlled conditions. This technique allows for the synthesis of a *copolymer that consists of PVC and ABS units*, resulting in a more intimate blend of the two polymers.

However, PVC (Polyvinyl Chloride) and ABS (Acrylonitrile Butadiene Styrene) are not inherently compatible polymers, which means they have limited miscibility and tend to phase separate when blended together. However, there are certain techniques that can improve their compatibility and promote a more homogeneous blend. Here are some methods to enhance the compatibility between PVC and ABS:

1. *Compatibilizers*: Compatibilizers or coupling agents can be added to the PVC-ABS blend to improve the interfacial adhesion between the two polymers. These additives act as a bridge between the PVC and ABS phases, promoting better mixing and reducing phase separation. Compatibilizers can include *maleic anhydride grafted polymers*, such as *maleic anhydride-grafted PVC* or *ABS*, which have reactive groups that can interact with both polymers and enhance their compatibility. (*Maleic anhydride, with the chemical formula  $C_2H_2(CO)_2O$ , is an organic compound and the acid anhydride of maleic acid. It exists as a colorless or white solid*

*with a pungent odor. The industrial production of maleic anhydride is carried out on a large scale, primarily for its applications in coatings and polymers (Lohbeck et al., 2000)).*

2. *Blending Conditions*: Optimizing the blending conditions, such as temperature, mixing time, and shear rate, can influence the compatibility of PVC and ABS. By selecting appropriate processing parameters, such as a higher temperature or longer mixing time, the polymer chains of PVC and ABS can have better chances to entangle and mix more effectively, improving the compatibility between the two polymers.

3. *Chemical Modifications*: Surface modification of either PVC or ABS can be performed to introduce functional groups that enhance compatibility. This can be achieved through various methods, including *plasma treatment*, *chemical grafting*, or introducing *reactive functional groups* through copolymerization or cross-linking. These modifications can improve the adhesion and compatibility between PVC and ABS at the molecular level.

4. *Blend Ratio*: The blend ratio of PVC and ABS can impact their compatibility. In some cases, a certain blend ratio may yield a more compatible blend. Through experimentation, different blend ratios can be tested to determine the optimal ratio that promotes better mixing and reduces phase separation.

In this research, the melt blending technique was utilized to produce a blend of ABS/PVC polymers at various ratios. It is important to note that the melt blending process alone does not guarantee compatibility between the two base polymers. However, there are several methods available to improve their compatibility, as listed above. In this study, we focus on investigating the effects of mechanical blending without employing additional compatibility-enhancing techniques. The specimens were fabricated using material extrusion techniques, and the response mechanical characteristics of the ABS/PVC blend polymers were evaluated. The objective is to understand the impact of mere mechanical blending on the mechanical properties of the specimens.

### **2.1.2. Carbon nanofibers**

Carbon nanofibers (CNFs) are nanostructures comprised of stacked cones or plates made of graphene layers. They are commonly synthesized through catalytical chemical vapor deposition (CCVD) or variations of chemical vapor deposition (CVD) methods, including thermal and

plasma-assisted decomposition of gas-phase molecules at elevated temperatures. In the synthesis process, carbon is deposited around transition metal catalyst particles on a substrate, leading to the growth of the nanofibers (Desmaris et al., 2015). Figure 2.3 provides a comparison of various carbon products.

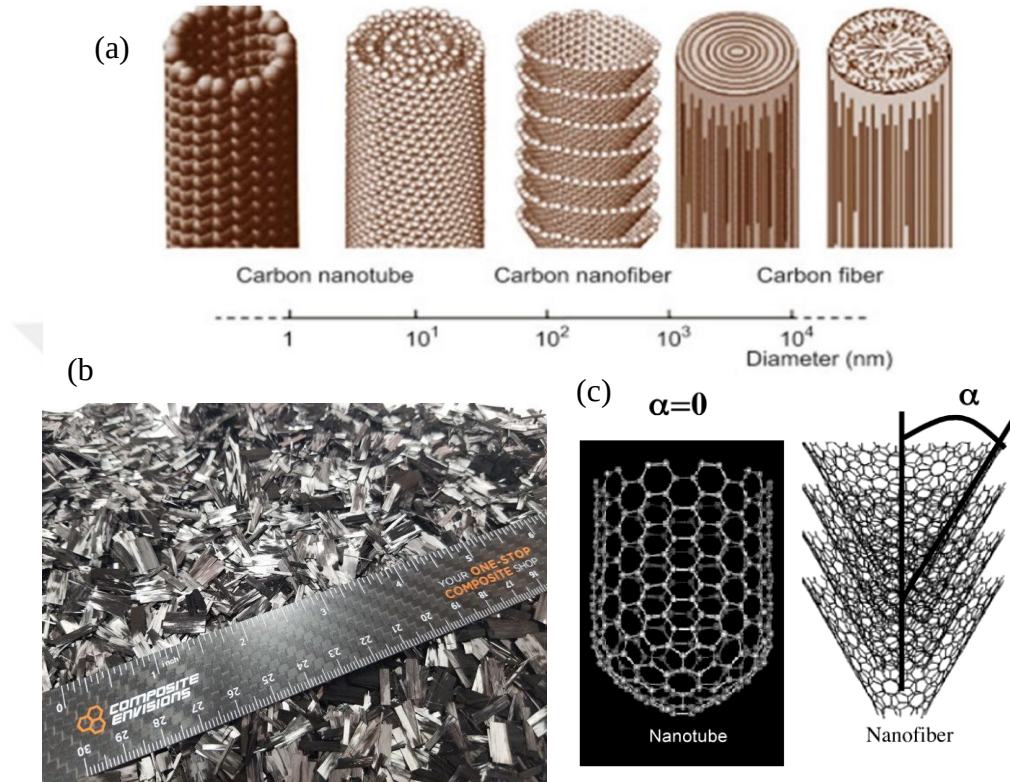


**Figure 2.3.** A comparison of different carbon products as additives; a) different configurations and size range of carbon products, b) chopped carbon fiber and c) a close view at carbon nanotubes and nanofibers.

Carbon nanotubes (CNTs) and carbon nanofibers (CNFs) are both carbon-based nanostructures, but they differ in their structural characteristics (Ngo et al., 2007). Here are the key differences between CNTs and CNFs:

1. *Structure:* Carbon nanotubes are cylindrical structures composed of rolled-up graphene sheets, forming a hollow tube. They can have a single-walled structure (SWCNT) consisting of a single layer of graphene or a multi-walled structure (MWCNT) with multiple concentric graphene layers. On the other hand, carbon nanofibers are solid cylindrical structures with graphene layers stacked in a plate-like or cone-like arrangement.

2. *Diameter*: Carbon nanotubes typically have diameters ranging from a few nanometers to a few tens of nanometers. They can be as thin as a single atom layer in the case of SWCNTs or can have larger diameters in the case of MWCNTs. Carbon nanofibers, on the other hand, have larger diameters ranging from several tens of nanometers to a few micrometers.

3. *Length*: Carbon nanotubes can grow to be very long, often reaching lengths of several micrometers to millimeters. They can form individual tubes or bundles of tubes. Carbon nanofibers, on the other hand, tend to have shorter lengths compared to nanotubes, typically in the range of a few micrometers.

4. *Morphology*: Carbon nanotubes have a tubular morphology with high aspect ratios, meaning their length-to-diameter ratio is typically very large. They can be straight or exhibit various degrees of curvature, such as helical or twisted structures. Carbon nanofibers, in contrast, have a more solid and fibrous morphology, resembling elongated particles or fibers.

5. *Synthesis*: Carbon nanotubes can be synthesized through different methods, including arc discharge, laser ablation, or chemical vapor deposition (CVD). The synthesis of carbon nanofibers also involves CVD techniques, but typically with variations in the growth conditions and catalysts to promote the formation of solid, fibrous structures.

Both carbon nanotubes and carbon nanofibers exhibit exceptional mechanical, electrical, and thermal properties. However, due to their structural differences, they may have varying performance characteristics and applications. Determining whether carbon nanofibers (CNFs) or carbon nanotubes (CNTs) are better for addition to polymers depends on the specific requirements of the application and the desired properties of the resulting composite material. Both CNFs and CNTs offer unique characteristics and advantages. Here are some factors to consider:

1. *Mechanical Properties*: Both CNFs and CNTs possess excellent mechanical properties, including high strength and stiffness. However, CNTs generally exhibit higher mechanical properties due to their tubular structure and high aspect ratio. If maximizing mechanical reinforcement is a priority, CNTs may be preferred. However, CNFs can still provide significant improvements in mechanical properties and may offer advantages in terms of their ease of handling and lower cost compared to CNTs.

2. *Electrical Conductivity*: CNTs have superior electrical conductivity compared to CNFs. If achieving high electrical conductivity in the composite material is crucial, CNTs are typically a better choice. They can enable applications such as conductive coatings, electrodes, or electromagnetic interference (EMI) shielding. CNFs, while less conductive, can still provide moderate electrical conductivity and may be suitable for applications where lower conductivity is acceptable or desired.

3. *Dispersion and Processing*: Achieving good dispersion of the nanofillers in the polymer matrix is important for optimal performance. CNTs, with their unique tubular structure, can pose challenges in achieving uniform dispersion due to their tendency to agglomerate. CNFs, being solid fibers, generally disperse more easily in the polymer matrix. The ease of dispersion and processing can influence the overall feasibility and efficiency of incorporating the nanofillers into the polymer.

4. *Cost Considerations*: CNTs are generally more expensive than CNFs due to the more complex synthesis processes involved. If cost is a significant factor, CNFs may offer a more cost-effective option while still providing significant property improvements.

Ultimately, the choice between CNFs and CNTs depends on the specific application requirements, desired properties, and cost considerations. Considering the range of products in the material extrusion process and the application of filaments in fabrication large scale specimens from prototypes to final products, and the nature of mixing of components of filaments through extrusion, CNFs have been selected as an additive in the composition of ABS/PVC in this research (Ning et al., 2015).

There are many different methods to make CNFs compatible with polymer matrix, some of which are summarized below (Jiminez & Jana, 2007).

1. *Surface Functionalization*: The surface of CNFs can be modified by introducing functional groups or coatings that improve the affinity between the CNFs and the polymer matrix. Functionalization techniques include oxidation, chemical grafting, or coating with surfactants or coupling agents. These modifications enhance the interfacial bonding and dispersion of CNFs within the polymer matrix.

2. *Polymer Matrix Modification*: Modifying the polymer matrix itself can improve the compatibility with CNFs. This can be done by incorporating functional groups or reactive

monomers into the polymer structure, allowing for better interaction with the CNFs. Polymer modifications can be achieved through copolymerization, blending with reactive polymers, or incorporating compatibilizers.

3. *Mechanical Mixing*: Mechanical mixing methods, such as high-shear mixing or sonication, can be used to disperse and distribute CNFs within the polymer matrix. These methods help break up agglomerates and promote better dispersion, leading to improved compatibility and mechanical properties.

4. *Solvent Mixing and Coating*: CNFs can be pre-treated by dispersing them in a solvent that is compatible with the polymer matrix. This pre-dispersion allows for more uniform mixing with the polymer during subsequent processing steps. Additionally, CNFs can be coated with a thin layer of polymer before blending with the matrix to enhance compatibility and prevent agglomeration.

5. *In-Situ Polymerization*: CNFs can be incorporated into the polymer matrix during the polymerization process. This method involves adding CNFs and monomers together, followed by in-situ polymerization to form a composite material. In-situ polymerization ensures good dispersion and interfacial bonding between the CNFs and the polymer matrix.

6. *Electrostatic Assembly*: Electrostatic assembly involves the use of electric charges to attract CNFs onto a polymer substrate or into a polymer matrix. By controlling the charge and surface properties, CNFs can be precisely positioned and dispersed within the polymer, improving compatibility and enhancing properties.

In this study, a mechanical mixing technique was employed to produce a blend of ABS/PVC polymers and CNFs at various ratios. It is worth mentioning that the sole use of the melt blending process does not guarantee strong bonding between the base polymers and the nanoadditives. However, there are several methods available to enhance their compatibility, as mentioned earlier. In this research, we specifically focused on investigating the effects of mechanical bonding and Vander Waals forces between the CNFs and the polymer molecules without employing additional compatibility-enhancing techniques. The nanocomposite filaments were fabricated using a melt blending and extrusion technique, and the mechanical properties of the 3D printed nanocomposite specimens were evaluated. The objective was to assess the impact of mechanical blending alone on the mechanical properties of the specimens.

## 2.2. Nanocomposite filament extrusion process

Composite filaments consisting of CNFs nanoparticle reinforced PVC/ABS polymers with varying fractions of reinforcement in the matrix and different mixing ratios of PVC and ABS polymers were produced using a melt blending and extrusion technique. The fabrication process steps are illustrated in Fig. 2.4. PVC polymer was added to the ABS polymer at various concentrations to achieve composite filaments with satisfactory printability. Based on preliminary experiments, the addition of PVC in the ABS matrix was limited to 20wt%. The extrusion process was performed using an extruder with an L/D ratio of 20, and the barrel and nozzle heater temperatures were set at approximately 205 °C. To ensure a stable filament diameter of  $1.75 \pm 0.03$  mm, a 1.82 mm nozzle, a water-cooling bath with a length of 50 mm, and an automatic filament winding system were utilized.

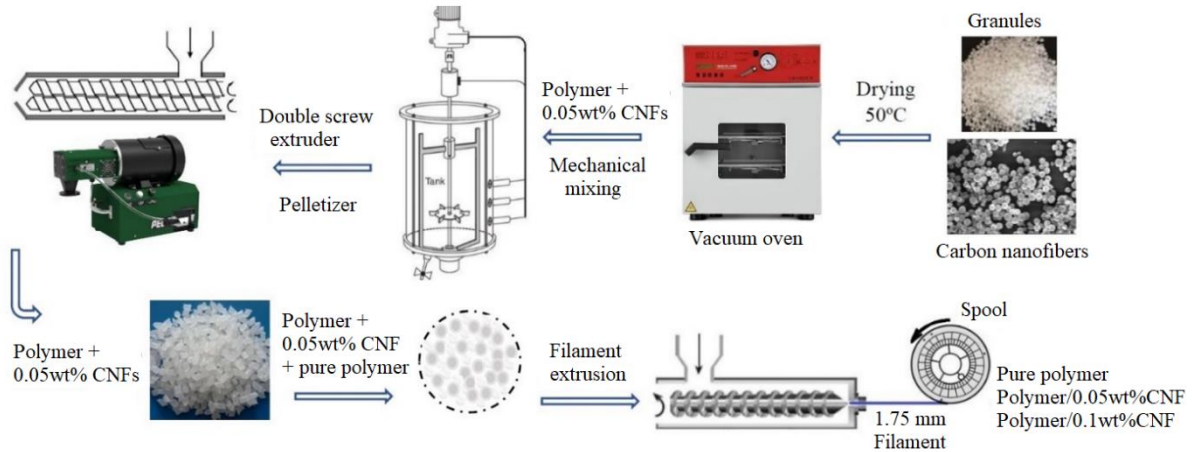


**Figure 2.4.** Schematic representation of fabrication steps of nanocomposite filaments using melt blending technique.

## 2.3. Fabrication of tensile and composite core-shell sandwich panel samples

The material extrusion process, specifically fused deposition modeling (FDM), was carried out using a single-head 3D printer equipped with a nozzle diameter of 0.4 mm and a table dimension of 250×220 mm. The FDM process involved fabricating a dog-bone specimen of ABS/0.05wt% CNF nanocomposite along the 1st principal axis, as illustrated in Figure 2.5. The orientation of the tensile samples during the material extrusion process, along with the three principal axes, is depicted in Figure 2.6. To conform to the FDM production mechanism, the dimensions of the tensile samples were adjusted following the D638-14 and D3039M-00 standards. The sample

design, as shown in Figure 2.6, enabled the characterization of the orthotropic mechanical properties of the 3D printed components.



**Figure 2.5.** Production of tensile test sample on a FlashForge material extrusion device.

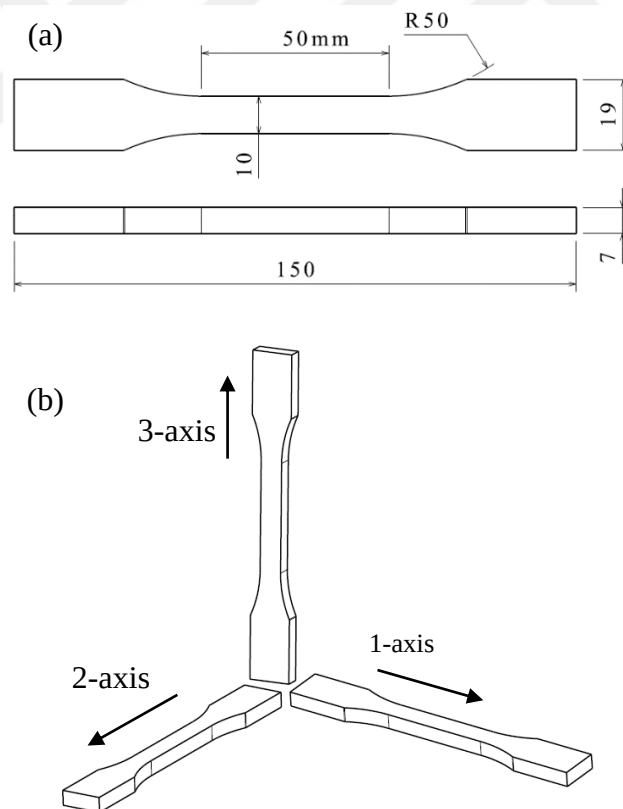


**Figure 2.6.** Tensile test sample for characterizing the orthotropic properties of 3D printing samples; a) Dimensions of dog-bone samples and b) Representation of sample orientation along the principal axes.

Special core structures, including honeycomb, triangular, and hybrid circular/triangular corrugated (HCTC) patterns, have been specifically designed for the sandwich panels. The size of the core patterns has been adjusted to maintain a constant mass for the structures. The designs of these core structures are illustrated in Fig. (2.7). Further details regarding the design and specifications of the core structures are discussed in Chapter 3. The composite core shell sandwich panels (CCSSPs) showcased in Fig. (2.8) feature core structures fabricated using pristine ABS filaments, adhering to specific material extrusion parameters, and carbon fiber reinforced composite shells.

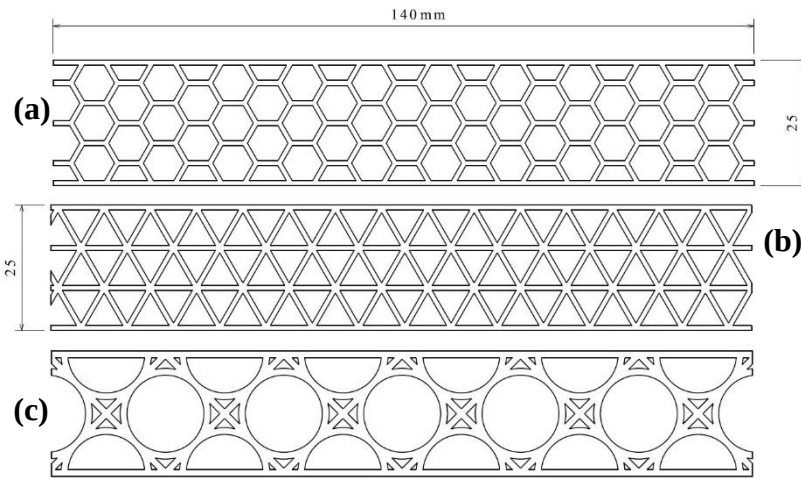


**Figure 2.7.** Various core structure designs of CCSSPs; a) Honeycomb core, b) Triangular core and c) Hybrid circular/triangular corrugated core structures.

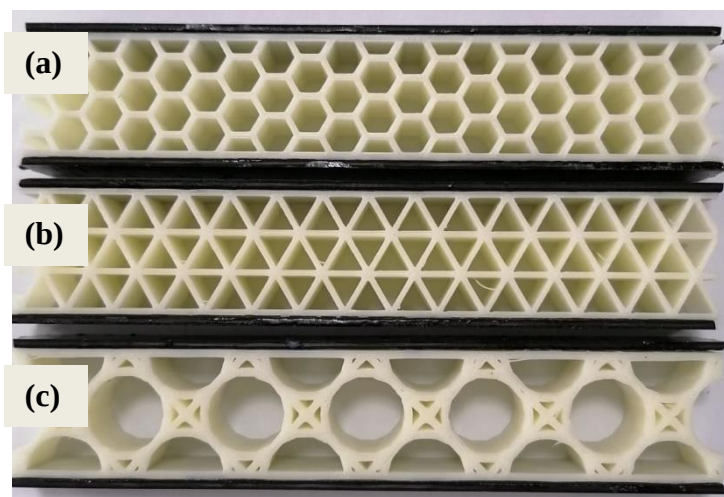


**Figure 2.8.** Fabricated CCSSPs of different core designs; a) honeycomb core, b) triangular core, and c) hybrid circular/triangular corrugated core structures.

The carbon fiber reinforced resin composite panels were utilized as the outer shell of the CCSSPs. These panels were produced using a hand layup and vacuum infusion technique. Three layers of carbon fiber fabric were laid up with a layer orientation of  $[0, 90, 0]$ . The layers were then molded using a plastic bag and subjected to vacuum pressure to facilitate resin transfer between the layers. Figure 2.9.a depicts the composite mold after the vacuum process. The resin was allowed to cure for 24 hours at room temperature. Subsequently, the composite panels were demolded and further cured at  $60^{\circ}\text{C}$  in a vacuum oven for 12 hours. To characterize the mechanical properties of the panels, the carbon fiber reinforced panels (CFRPs) were cut into dog-bone and rectangular samples using water-jet cutting technique (Fig. 2.9.b). Tensile tests were conducted on the CFRP samples to obtain the engineering constants required for the outer shell of the CCSSPs in 3-point bending finite element analyses (Fig. 2.9.c). An example of a tensile test result for CFRP is illustrated in Fig. 2.10. Further details regarding the engineering constants are presented in the subsequent chapter.

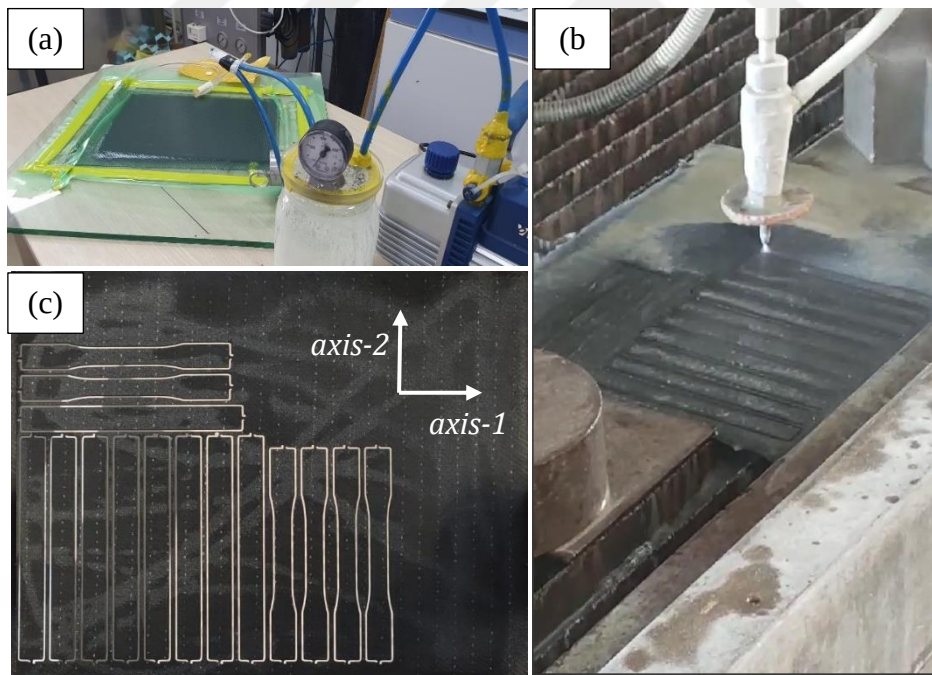


**Figure 2.9.** The fabrication process of carbon fiber reinforced resin composite panel (CFRP); a) vacuum infusion process, b) water jet cutting of CFRP and c) tensile test samples and shell of core shell structure.

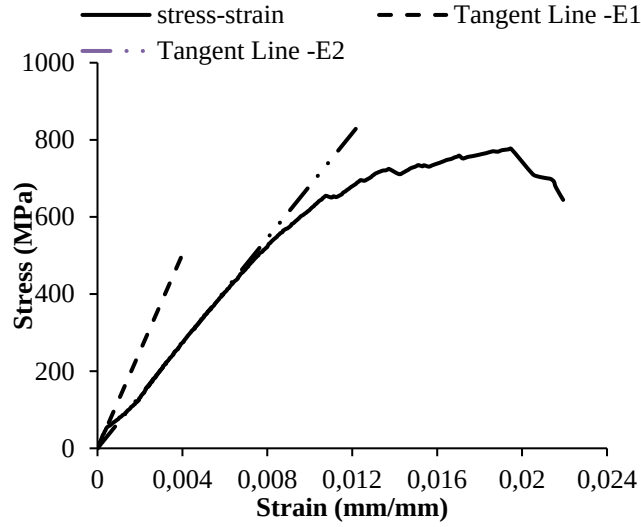


**Figure 2.10.** Stress – strain curve of CFRP tensile test sample (*along the 1st principal axis*).

The interlaminar shear modulus has been determined with semi-empirical stress partitioning parameter technique (SSP), which is shown in Eq. (2.1) (Tsai & Hahn, 1980).

$$G_{23} = G_m \frac{V_f + \eta(1-V_f)}{\eta_4(1-V_f) + V_f G_m / G_f} \quad (2.1)$$

$$\text{with } \eta_4 = \frac{3 - 4\nu_m + G_m / G_f}{4(1 - \nu_m)}$$

where,  $V_f$  is the volume fraction of the carbon fibers,  $G_m$  and  $G_f$  are the shear modulus of the resin matrix and the carbon fiber fabric, respectively.

In order to obtain the elastic modulus perpendicular to the fabric orientation, the semi-empirical Halpin-Tsai formula, as in Eq. (2.2) was employed,

$$E_2 = E_m \left[ \frac{1 + \xi \eta V_f}{1 - \eta V_f} \right] \quad (2.2)$$

$$\text{with } \eta = \frac{(E_f / E_m) - 1}{(E_f / E_m) + \xi}$$

where,  $\xi$  is an empirical parameter obtained by curve-fitting with the results of an analytical solution. The value  $\xi = 2$  usually gives good fit for the case of circular or square fibers. The  $V_f$  of composite panels was set to 54%.

## 2.4. Design of experiments

Some of the main process variables in FDM, include the extrusion rate (*ER*), printing orientation (*raster orientation, PO*) and composition of the polymer (*ratio of the PVC in the ABS matrix, PR*), which are taken in three levels as shown in Table (2.1). The material composition has been considered according to the PVC ratio (*PR*) and the concentration of carbon nanofibers (*nanoparticle ratio, NP*) in the ABS matrix. The design of experiments has been conducted based on modified central-composite surface response (CCSR) method for 4-parameters at 3-levels, in which the central levels have been reduced to one run and 4 sets of parameters were added by comparing the parameter runs for CCSR and Taguchi  $L_9$  orthogonal array to raise the number of data that are available in modeling the response variables of the fabricated component. The set of normalized parameters and their levels are summarized in Table (2.2). In this table, the included parameter runs of Taguchi  $L_9$  orthogonal array are represented in bold.

**Table 2.1.** Material extrusion process parameters for tensile test samples and composite panel core structure fabrication.

|                                         |              |
|-----------------------------------------|--------------|
| Temperature of nozzle (°C)              | 235          |
| Temperature of bed (°C)                 | 110          |
| Filling ratio (%)                       | 100          |
| Extrusion rate (mm/s), <i>ER</i>        | 20, 40, 60   |
| Printing orientation (°), <i>PO</i>     | 0, 35, 70    |
| PVC polymer ratio (wt%), <i>PR</i>      | 0, 10, 20    |
| Carbon nanofiber ratio (wt%), <i>NP</i> | 0, 0.05, 0.1 |

**Table 2.2.** Modified central-composite surface response (CCSR) design of FDM and material composition parameter sets for material extrusion process of tensile samples and core structure of composite panels.

| <b>Run</b> | <b><i>ER</i></b> | <b><i>PO</i></b> | <b><i>PR</i></b> | <b><i>NP</i></b> |
|------------|------------------|------------------|------------------|------------------|
| 1          | 1                | 1                | 1                | -1               |
| 2          | -1               | -1               | 1                | -1               |
| 3          | 1                | 0                | 0                | 0                |
| 4          | 1                | -1               | -1               | 1                |
| 5          | 0                | 0                | 0                | 0                |
| 6          | -1               | 1                | 1                | 1                |
| 7          | -1               | 1                | 1                | -1               |
| 8          | 0                | 1                | 0                | 0                |
| 9          | 0                | 0                | 0                | 0                |
| 10         | 1                | 1                | -1               | -1               |
| 11         | -1               | 1                | -1               | 1                |
| 12         | -1               | -1               | 1                | 1                |
| 13         | 1                | 1                | 1                | 1                |
| 14         | 0                | -1               | 0                | 0                |
| 15         | 1                | -1               | -1               | -1               |
| 16         | 1                | -1               | 1                | 1                |
| 17         | 0                | 0                | 0                | 1                |
| 18         | -1               | 1                | -1               | -1               |
| 19         | 0                | 0                | 1                | 0                |
| 20         | 0                | 0                | 0                | -1               |
| 21         | 0                | 0                | -1               | 0                |
| 22         | -1               | 0                | 0                | 0                |
| 23         | -1               | -1               | -1               | 1                |
| 24         | 1                | -1               | 1                | -1               |
| 25         | 1                | 1                | -1               | 1                |
| 26         | -1               | -1               | -1               | -1               |
| 27         | 0                | -1               | 0                | 1                |
| 28         | 0                | 0                | 1                | -1               |
| 29         | 0                | 1                | -1               | 0                |
| 30         | 1                | -1               | 1                | 0                |
| 31         | 1                | 0                | -1               | 1                |
| 32         | 1                | 1                | 0                | -1               |

## 2.5. Tensile and 3-point bending experiments

All the uniaxial tensile of dog-bone shaped tensile samples (*employed for finding the mechanical characteristics of 3D printed specimens*) and 3-point bending of CCSSPs (*employed to quantify the flexural characteristics of composite core shell structures to validate the results of finite element analyses*) have been conducted at room temperature on a Shimadzu tensile test machine with a capacity of 100 KN. Because of the layered deposition production in additive manufacturing of FDM technique, the structure of the printed tensile test samples is symmetric with respect to planes of 1-3 and 2-3 planes as shown in Fig. 2.6. These planes of symmetry provide the orthogonally isotropic properties of the printed structure. The experiments have been conducted at constant displacement rate of 1 mm/min to satisfy the quasi-static loading conditions. The 3-point bending experiments were conducted according to the ASTM D7249 standard, with the overall length of the sample of 140 mm and the span length of 120 mm (Fig. 2.11). A view of the tensile test and 3-point bending experiments are shown in figure 2.12.

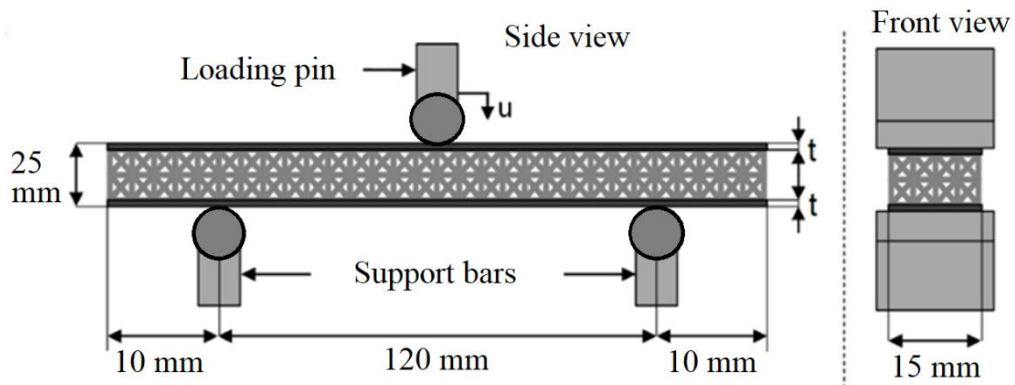


**Figure 2.11.** Schematic representation of 3-point bending experiment set up of CCSSPs in accordance to ASTM D7249.

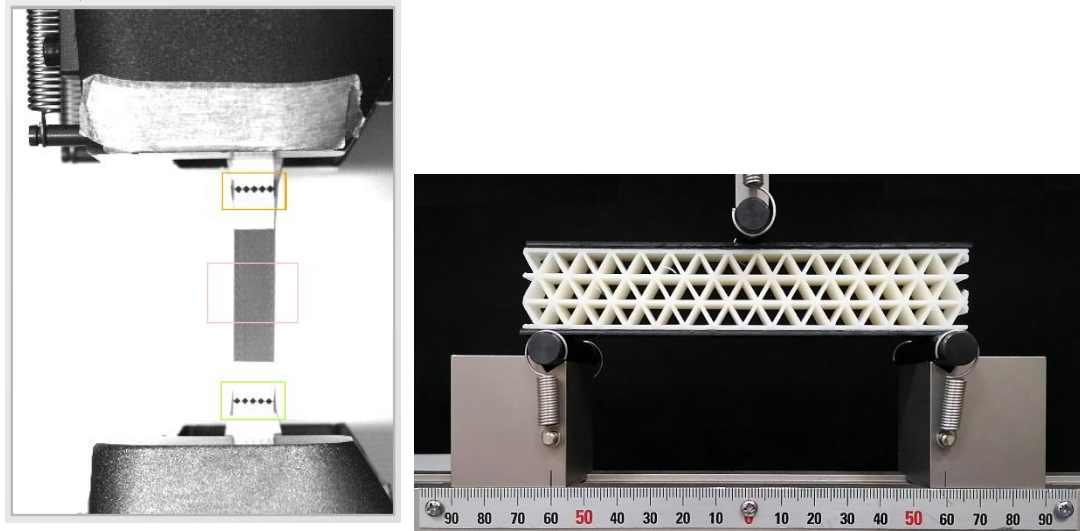


**Figure 2.12.** Views of experiments on Shimadzu uniaxial tensile test machine; a) uniaxial tensile test of dog-bone sample and b) 3-point bending of CCSSPs.

### 3. NUMERICAL AND MODELING TECHNIQUES

This section provides an overview of the core-shell design configurations, the development of core structures for composite sandwich panels, and the steps involved in defining the 3-point loading model in the Abaqus environment. The initial analysis involves comparing the loading-deformation response of the sandwich panels under 3-point bending and evaluating the von-Mises stresses in critical areas of the core structures during deformation. These results are used to identify the core design that exhibits the highest stiffness and load carrying capacity among the evaluated structures. Subsequently, the effects of the mechanical properties of the 3D printed core structure, considering various printing parameters and polymer compositions, on the performance of the composite sandwich panels under quasi-static 3-point bending conditions are investigated. Finite element (FE) analyses of the core structures are conducted using experimentally obtained mechanical properties. The simulations are validated by comparing the load-displacement results obtained from the FE analyses with the experimental data.

#### 3.1. Design of core structure

##### State of art of core lattice design

The performance of sandwich structures is highly dependent on the configuration of the structure and the choice of materials (Sahu et al., 2022). Sandwich structures offer numerous advantages, including improved energy absorption properties, high stiffness-to-weight ratios, excellent ballistic resistance, and effective thermal and acoustic insulation. These advantages make sandwich structures widely applicable in various fields such as automotive and aerospace engineering. The key to successful implementation of core-shell structures lies in the design of the core structure itself. Figure 3.1 illustrates different types of core structures commonly used, including truss, honeycomb, foam, and corrugated structures, each suited for specific applications. Honeycomb and corrugated cores are examples of periodically repeated inner structures. Honeycomb cores, such as hexagonal, square, or honeycomb cores with different cell shapes, are typically closed-cell structures. In contrast, corrugated cores feature open channels in one direction, as depicted in Fig. 3.1.d. Each core design offers unique characteristics and performance attributes, which will be further discussed in the following sections.

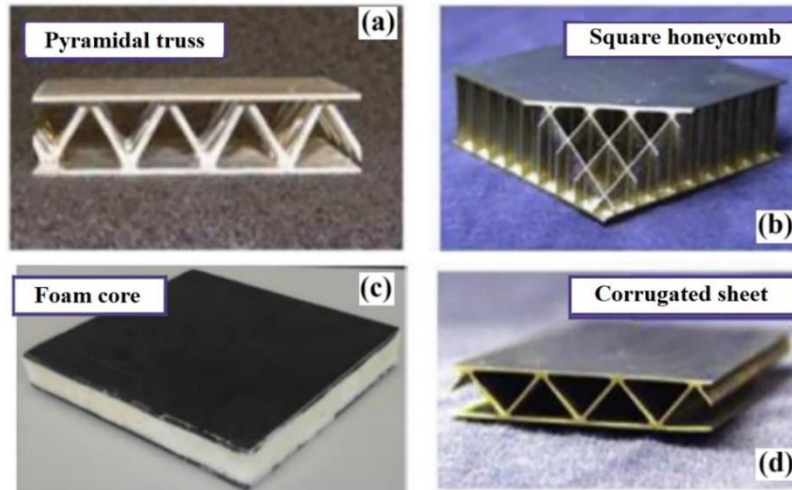


**Figure 3.1.** Various core shell sandwich structures: (a) pyramidal truss, (b) square honeycomb, (c) foam core, and (d) triangular corrugated sheet (Feng et al., 2020).

### 3.1.1. Conventional core structures

#### Truss core.

Truss core sandwich structures have a long history and are widely utilized in various applications. Traditional truss core designs, including tetrahedral, pyramidal, Kagome, and X-type configurations (Fig. 3.2.a – d) (Zhang et al., 2017), (Jiang et al., 2016), have been commonly employed. However, these lattice structures are better suited for manufacturing methods such as casting or metal sheet forming, rather than additive manufacturing (AM) techniques like Fused Deposition Modeling (FDM), which is the focus of this study. The use of FDM in fabricating truss core structures can result in weaker interlayer bonding, potentially impacting the mechanical properties of the produced core shell structures.

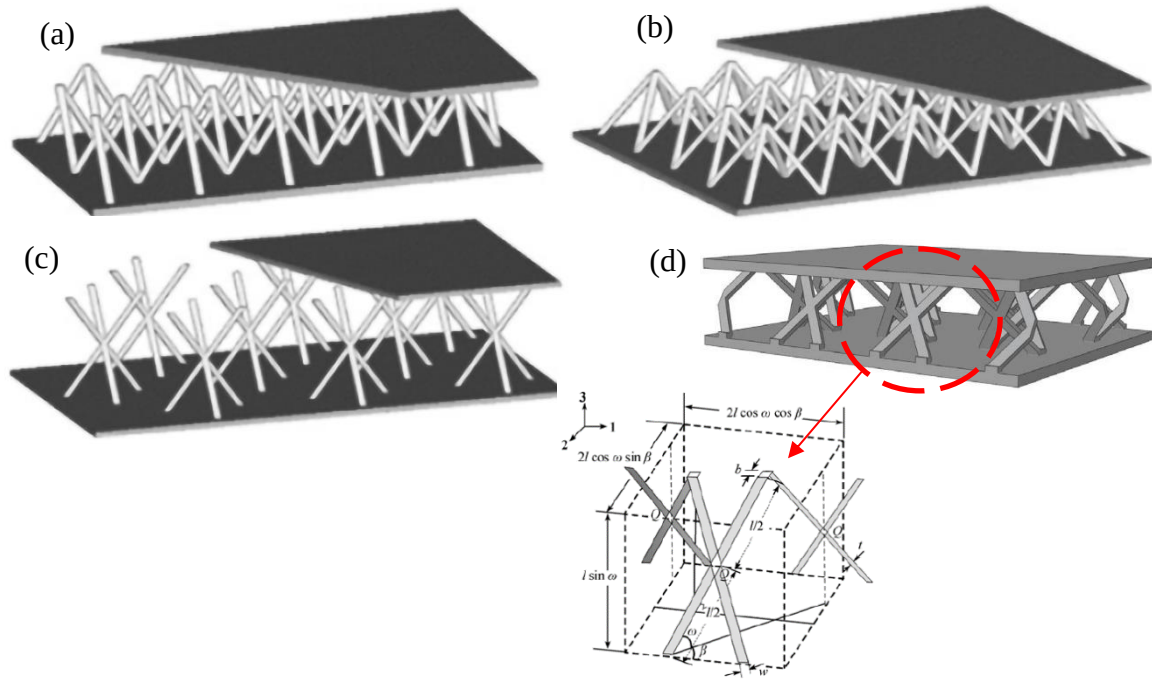


**Figure 3.2.** Sketches of (a) tetrahedral, (b) pyramidal and (c) 3-D Kagome and (d) X-type unite lattice core sandwich panel structures (Zhang et al., 2017), (Jiang et al., 2016).

### Corrugated core.

Corrugated sandwich structures find extensive applications in industries such as aeronautics, aerospace, naval, civil engineering, and automotive, thanks to their remarkable load-bearing and energy-absorbing capabilities. The corrugated core, positioned between the face sheets, can adopt various geometries, including rectangular, triangular, trapezoidal, arc-tangent, and sinusoidal cores, as depicted in Fig. 3.3 (Rong et al., 2018). Additive manufacturing (AM) techniques are particularly suitable for producing these structures, as the cross-section of the core can be sliced into continuous layers that faithfully represent the internal architecture of the corrugated pattern (Zaharia et al., 2020), (Basurto-Vázquez et al., 2021). This enables precise fabrication of the intricate core structure, leading to enhanced performance and design flexibility in AM-produced corrugated sandwich structures.

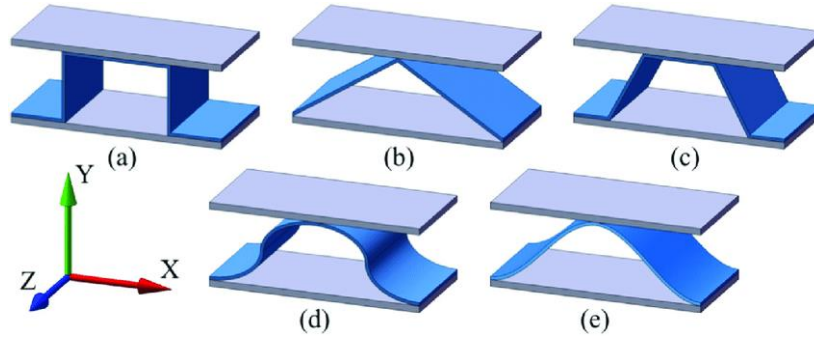


**Figure 3.3.** Different unit cells of corrugated sandwich cores: (a) rectangular, (b) triangular, (c) trapezoidal, (d) arc-tangent, and (e) sinusoidal (Zhang et al., 2019).

### Honeycomb core.

A typical honeycomb sandwich structure is composed of a hexagonal honeycomb core layer sandwiched between two thin plates forming the face sheets of the structure (Fig. 3.4(a)). These sandwich structures offer numerous advantages, including lightweight construction, increased flexural rigidity, improved out-of-plane strength and stiffness, and enhanced stability compared to conventional structures (Feng et al., 2020). In this design, the face sheets primarily carry the flexural load, while the core is responsible for bearing the normal and shear loads in the planes perpendicular to the cellular core. Alongside the conventional honeycomb core, various other honeycomb core designs have been introduced in recent years. One notable example is the center symmetric auxetic multi reentrant honeycomb structure developed by Lira et al. (Fig. 3.4(b) and (c)) (Lira et al., 2009). This innovative structure exhibits a negative Poisson's ratio (NPR) effect, resulting in higher fracture toughness, improved indentation resistance, enhanced shear modulus, superior vibration absorption, and lower fatigue crack propagation. The introduction of such honeycomb core designs expands the possibilities for tailoring the mechanical properties and performance of honeycomb sandwich structures in different applications.

Another variation is the combination of regular honeycomb and auxetic structures, as designed by Ingrole et al. (Fig. 3.4(d) and (e)) (Ingrole et al., 2017). These auxetic honeycomb structures have been claimed to possess higher compressive strength and greater energy absorption capabilities compared to other structures. Overall, honeycomb sandwich structures, including both conventional and auxetic designs, offer a range of advantages in terms of mechanical performance and can find applications in various industries.

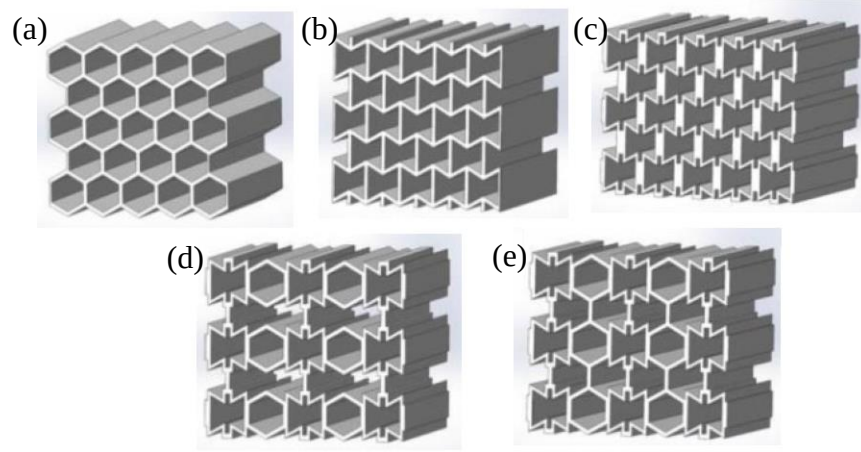


**Figure 3.4.** Various honeycomb core structures: (a) Traditional honeycomb, (b) Reentrant auxetic honeycomb, (c) Auxetic-strut honeycomb, (d, e) Auxetic honeycomb variations (Feng et al., 2020), (Lira et al., 2009), (Ingrole et al., 2017).

### 3.1.2. Novel core structure

#### Derivative core.

Figure 3.5 presents both the conventional Y-shape unit core and sandwich structure. The Y-shape core is designed with folded regions near the edges, which contribute to improved bonding between the face sheets and the core (Feng et al., 2020). The mechanical properties of Y-shaped cores are notably influenced by geometric parameters and relative density (Liu et al., 2018). Feng et al. (2020) highlighted the key parameters characterizing the Y-shaped core geometry, as depicted in Figure 3.5. These parameters include the thickness ( $t$ ) of the constituent members, the height ( $h$ ) of the Y-shaped core leg, the inclined angle ( $\alpha$ ) of the Y-flanges, the web size ( $e$ ), and the overall height ( $H$ ).

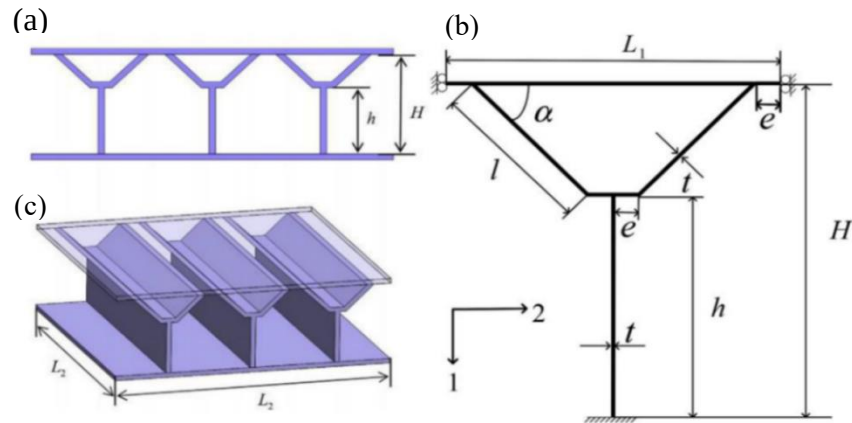


**Figure 3.5.** Schematic representation of a Y-shaped core sandwich structure: (a) Cross-section, (b) 3D geometric model, and (c) Unit cell (Liu et al., 2018).

The performance of Y-shaped cores has garnered significant attention in recent years, with several studies focusing on their mechanical behavior and practical applications. Liu et al. (2018) conducted comprehensive research on all-composite sandwich structures incorporating Y-shaped cores. Through hot-press molding, they explored the impact of relative density on the mechanical properties by subjecting the Y-shaped core sandwich panels to out-of-plane compressive tests across a range of relative densities (5.34% to 10.53%). The study examined failure modes, stress-strain behavior, mechanical properties, and energy absorption capacity, providing valuable insights into the influence of relative density on the core structure.

In another investigation, St-Pierre et al. (2015) evaluated the response of sandwich panels with Y-frame cores and compared them to panels with corrugated cores under low-velocity impact conditions. The results indicated comparable performance between the Y-frame core and corrugated core structures. Additionally, Rubino et al. (2010) focused on the quasi-static three-point bending behavior of simply supported and clamped sandwich structures with Y-frame cores. Their experimental study demonstrated similar responses between sandwich beams with Y-frame or corrugated cores under various loading scenarios, including clamped and simply supported three-point bending as well as indentation. From a strength perspective, both Y-frame and corrugated cores exhibited similar quasi-static performances.

### **Hybrid core.**

Ultralight sandwich structures featuring 2D prismatic or 3D lattice truss cores, such as honeycombs, corrugations, and pyramidal trusses, are renowned for their exceptional mechanical stiffness, strength, and impact resistance (Han et al., 2016a), (Han et al., 2016b), (Hu, 2016), (Yang, 2016). To further enhance these properties, hybrid lattice-cored sandwiches can be created by incorporating different materials into the interstices of the lattice. Han et al. (2016a, 2016b) conducted a study on a honeycomb-corrugate hybrid core by filling the interstices of aluminum corrugations with precision-cut trapezoidal aluminum honeycomb blocks (Fig. 3.6). These blocks were effectively bonded together using epoxy glue, forming a cohesive hybrid core. Subsequently, the hybrid core underwent rigorous testing under out-of-plane compression, transverse shear, and three-point bending loadings. The study unveiled the positive interaction effects between the corrugated plates and honeycomb walls, resulting in enhanced resistance against buckling and improved capacity to withstand bulk crushing at large plastic deformations. This research showcased the potential of hybrid lattice-cored structures to augment the mechanical performance of ultralight sandwich systems.

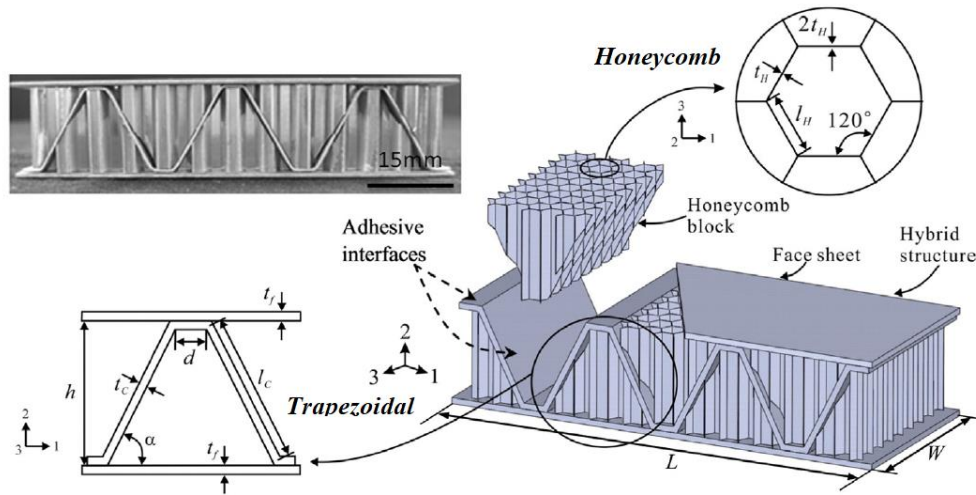


**Figure 3.6.** Schematic of a hybrid metallic core sandwich structure composed of corrugated plates, trapezoidal blocks, and honeycomb blocks (Han et al., 2016a), (Han et al., 2016b).

Hu et al. (2016) conducted a comprehensive investigation on a unique carbon fiber reinforced composite (CFRC) lattice truss sandwich panel (LTSP) with a corrugated core, fabricated using the compression molding process (Fig. 3.7). The study revealed that the mold pressing process effectively increased the fiber fraction within the lattice structure. Additionally, the co-curing of the core and CFRC facesheets, along with the enlarged contact area resulting from the corrugation design, substantially enhanced the shear strength and mitigated strut fracture and buckling failures.

In a separate study, Yang et al. (2016) focused on evaluating the damping and stiffness efficiency of hybrid sandwich panels. The base structure of these panels consisted of 2D truss patterns made from 2A12-T4 aluminum alloy, connected to woven carbon fiber/epoxy resin composite facesheets using J-272 adhesives (Fig. 3.8). The authors explored different integration approaches for incorporating damping agents within the core-shell structures. Type I involved the insertion of a viscoelastic damping sheet between the laminas of the composite facesheets. Type II entailed filling the voids of the pyramidal truss cores with effective damping materials like hard polyurethane foam (HPF), soft polyurethane foam (SPF), and silicon rubber. Type III combined the approaches used in types I and II. The results demonstrated that specimens of type II-HPF and -SPF exhibited superior damping and stiffness efficiency compared to other conventional or hybrid structures, highlighting the potential of such configurations for enhancing the dynamic properties of sandwich panels.

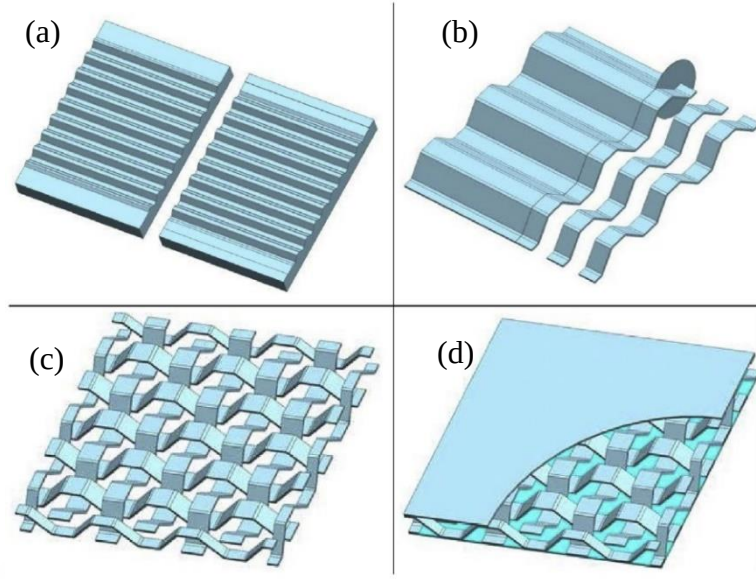


**Figure 3.7.** Fabrication process of a corrugated lattice truss sandwich panel: (a) Compression molding of CFRC, (b) Cutting corrugated panel into strips, (c) Assembly of corrugated strips in truss core, and (d) Adhesion of facesheets to the truss core (Hu et al., 2016).

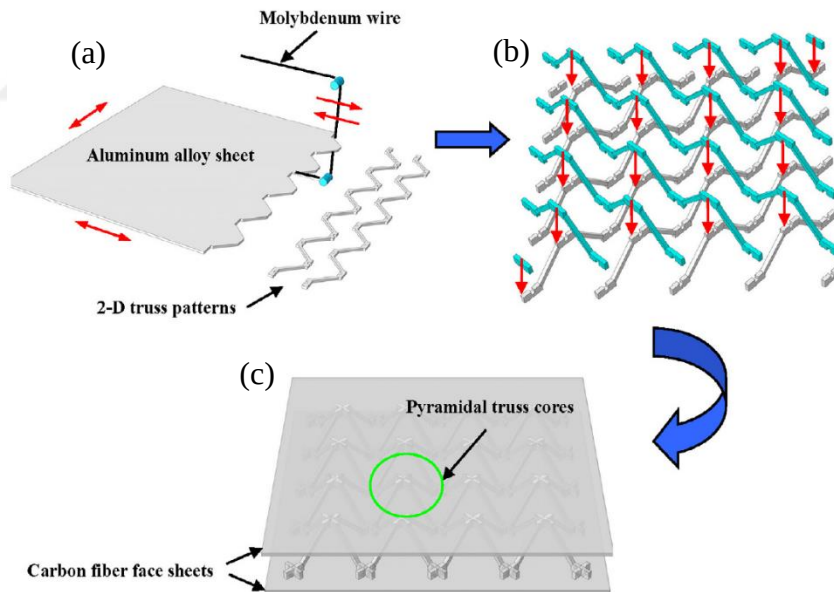
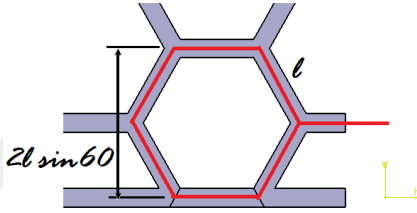
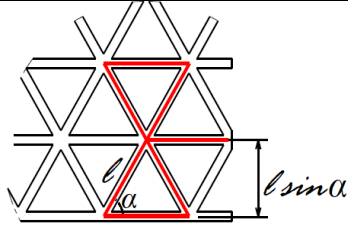
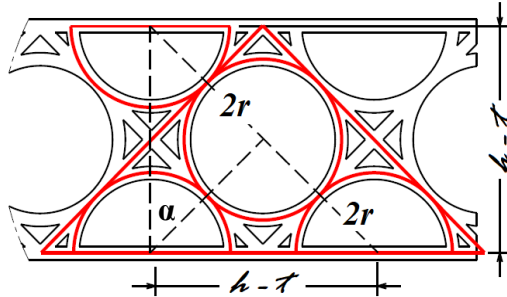


**Figure 3.8.** Fabrication process of pyramidal truss sandwich panels: (a) Wire-cutting of 2-D truss patterns, (b) Assembly of truss patterns, and (c) Joining the composite face sheets and the core with adhesive (Yang et al., 2016).

### 3.1.3. Studied core structure

In this investigation, the flexural behavior of two commonly used honeycomb and triangular core structures was compared to a novel hybrid circular/triangular corrugated (HCTC) core. The design specifications of the core structures are provided in Table (3.1), while the dimensions and isometric views of the cores are depicted in Fig. 3.9. To ensure a fair comparison among the different core structures, the thickness of the grids and the cell sizes were determined using Eqs. (3.1) - (3.3), while keeping other dimensions constant. These calculations were based on maintaining a constant relative mass of the cored structures compared to the solid structure.

**Table 3.1.** Configurations and dimensions of core cells for different core designs.

| Core cell type                        | Configuration                                                                       | Dimensions and calculations                                                                                                                                                                                                              |
|---------------------------------------|-------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Honeycomb core                        |   | $h = (2l \sin 60) \times n + t \quad (3.1)$ <p>where <math>t = 1.3 \text{ mm}</math> and therefore,<br/> <math>l = 4.56 \text{ mm}</math></p> $m_{rel} = \frac{m_{cored}}{m_{filled}} = 36.4\%$                                          |
| Triangular core                       |  | $h = (l \sin \alpha) \times n + t \quad (3.2)$ <p>where <math>t = 1 \text{ mm}</math> and therefore,<br/> <math>l = 9.24 \text{ mm}</math></p> $m_{rel} = \frac{m_{cored}}{m_{filled}} = 36.4\%$                                         |
| Hybrid circular/triangular corrugated |  | $\cos \alpha = \frac{h-t}{2(2r)} \rightarrow r = \frac{h-t}{2\sqrt{2}} \quad (3.3)$ <p>where <math>t = 1.36 \text{ mm}</math> and therefore,<br/> <math>r = 8.36 \text{ mm}</math></p> $m_{rel} = \frac{m_{cored}}{m_{filled}} = 36.4\%$ |

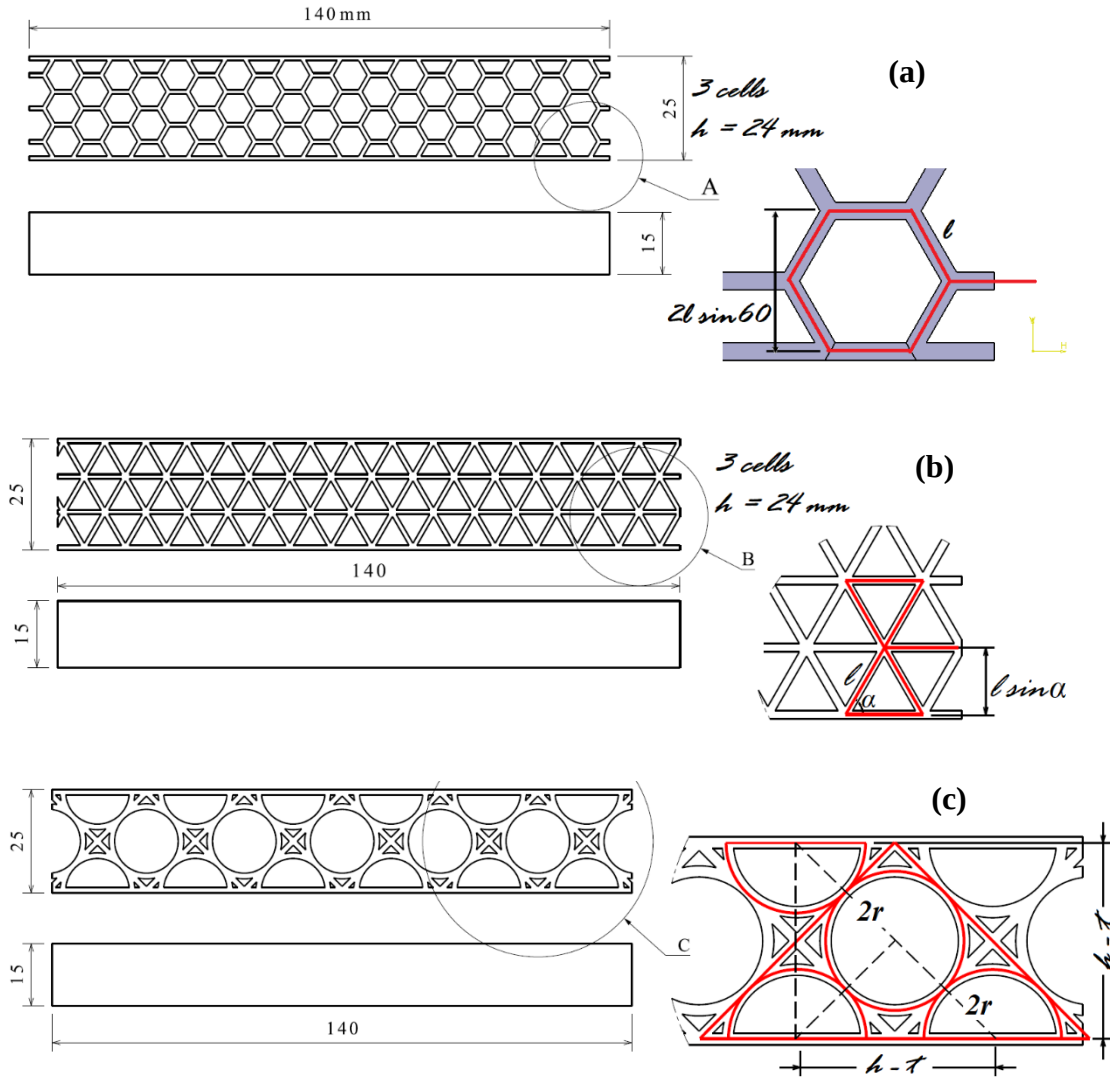


**Figure 3.9.** Configurations and dimensions of core cells for different core designs; a) honeycomb core, b) triangular core, and c) hybrid circular/triangular corrugated (HCTC) core.

### 3.2. Finite element analysis of core-shell structure

This section outlines the steps taken to develop finite element models (FEM) for the analysis of the core shell structures designed and discussed in the previous section, specifically under 3-point bending conditions. The results obtained from these analyses were used to determine the most suitable core structure based on its flexural loading and von Mises stress characteristics. The FEM of the selected core structure was then utilized to evaluate the impact of material extrusion parameters, including extrusion rate, printing orientation, PVC polymer mixing ratio, and CNF nanoadditive concentration in the matrix, on the flexural response of the core shell structures.

### 3.2.1. Steps of finite element analyses

The initial step in this process involves defining the geometry of the core structure and the fiber/resin composite as the face sheets within the part domain. For this purpose, the CAD models of the core structure, along with the shells of 1.9 mm thickness, were imported as STP files into the part module of Abaqus/CAE software. The face sheets were subsequently partitioned using datum planes, as depicted in Fig. 3.10. The pins, with a diameter of 10 mm, were defined as discrete – rigid elements. They were then assembled, as shown in Fig. 3.11, in a 3-point bending configuration, with the lower pins positioned 120 mm apart, following the specifications outlined in the standard (Xia et al., 2022).

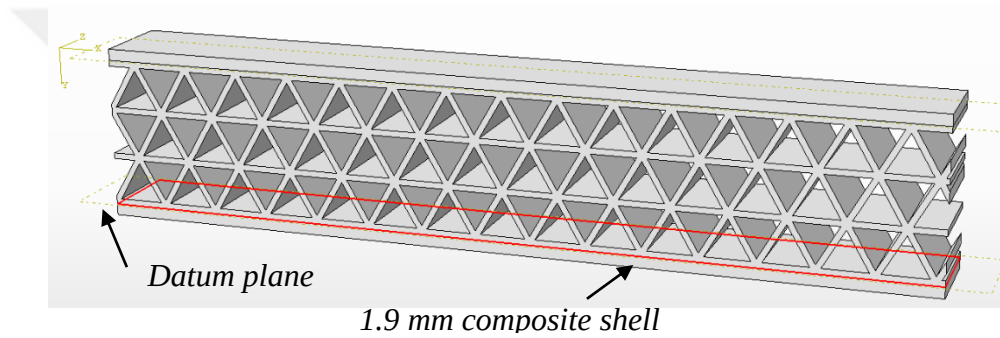


**Figure 3.10.** Definition of datum plane and partition of shell planes on both sides of the triangular core structure.

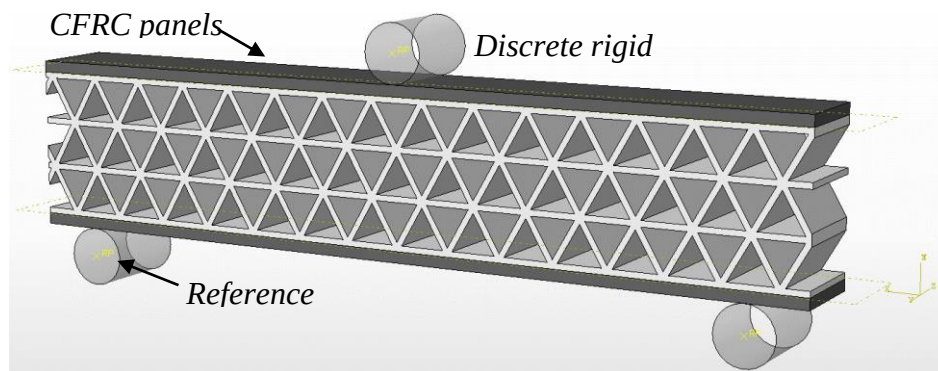


**Figure 3.11.** Assembly of composite core shell structure with discrete – rigid pins and definition of reference points.

To determine the core structure that exhibits the best response in terms of flexural loading and von Mises stress developed in the core grids, the material properties obtained for set-1 of the

material extrusion parameters, as presented in the RMS-32 design in the previous chapter, were assigned as engineering constants for the core of various honeycomb, triangular, and HCTC core structures. The properties of the shells were defined using experimentally obtained engineering constants for carbon fiber reinforced resin panels (CFRP). These CFRPs were manufactured through vacuum infusion molding and tested under quasi-static uniaxial tensile loading. The specific engineering constants for the CFRPs are outlined in Table (3.2).

**Table 3.2.** Mechanical properties of the core structure and the CFRF panels of the composite core shell structures

| Engineering constants       | $E_1$<br>(GPa) | $E_2$<br>(GPa) | $E_3$<br>(GPa) | $\nu_{12}$ | $\nu_{13}$ | $\nu_{23}$ | $G_{12}$<br>(GPa) | $G_{13}$<br>(GPa) | $G_{23}$<br>(GPa) |
|-----------------------------|----------------|----------------|----------------|------------|------------|------------|-------------------|-------------------|-------------------|
| Core structure <sup>1</sup> | 2.077          | 2.342          | 2.345          | 0.207      | 0.426      | 0.480      | 0.86              | 0.728             | 0.792             |
| CFRC <sup>2</sup> shell     | 125.80         | 122.425        | 8.226          | 0.145      | 0.459      | 0.336      | 54.936            | 43.113            | 3.233             |

<sup>1</sup>the engineering constants were defined as the mechanical properties obtained for the tensile test samples fabricated based on set-1 parameters of RSM-32 design of experiments.

<sup>2</sup>carbon fiber reinforced composite shell

In Fig. 3.12, reference points (RPs) were assigned to each pin, and a coupling constraint was established between each pin and its corresponding pin. The interaction between the outer surfaces of the rigid pins (*acting as the master*) and the contacting surfaces of the CFRPs (*acting as slaves*) was defined with a coefficient of friction of 0.2 for the tangential behavior and hard contact for the normal behavior. This setup allows for the separation of surfaces after the initial contact.

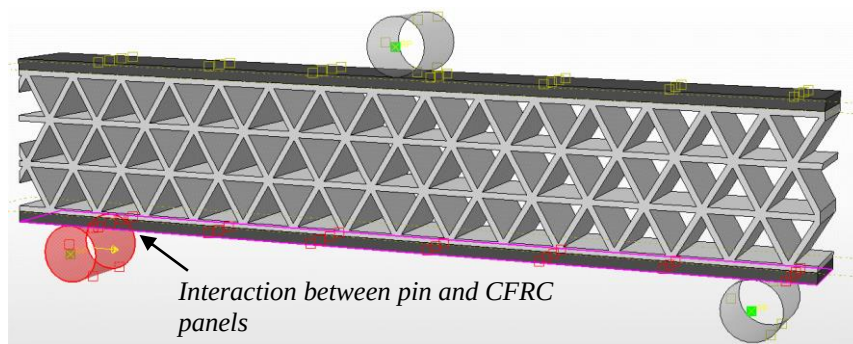


**Figure 3.12.** Definition of interaction between the external surface of pin (*as master*) and lower surface of the CFRP (*as slave*).

In addition, as depicted in Fig. 3.13, the boundary conditions (BCs) for the 3-point bending models were defined as rotational and displacement constraints at the reference points (RPs) of the pins. The degrees of freedom for the pins were restricted, except for the displacement of the upper pin along the z-axis. A velocity/angular velocity *BC* was applied to the upper pin along the z-axis, with a constant displacement rate of 1 mm/min, to simulate the quasi-static loading of the 3-point bending composite core shell structure during the experiments.

Furthermore, 30 steps were defined, with each step taking 10 seconds, allowing the moving pin to achieve a downward displacement of 5 mm to measure the flexural response of the core shell structures. To capture the behavior of the structures under quasi-static loading conditions, a *history output* was assigned to record the reaction load along the z-axis and the displacement of the upper pin at the reference point of the upper pin. This data was used to generate load-displacement curves for the core shell structures.

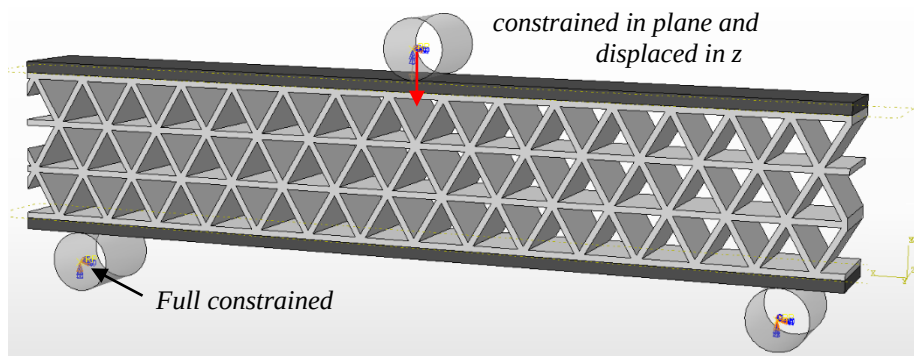


**Figure 3.13.** Definition of boundary conditions of the 3-point bending model at the reference points of pins.

A typical meshing for the HCTC core shell structure is represented in Fig. 3.14. As shown in this figure, depending on the configuration, each instance of the assembly was meshed with different type of elements represented in Table (3.3). The discrete-rigid pins and CFRP shells were assigned seed sizes of 1 mm. For the core structures, seed sizes were selected to ensure a uniform distribution of elements throughout the structure, as outlined in Table (3.4).

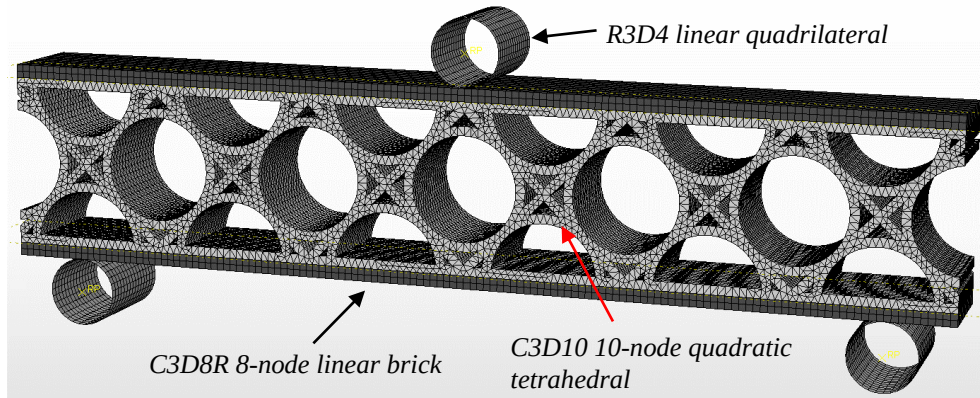


**Figure 3.14.** Meshing of the hybrid circular/triangular corrugated composite core shell structure with different element types for various sections.

**Table 3.3.** Type of the elements and size of the seeds for instances of the assembly of composite core shell structures.

| Assembly instance    |            | Element type       | Total number of elements | Size of seeds (mm) |
|----------------------|------------|--------------------|--------------------------|--------------------|
| Core structure       | Honeycomb  | C3D10 <sup>1</sup> | 94,654                   | 1.3                |
|                      | Triangular | C3D10              | 222,013                  | 1                  |
|                      | HCTC       | C3D10              | 157,905                  | 1                  |
| CFRC shell           |            | C3D8R <sup>2</sup> | 8,400                    | 1                  |
| Discrete – rigid pin |            | R3D4 <sup>3</sup>  | 1,395                    | 1                  |

<sup>1</sup> 10-node quadratic tetrahedron

<sup>2</sup> 8-node linear brick

<sup>3</sup> linear quadrihedral

### 3.2.2. Flexural response and stress distribution in core structures

The initial results of deformation and von Mises stress distribution in the core structures under a 5 mm displacement of the loading pin in the 3-point bending experiments of composite core shell structures are presented in Figs. 3.15 to 3.17. An important observation to note is that, regardless of the ultimate strength of the core material, the triangular core structure exhibits significantly higher stress levels and extensive deformations compared to the honeycomb and HCTC cores. However, the maximum von Mises stress in the HCTC core is approximately half of the corresponding stress observed in the honeycomb core, indicating the effectiveness of the hybrid core design in distributing the load throughout the core shell structure.

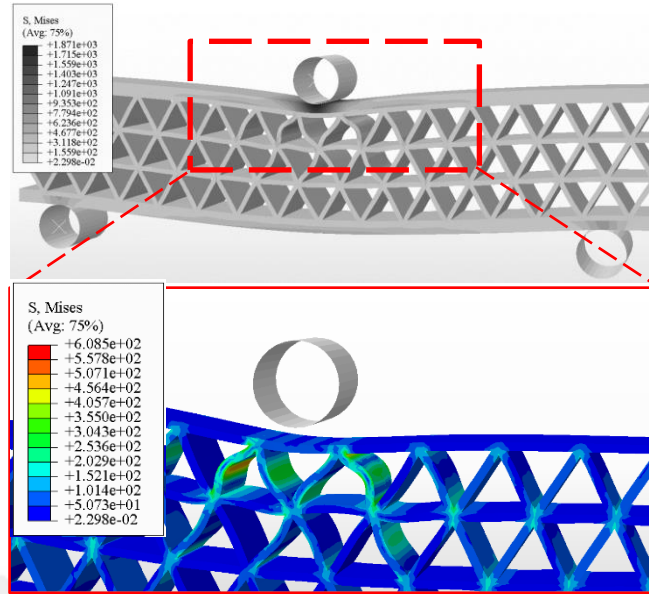


**Figure 3.15.** 3D representation of deformation and von-Mises stress distribution of triangular core structure in FEM of 3-point bending at 5 mm displacement of central pin.

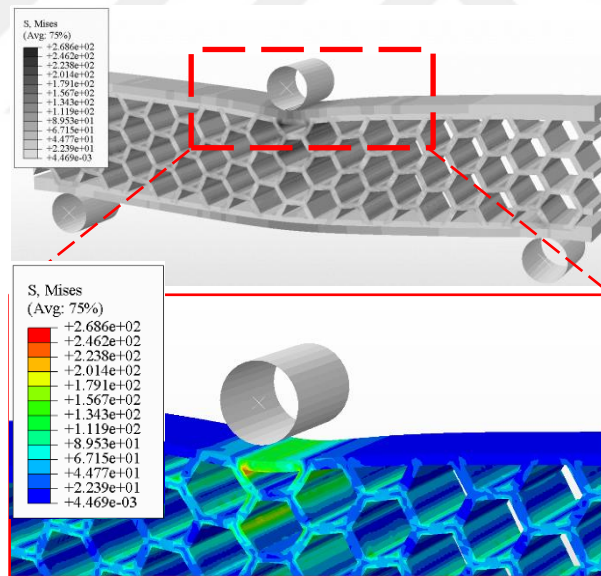


**Figure 3.16.** 3D representation of deformation and von-Mises stress distribution of triangular core structure in FEM of 3-point bending at 5 mm displacement of central pin.

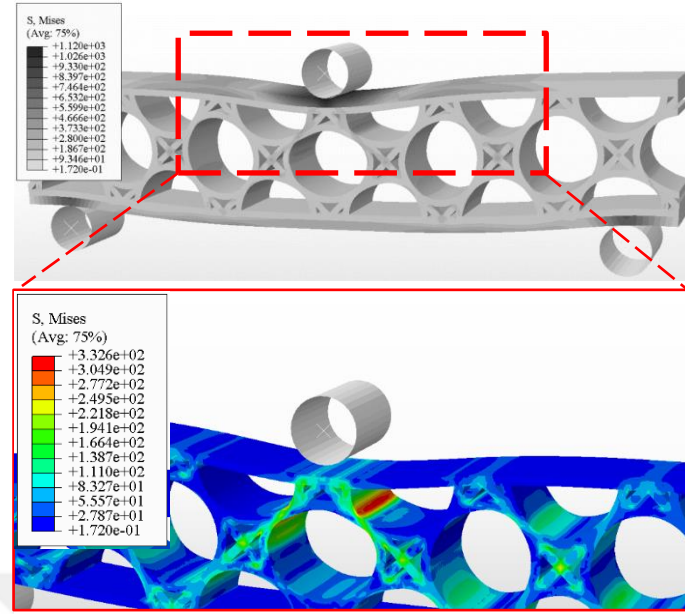


**Figure 3.17.** 3D representation of deformation and von-Mises stress distribution of triangular core structure in FEM of 3-point bending at 5 mm displacement of central pin.

To further investigate the effectiveness of the introduced HCTC core design in improving the flexural properties of the composite core shell structures, the force – displacement diagrams obtained from the reference point of the central pin and the von Mises stress distributions along defined paths at critical locations of the core structures were compared for different core types. Critical stress regions of the cores were identified and paths were defined accordingly, as shown in Fig. 3.18. The maximum von Mises stresses along these paths were plotted against the displacement of the central pin. The finite element results of the deformation load and the maximum von Mises stress versus displacement in the 3-point bending configuration are presented in Fig. 3.19. It is worth mentioning that the properties of the fabricated samples in the material extrusion process, based on the set-1 of the RSM-32 design of experiments, were incorporated as engineering constants for the core material.

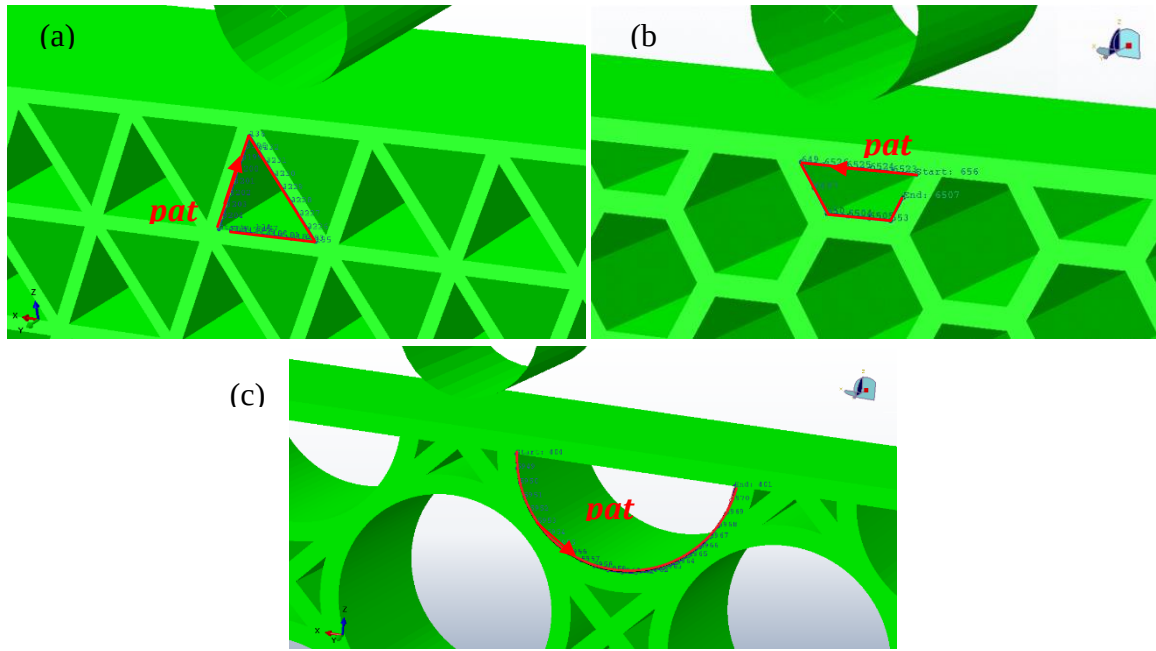


**Figure 3.18.** Definition of path at critical regions of core structures; a) triangular, b) hexagonal, and c) hybrid circular/triangular corrugated cores.

Figure 3.19.a shows the deformation loading versus the displacement of the central pin in the 3-point bending analyses of different core structures. It is evident that the honeycomb core structure exhibited significantly lower flexural response compared to the triangular and HCTC structures. On the other hand, although the triangular core design displayed a higher slope of the deformation curve and maximum loading than the HCTC core, the variation of von Mises stresses versus deformation was nonlinear in the former structure, reaching maximum levels after 4 mm displacement of the loading pin (Fig. 3.19.b). This nonlinear behavior can be attributed to excessive deformation of the ribs in the triangular grids located just below the loading center during the 3-point bending analysis, as depicted in Fig. 3.16. These observations demonstrate the effectiveness of the HCTC core as a viable design for composite core shell structures. As a result, all subsequent investigations on the effects of material extrusion parameters on the flexural response and the parameter optimization process have been conducted exclusively using the HCTC core as the selected core design.

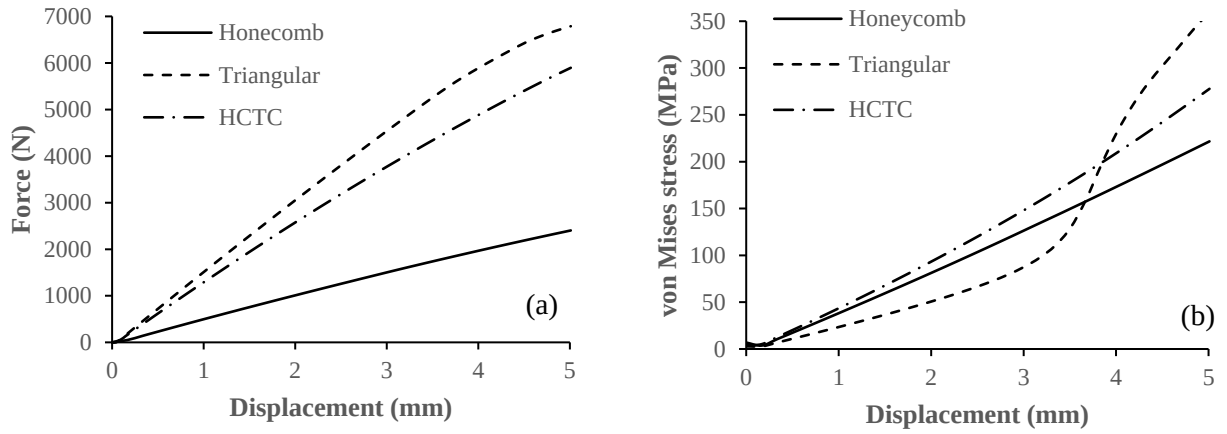


**Figure 3.19.** Results of 3-point bending analyses of different core structures; a) reaction loading of loading pin and b) maximum von Mises stress at critical spot of the core grids versus the displacement.

### 3.3. Regression modeling and optimization of mechanical properties

#### 3.3.1. Hybrid ANN/Bayesian modelling of response variables

The Artificial Neural Network (ANN) is a computational model that emulates the functioning of the human brain's biological neural network. It consists of interconnected neurons organized in input, hidden, and output layers. ANN is recognized as an effective approach for modeling complex nonlinear relationships between inputs and outputs in various processes (Oskui et al., 2016). In this study, a multilayer feed-forward back-propagation ANN architecture, depicted in Fig. 3.20, is employed to model the mechanical variables of 3D printed tensile samples and core-shell structures of fabricated ABS/PVC/CNF nanocomposites in the material extrusion process. The input layer comprises four neurons ( $ER$ ,  $PO$ ,  $PR$ ,  $NP$ ), representing the extrusion ratio, printing orientation, PVC polymer ratio, and CNF nanoadditives concentration, respectively. The output layer consists of a single neuron,  $\hat{y}$ , representing the response variable. Thus, separate regression equations are developed to model the response variables of interest, including the in-plane and out-of-plane modulus of elasticity and ultimate strength of dog-bone tensile samples, as well as the 3-point bending properties of flexural modulus and maximum loading in response to a 5 mm displacement of the loading pin.

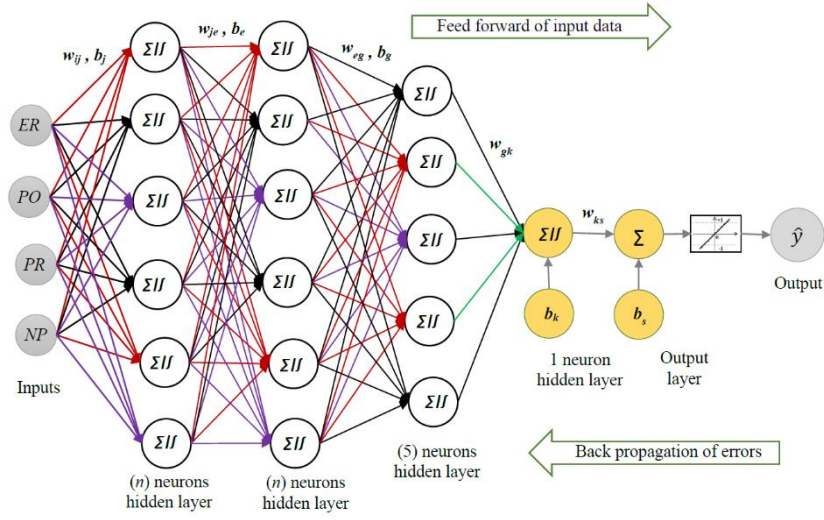


**Figure 3.20.** Architecture of a feed-forward back-propagation ANN with 4 hidden layers for modeling the mechanical response variables of samples in the material extrusion process.

As depicted in Figure 3.20, the neurons in each layer are interconnected with adjacent layers through weighted factors denoted as  $w_{\alpha\beta}$  ( $\alpha = i, j, e, g, k, s$ ;  $\beta = j, e, g, k, s$ ), which signify the significance of each factor. The inputs of each neuron are determined by the weighted sum of incoming signals and a bias term represented as  $b_{\alpha i}$  ( $\alpha = j, e, g, k, s$ ;  $i = \text{neuron number}$ ) to adjust the output of the layer using a transfer function. To determine the training and transfer functions, the number of neurons in the first two hidden layers, and the training rate of the ANN algorithm, a hyperparameter optimization was conducted using the Bayesian optimization approach.

Among various optimization algorithms for hyperparameters, grid search, random search, and Bayesian optimization are widely employed techniques (Wu et al., 2019), (Jiménez et al., 2009). Grid search exhaustively examines all possible combinations of hyperparameter values to select the optimal set. While this approach covers the entire search space, it becomes computationally exhaustive and inefficient as the number of hyperparameters increases, making it suitable for smaller networks with a limited number of hyperparameters. Random search, on the other hand, selects random combinations of hyperparameters, resulting in quicker optimal responses, but there is no guarantee of obtaining the best solution.

Both grid search and random search are blind techniques, as they do not utilize data from previous trials to inform the selection of subsequent hyperparameter values. In contrast, Bayesian optimization intelligently incorporates knowledge from previous trials to guide the

selection of hyperparameter values. Instead of blindly exploring the hyperparameter space, the Bayesian optimization algorithm makes informed decisions. Therefore, in this study, the Bayesian optimization approach was employed to optimize the hyperparameters of the ANN model.

The Bayesian optimization algorithm consists of two main components: a probabilistic model for the objective function and an acquisition function for evaluating the "quality" of a candidate point and selecting the next point to evaluate. The optimization process begins with an initial probability distribution, known as the prior, over the objective function that is to be optimized. As evaluations of the objective function are made at different candidate points, the distribution over possible functions, now referred to as the posterior, becomes more focused and precise.

The posterior distribution is then used to construct an acquisition function, which quantifies the desirability of exploring different candidate points. In other words, the probabilistic model provides a Bayesian posterior probability distribution that characterizes potential values of the objective function at each candidate point. After the objective function is observed at a new candidate point, the posterior distribution is updated to incorporate this new information. Based on the current posterior distribution, the acquisition function determines the next candidate point to be evaluated, optimizing the trade-off between exploration (sampling uncertain regions) and exploitation (sampling promising regions).

By iteratively updating the posterior distribution and selecting the next query point using the acquisition function, the Bayesian optimization algorithm guides the search towards regions of the parameter space that are likely to yield better objective function values. This iterative process continues until a stopping criterion is met or a satisfactory solution is found.

To prevent overtraining or overfitting of the ANN model, several techniques were employed, including early stopping and regularization methods. In particular, Bayesian regularization backpropagation and a modified performance function were utilized as part of the training process. The modified performance function aimed to improve the evaluation metrics, such as the root mean squared error (RMSE), adjusted  $R^2$  for the training data, and the overall model. This was achieved by incorporating an additional component that considered the RMSE,  $R^2_{\text{train}}$ , and  $R^2_{\text{all}}$  of the developed ANN (Pashmforoush, 2022), (Bai et al., 2018).

The optimization parameters used in the search for the optimal ANN configuration are detailed in Table (3-4). These parameters, such as the number of neurons in hidden layers ( $n$ ), the transfer function between layers, the training function, and the training rate, were evaluated

using a MATLAB code. The objective was to identify the combination of these parameters that would minimize the RMSE and maximize the adjusted  $R^2$  for both the training data and the entire model, serving as performance metrics for assessing the ANN's accuracy and generalization capability.

**Table 3.4.** ANN/Bayesian hyperparameter optimization in modeling of response variables of 3D printed ABS/PVC/CNF nanocomposites.

| Parameter                                                                                                                                         | Ranges/Functions                                                                                                                                                                                                                                              |
|---------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Number of neurons                                                                                                                                 | $n, n^*, 5, 1$                                                                                                                                                                                                                                                |
| Transfer functions                                                                                                                                | <i>tansig</i> “Symmetric sigmoid”<br><i>logsig</i> “Logarithmic sigmoid”<br><i>softmax</i> “Soft max”                                                                                                                                                         |
| Training function                                                                                                                                 | <i>trainlm</i> (Levenberg-Marquardt)<br><i>trainscg</i> (Scaled conjugate gradient)<br><i>traingdm</i> (Batch Gradient Descent with Momentum)<br><i>traingda</i> (Gradient descent with adaptive learning rate)<br><i>trainrp</i> (Resilient Backpropagation) |
| Performance merits                                                                                                                                | $RMSE, R_{train}^2, R_{all}^2$                                                                                                                                                                                                                                |
| Learning rate                                                                                                                                     | 0.001 – 0.5                                                                                                                                                                                                                                                   |
| Maximum epoch                                                                                                                                     | 1000                                                                                                                                                                                                                                                          |
| Performance goal                                                                                                                                  | $1 \times 10^{-7}$                                                                                                                                                                                                                                            |
| *n is determined as a number between 1-30 based on the MSE and maximum adjusted- $R^2$ values of training network obtained at the minimum epochs. |                                                                                                                                                                                                                                                               |
| **Conjugate gradient backpropagation                                                                                                              |                                                                                                                                                                                                                                                               |

The output layer was configured with a linear transfer function (*purelin*) that enables the production of values beyond the normalized range of  $[-1, 1]$ . This transfer function is commonly employed for function fitting tasks. The mathematical representation of the resulting model for each response variable of the 3D printed samples can be described by Eq. (3.4).

$$\hat{y} = f_5 \left\{ \sum_{k=1}^{m_4} w_{ks} \cdot f_4 \left\{ \sum_{g=1}^{m_3} w_{gk} \cdot f_3 \left\{ \sum_{e=1}^{m_2} w_{eg} \cdot f_2 \left\{ \sum_{j=1}^{m_1} w_{je} \cdot f_1 \left\{ \sum_{i=1}^n w_{ij} \cdot X_i + b_j \right\} + b_e \right\} + b_g \right\} + b_k \right\} + b_s \right\} \quad (3.4)$$

In Eq. (3.4),  $X_j$  represents the input parameters, and  $\hat{y}$  corresponds to the output variable. The weights between the successive layers, namely  $w_{ij}$ ,  $w_{je}$ ,  $w_{eg}$ ,  $w_{gk}$ , and  $w_{ks}$ , are associated with the connections between the respective layers denoted by letters  $i, j, e, g, k$ , and  $s$ . The bias of each neuron in different layers is represented by the parameter  $b$ . The transfer functions  $f_i$  ( $i = 1-4$ )

are determined through the hyperparameter optimization process, while the transfer function  $f_5$  is the purelin function.

The ANN model was trained using 70% of the experimental data, while the remaining 30% was used for testing and validation. All input and output parameters were normalized within the range of [-1, 1] to enhance the consistency of the obtained models for the response variables of the 3D printed samples.

The finalized training parameters for the ANN model, including the values of control variables such as RMSE, adjusted- $R^2$ , and the *minimum number of epochs* required to satisfy the training metrics for modeling the response variables of interest in the 3D printed samples, are summarized in Tables (3.5) and (3.6).

**Table 3.5.** Results of Bayesian optimization of hyperparameters of ANN models.

| Response mode           | ANN response variables      | ANN parameters       |               |                   |                   |
|-------------------------|-----------------------------|----------------------|---------------|-------------------|-------------------|
|                         |                             | n – number of layers | training rate | training function | transfer function |
| In-plane properties     | Elastic modulus, $E_1$      | 50                   | 0.0060439     | <i>trainlm</i>    | <i>logsig</i>     |
|                         | Ultimate strength, $S_{u1}$ | 49                   | 0.0913        | <i>trainlm</i>    | <i>tansig</i>     |
| Out-of-plane properties | Elastic modulus, $E_3$      | 40                   | 0.49739       | <i>trainlm</i>    | <i>tansig</i>     |
|                         | Ultimate strength, $S_{u3}$ | 24                   | 0.14572       | <i>trainlm</i>    | <i>tansig</i>     |
| Flexural properties     | Flexural modulus, $E_f$     | 50                   | 0.042495      | <i>trainlm</i>    | <i>logsig</i>     |
|                         | Maximum loading, $F_{max}$  | 28                   | 0.0010117     | <i>trainlm</i>    | <i>logsig</i>     |

Furthermore, the performance of the ANN models was evaluated using the loss response as the performance criterion with respect to the RSM-32 experimental data. The results for testing, training, and validation of the ANN models for selected response variables are presented in Figs. 3.21 - 3.22. The rapid convergence of the loss parameters with respect to the number of iterations indicates that the developed models provide a good fit to the response variables of the fabricated nanocomposites. In particular, the in-plane properties of modulus of elasticity ( $E_1$ ) and ultimate strength ( $S_{u1}$ ) correspond to the tensile samples fabricated horizontally on the 3D machine table along the main axis-1, while the out-of-plane properties of  $E_3$  and  $S_{u3}$  represent the properties of the tensile samples fabricated vertically with respect to the 3D machine table along the main axis-3.

Additionally, the flexural modulus and maximum flexural loading in response to a 5 mm displacement of the loading pin in 3-point bending were obtained through finite element analyses of the hybrid circular/triangular corrugated (HCTC) core shell structure. As depicted in Figs. 3.21 and 3.22, the adjusted- $R^2$  values indicate a strong correlation between the dependent parameters and the independent response variables, demonstrating the high precision of the developed ANN models in predicting the response variables of the 3D printed samples. Moreover, Figs. 3.23 and 3.24 illustrate the rapid convergence of the loss parameters, affirming that the developed models accurately capture the mechanical and flexural properties of the fabricated ABS/PVC/CNF nanocomposites.

**Table 3.6.** ANN response variables at critical running epochs that satisfy the evaluation metrics.

| ANN response variables | Response variables    |                        |                         |                        |                       |                       |
|------------------------|-----------------------|------------------------|-------------------------|------------------------|-----------------------|-----------------------|
|                        | In-plane properties   |                        | Out-of-plane properties |                        | Flexural properties   |                       |
|                        | $E_1$                 | $S_{u1}$               | $E_3$                   | $S_{u3}$               | $E_f$                 | $F_{max}$             |
| Epochs                 | 124                   | 294                    | 58                      | 34                     | 76                    | 22                    |
| Final MSE              | $5.27 \times 10^{-4}$ | $5.47 \times 10^{-10}$ | $3.18 \times 10^{-4}$   | $1.917 \times 10^{-6}$ | $7.29 \times 10^{-7}$ | $4.08 \times 10^{-8}$ |
| $R^2_{train}$          | 0.907                 | 0.885                  | 0.982                   | 0.942                  | 0.919                 | 0.918                 |
| $R^2_{val}$            | 0.996                 | 1                      | 0.999                   | 0.935                  | 1                     | 1                     |
| $R^2_{test}$           | 0.995                 | 1                      | 0.985                   | 1                      | 1                     | 0.946                 |
| $R^2_{all}$            | 0.923                 | 0.91                   | 0.988                   | 0.948                  | 0.931                 | 0.93                  |

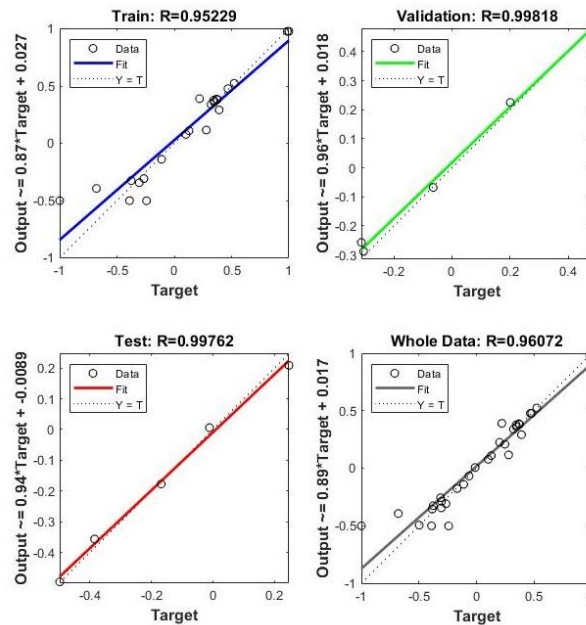


**Figure 3.21.** Results of regression, showing the correlation between the output and the target data in ANN training for modeling of modulus of elasticity,  $E_1$ .

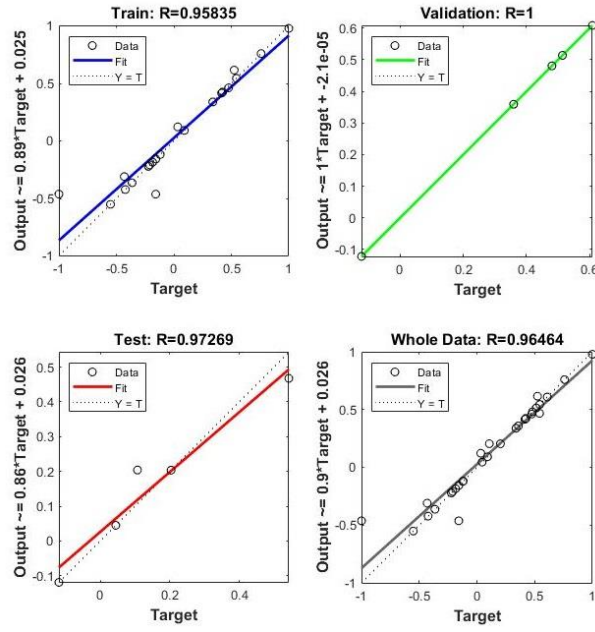


**Figure 3.22.** Results of regression, showing the correlation between the output and target data in ANN training for modeling maximum flexural loading of 3-point bending at 5 mm displacement,  $F_{max}$ .

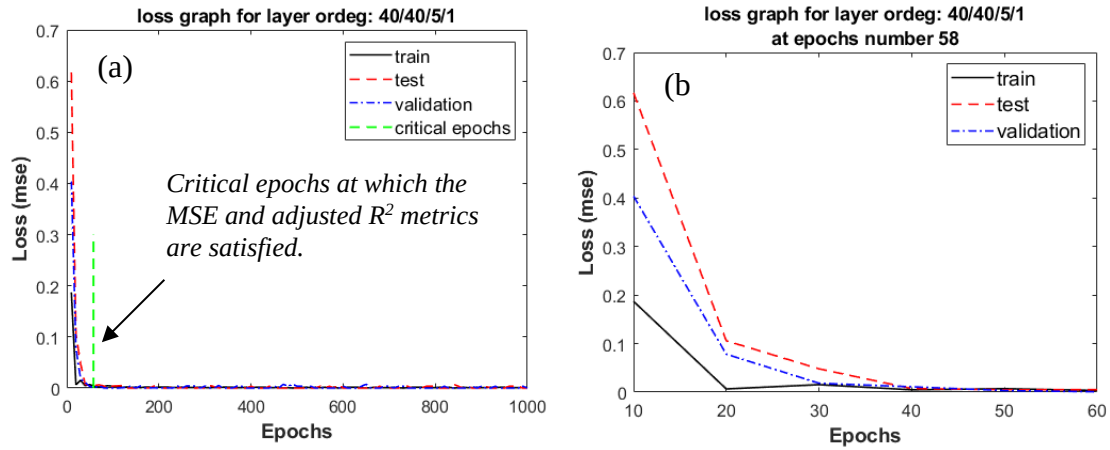


**Figure 3.23.** Loss parameters versus the number of epochs in modeling of  $E_3$ ; a) total range of ANN iterations and b) maximum number of epochs to meet the training metrics.

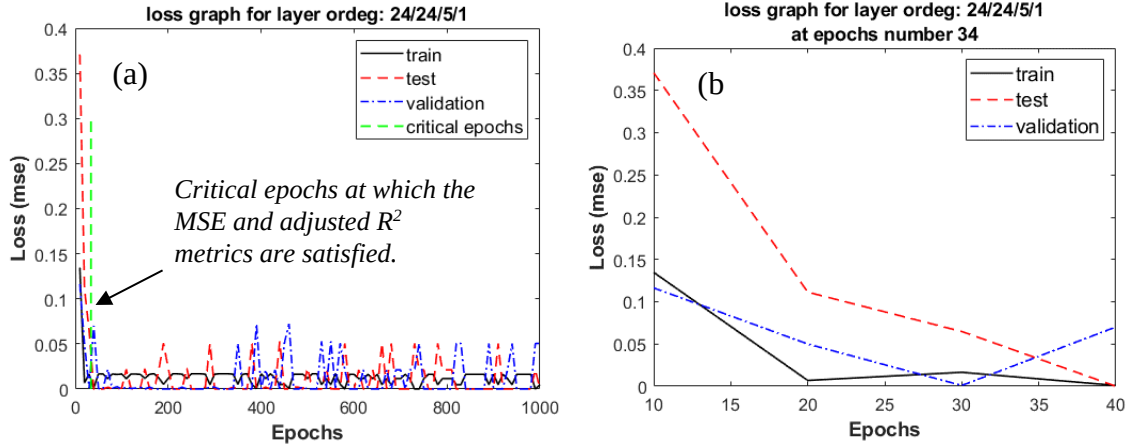


**Figure 3.24.** Loss parameters versus the number of epochs in modeling of  $Su_3$ ; a) total range of ANN iterations and b) maximum number of epochs to meet the training metrics.

### 3.3.2. Optimization of mechanical properties of 3D printed samples using ACO

The communication observed in nature, where insects deposit pheromones to communicate with other members of their swarm, has inspired various optimization techniques. While these techniques may not replicate all aspects of natural pheromone communication, they have proven effective in solving computational problems that involve finding optimal paths. One such technique is ant colony optimization (ACO), which aims to find the shortest path to the desired solution (Yang & Karamanoglu, 2020).

To apply ACO, the problem is transformed into an algorithm that seeks to find the optimal solution through an iterative process. In this algorithm, each ant initially constructs a solution by randomly selecting edges to form a local solution. The paths constructed by different ants are then compared, and the pheromone level of each edge is updated accordingly. This iterative process allows the algorithm to gradually converge towards the optimal solution. The steps involved in the ACO algorithm can be summarized as follows:

#### Selection of the edge between the states

Each ant  $k$  constructs an edge from current state  $x_{i,j}$  to next state  $x_{i,j+1}$ , in which  $i$  represents the iteration number and  $j$  represents the step number. Therefore, each ant computes a set of feasible expansions in each solution to its local objective,  $obj^{k,i}$ , in each iteration and moves in one of these solutions based on its probability,  $P_{j,j+1}^{k,i}$ . The probability depends on two parameters of desirability of the path,  $\eta_{j,j+1}$ , and the pheromone level,  $\tau_{j,j+1}$ , in the form of the following equation:

Each ant  $k$  constructs an edge from the current state  $x_{ij}$  to the next state  $x_{i,j+1}$ , where  $i$  represents the iteration number and  $j$  represents the step number. During each iteration, each ant evaluates a set of feasible expansions to its local objective,  $obj^{k,i}$ , and selects a solution based on the probability  $P_{j,j+1}^{k,i}$ . This probability is determined by two parameters: the desirability of the path,  $\eta_{j,j+1}$ , and the pheromone level,  $\tau_{j,j+1}$ , following the equation:

$$P_{j,j+1}^{k,i} = \frac{\tau_{j,j+1}^\alpha \eta_{j,j+1}^\beta}{\sum (\tau_{j,j+1}^\alpha)(\eta_{j,j+1}^\beta)} \quad (3.5)$$

where  $\tau_{j,j+1}$  is the amount of pheromone deposited between states  $j$  and  $j+1$ ,  $\alpha > 0$  is the parameter that controls the influence of  $\tau_{j,j+1}$ ,  $\eta_{j,j+1}$  is the desirability of each edge that depends on the  $d_{j,j+1}$ , distance between the states  $j$  and  $j+1$ , and  $\alpha$  and  $\beta$  are parameters that control the influence of the pheromone level ( $\tau_{j,j+1}$ ) and desirability of the path ( $\eta_{j,j+1}$ ), respectively. The numerator represents the attractiveness of the path based on the pheromone level and desirability, while the denominator ensures that the probabilities of all feasible expansions sum up to 1. By utilizing these probabilities, each ant makes informed decisions on which path to follow in constructing its solution.

### Update the pheromone level of edges

The pheromone levels on the trails are updated after all ants complete their tours. The decision to increase or decrease the pheromone level is based on the quality of the solution. As ants converge to a solution, the pheromone amount on good tours gradually increases. Additionally, a portion of the pheromone evaporates from low-quality tours to enhance the effectiveness of depositing pheromone on good tours. These rules can be expressed mathematically using the following equation:

$$\tau_{j,j+1} \leftarrow (1 - \rho)\tau_{j,j+1} + \sum_{k=1}^N \Delta\tau_{j,j+1}^{k,i} \quad (3.6)$$

Here,  $\tau_{j,j+1}$  represents the pheromone level on the trail between states  $j$  and  $j+1$ . The parameter  $\rho$  ( $0 < \rho < 1$ ) denotes the evaporation rate, determining the amount of pheromone that evaporates from the trails.  $\Delta\tau_{j,j+1}^{k,i}$  represents the pheromone deposit made by ant  $k$  on the trail between states  $j$  and  $j+1$ . The pheromone levels are updated by considering the contributions from all ants.

$$\Delta\tau_{j,j+1}^{k,i} = \begin{cases} \frac{Q}{L_k} & \text{if ant } k \text{ uses the tour between } j \text{ and } j+1 \text{ states} \\ 0 & \text{otherwise} \end{cases} \quad (3.7)$$

where  $Q$  is a constant (often 1) and  $L_k$  is the cost of ant  $k$ .

In this study, a computer code was developed in MATLAB based on the ACO model described above to optimize the mechanical properties of fabricated samples in uniaxial tensile loading of dog-bone samples and 3-point bending of core-shell structures. The ACO parameters applied in this program are specified in Table (3.7). It is important to note that the ACO program was iterated 2000 times, and the best solution obtained by the ants was reported as the response of the model.

**Table 3.7.** ACO model parameters for optimization of mechanical properties of fabricated material extrusion samples.

| Parameter                                          | Range of variable |
|----------------------------------------------------|-------------------|
| Ant swarm population ( $N$ )                       | 20                |
| Permissible discrete value of each design variable | 50                |
| Pheromone decay parameter ( $\rho$ )               | 0.5               |
| Desirability (scaling) factor ( $\eta$ )           | 2                 |
| Control factors $\alpha$ and $\beta$               | 1                 |
| Maximum iteration value of each run                | 100               |
| Maximum run of models                              | 2000              |

## 4. RESULTS and DISCUSSION

In this chapter first the mechanical properties of tensile test samples fabricated at different orientations of principal axes under the material extrusion parameters, specified according to the central composite surface response (CCSR) design of experiments, have been presented in the form of engineering constants of fabricated samples. Later, the results of finite element modeling of 3-point bending of composite core shell sandwich panels (CCSSP), with hybrid circular/triangular corrugated (HCTC) core structure, have been presented in the form of flexural modulus and maximum flexural loading of sandwich panels with mechanical properties of the core defined using engineering constants of 3D printed samples. The discussions include the variation of mechanical and flexural response of tensile samples and CCSSP specimens in response to the variations in material extrusion parameters, including extrusion rate (ER), printing orientation (PO), PVC polymer ratio (PR) and concentration of carbon nanofiber in the matrix (CNF).

### 4.1. Results of tensile tests and 3-point bending simulations

The results of uniaxial tensile experiments of samples fabricated along the principal axes, as shown in Fig. 4.1, and under the material extrusion parameters, represented in Table 4.1, are summarized in the form of engineering constants in Table 4.2. It might be worth noting that the experimental sets for the material extrusion process have been determined based on the central composite surface response (CCSR) method, as described in chapter 2.

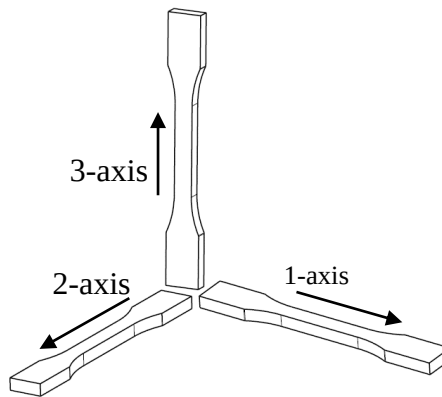


**Figure 4.1.** Schematic representation of sample orientation along the principal axes in 3D printing process of tensile test specimens.

The obtained experimental data, in the form of engineering constants, represented in Table 4.2 have been employed as the material properties of hybrid circular/triangular corrugated (HCTC) core in 3-point bending modeling of composite core shell sandwich panels (CCSSP). The response variables, in the form of flexural modulus ( $E_f$ ) and maximum flexural loading ( $F_{max}$ ) for 5 mm displacement of the central pin were reported as the result of 3-point bending simulations in Table 4.3.

All the mechanical properties obtained by uniaxial tensile tests and the flexural properties obtained through finite element modeling of 3-point bending of CCSSPs, of different core properties according to the CCSR approach, have been subjected to regression modeling based on the hybrid ANN/Bayesian artificial intelligent (AI) algorithm described in previous chapter. The obtained models were employed to obtain the variation of response variables of interest of fabricated samples using material extrusion process in the form of bar-charts and surface responses as described in subsequent sections. The response variables here to represent and discuss include; the in-plane mechanical properties and flexural response of fabricated samples in response to the variations in the input parameters of *extrusion rate (ER)*, *printing orientation (PO)*, *PVC polymer ratio (PR)* and *concentration of carbon nanofiber in the matrix (CNF)*. The response variables of the fabricated 3D printed samples, including in-plane (along the 1<sup>st</sup> axis) and out-of-plane (along the 3<sup>rd</sup> axis) modulus of elasticity and ultimate strength, and the CCSSP specimens, including the flexural modulus and loading, have been subjected to the optimization algorithms to obtain the set of material extrusion parameters by which the response variables were maximized in an individual and an accumulative approach, separately.

**Table 4.1.** The central composite surface response (CCSR) design of material extrusion parameters in 3D printing of tensile specimens.

| <b>Run</b>       | <b><i>ER</i></b> | <b><i>PO</i></b> | <b><i>PR</i></b> | <b><i>NP</i></b> |
|------------------|------------------|------------------|------------------|------------------|
| 1                | 60               | 70               | 20               | 0                |
| 2                | 20               | 0                | 20               | 0                |
| 3                | 60               | 35               | 10               | 0.05             |
| 4                | 60               | 0                | 0                | 0.1              |
| 5                | 40               | 35               | 10               | 0.05             |
| 6                | 20               | 70               | 20               | 0.1              |
| 7                | 20               | 70               | 20               | 0                |
| 8                | 40               | 70               | 10               | 0.05             |
| 9                | 40               | 35               | 10               | 0.05             |
| 10               | 60               | 70               | 0                | 0                |
| 11               | 20               | 70               | 0                | 0.1              |
| 12               | 20               | 0                | 20               | 0.1              |
| 13               | 60               | 70               | 20               | 0.1              |
| 14               | 40               | 0                | 10               | 0.05             |
| 15               | 60               | 0                | 0                | 0                |
| 16               | 60               | 0                | 20               | 0.1              |
| 17               | 40               | 35               | 10               | 0.1              |
| 18               | 20               | 70               | 0                | 0                |
| 19               | 40               | 35               | 20               | 0.05             |
| 20               | 40               | 35               | 10               | 0                |
| 21               | 40               | 35               | 0                | 0.05             |
| 22               | 20               | 35               | 10               | 0.05             |
| 23               | 20               | 0                | 0                | 0.1              |
| 24               | 60               | 0                | 20               | 0                |
| 25               | 60               | 70               | 0                | 0.1              |
| 26               | 20               | 0                | 0                | 0                |
| 27               | 40               | 0                | 10               | 0.1              |
| <b><u>28</u></b> | 40               | 35               | 20               | 0                |
| <b><u>29</u></b> | 40               | 70               | 0                | 0.05             |
| <b><u>30</u></b> | 60               | 0                | 20               | 0.05             |
| <b><u>31</u></b> | 60               | 35               | 0                | 0.1              |
| <b><u>32</u></b> | 60               | 70               | 10               | 0                |

**Table 4.2.** Results of tensile tests of samples printed along the 1-axis under the FDM parameters of CCSR design.

|           | Modulus of elasticity (MPa) |        |        | Ultimate strength (MPa) |        |        | Poisson's ratio |            |            |
|-----------|-----------------------------|--------|--------|-------------------------|--------|--------|-----------------|------------|------------|
| Set       | $E_1$                       | $E_2$  | $E_3$  | $Su_1$                  | $Su_2$ | $Su_3$ | $\nu_{12}$      | $\nu_{13}$ | $\nu_{23}$ |
| 1         | 2077.1                      | 2342.3 | 2345.2 | 29.5                    | 25.3   | 5      | 0.207           | 0.426      | 0.480      |
| 2         | 2616.8                      | 2237.1 | 2347.7 | 27.65                   | 26.37  | 4.76   | 0.356           | 0.445      | 0.380      |
| 3         | 1942.8                      | 1951.6 | 1643.7 | 27.09                   | 27.37  | 5.08   | 0.451           | 0.422      | 0.424      |
| 4         | 2324.1                      | 2355.4 | 1653   | 30.71                   | 29.95  | 6.09   | 0.478           | 0.527      | 0.534      |
| 5         | 1640.1                      | 1665.6 | 1439.6 | 21.39                   | 22.28  | 4.03   | 0.519           | 0.253      | 0.257      |
| 6         | 2126.1                      | 2090.8 | 1766.6 | 28.12                   | 25.13  | 4.6    | 0.422           | 0.424      | 0.417      |
| 7         | 2313.3                      | 2455.6 | 1425.8 | 26.13                   | 27.94  | 2.7    | 0.205           | 0.440      | 0.467      |
| 8         | 2194.8                      | 1900.1 | 1605.5 | 28.91                   | 24.19  | 3.69   | 0.394           | 0.314      | 0.272      |
| 9         | 1939.8                      | 1934.1 | 1650   | 28.91                   | 25.8   | 3.85   | 0.487           | 0.477      | 0.476      |
| 10        | 2315.8                      | 2336.5 | 2179.9 | 35.37                   | 31.82  | 13.07  | 0.287           | 0.425      | 0.429      |
| 11        | 2289.8                      | 2252.8 | 1629.7 | 30.44                   | 31.15  | 6      | 0.481           | 0.403      | 0.397      |
| 12        | 2302.5                      | 2395.9 | 1500   | 27.65                   | 28.44  | 4.59   | 0.489           | 0.396      | 0.412      |
| 13        | 2049                        | 2057.5 | 1809.5 | 28.67                   | 25.75  | 7.4    | 0.347           | 0.316      | 0.317      |
| 14        | 2252.8                      | 2258.9 | 1356   | 28.52                   | 30.57  | 2.2    | 0.454           | 0.475      | 0.476      |
| 15        | 1946.9                      | 1778.1 | 2294.3 | 27.82                   | 31.54  | 10.91  | 0.377           | 0.326      | 0.298      |
| 16        | 2100                        | 2080   | 1647.5 | 27.11                   | 27.27  | 6.16   | 0.393           | 0.421      | 0.417      |
| 17        | 2001.4                      | 2172.1 | 1693.8 | 28.6                    | 29.54  | 6.54   | 0.406           | 0.451      | 0.490      |
| 18        | 2623.3                      | 2452   | 2603   | 36.17                   | 34.03  | 11.88  | 0.391           | 0.422      | 0.395      |
| 19        | 1981.5                      | 1853.5 | 1556.1 | 27.6                    | 25.44  | 3.62   | 0.419           | 0.471      | 0.441      |
| 20        | 2389.1                      | 2305.1 | 2567.8 | 31.68                   | 31.58  | 7.86   | 0.356           | 0.406      | 0.391      |
| 21        | 1887.1                      | 2053   | 1832.7 | 30.93                   | 30.22  | 7.96   | 0.413           | 0.309      | 0.336      |
| 22        | 2181.9                      | 1858.4 | 1494.7 | 31.13                   | 26.79  | 4.54   | 0.454           | 0.309      | 0.264      |
| 23        | 2240                        | 2163.3 | 1603.8 | 31                      | 31.93  | 6.49   | 0.411           | 0.392      | 0.379      |
| 24        | 1978.5                      | 1976   | 1375   | 21.6                    | 21.74  | 4.79   | 0.304           | 0.491      | 0.490      |
| 25        | 1797.7                      | 1910   | 1560.5 | 27.33                   | 28.79  | 7.67   | 0.486           | 0.343      | 0.365      |
| 26        | 2301                        | 2397.5 | 2436.2 | 33.23                   | 33.8   | 14.8   | 0.375           | 0.395      | 0.411      |
| 27        | 2230.6                      | 2289.9 | 1736.3 | 30.94                   | 30.5   | 5.38   | 0.386           | 0.212      | 0.218      |
| <u>28</u> | 1982.3                      | 1836.4 | 1445.3 | 23.94                   | 22.45  | 3.74   | 0.435           | 0.313      | 0.290      |
| <u>29</u> | 2362                        | 2158.5 | 1869.3 | 31.93                   | 29.8   | 8.4    | 0.394           | 0.428      | 0.391      |
| <u>30</u> | 2268.8                      | 2595.5 | 1484.7 | 28.63                   | 28.67  | 3.56   | 0.457           | 0.408      | 0.467      |
| <u>31</u> | 2012.7                      | 1967   | 1616.6 | 28.78                   | 29.3   | 7.62   | 0.381           | 0.367      | 0.359      |
| <u>32</u> | 2368.1                      | 2552.8 | 2889.8 | 31.11                   | 29.07  | 8.6    | 0.47            | 0.384      | 0.414      |

**Table 4.3.** Results of finite element analyses flexural response of composite core shell structures with HCTC core design of samples printed along the 1-axis under the FDM parameters of CCSR design

| Set | $E_f$ (MPa) | $F_{max}$ (N) | Set       | $E_f$ (MPa) | $F_{max}$ (N) |
|-----|-------------|---------------|-----------|-------------|---------------|
| 1   | 2,308.7     | 5,439.8       | 17        | 2,367.19    | 5,612         |
| 2   | 2,577.17    | 6,070.84      | 18        | 2,815.51    | 6,617.32      |
| 3   | 2,250.01    | 5,331.49      | 19        | 2,260.22    | 5,344.19      |
| 4   | 2,555.54    | 6,066.15      | 20        | 2,638.84    | 6,205.58      |
| 5   | 1,912.23    | 4,512.24      | 21        | 2,195.98    | 5,181.96      |
| 6   | 2,399.07    | 5,660.85      | 22        | 2,294.77    | 5,369.9       |
| 7   | 2,616.43    | 6,105.86      | 23        | 2,460.5     | 5,779.19      |
| 8   | 2,326.92    | 5,436.47      | 24        | 2,308.69    | 5,439.8       |
| 9   | 2,269.25    | 5,398.88      | 25        | 2,102.93    | 4,984.5       |
| 10  | 2,613.84    | 6,137.64      | 26        | 2,602.78    | 6,135.79      |
| 11  | 2,512.76    | 5,921.31      | 27        | 2,430.59    | 5,677.74      |
| 12  | 2,549.06    | 6,010.75      | <u>28</u> | 2,180.3     | 5,119.71      |
| 13  | 2,302.93    | 5,399.23      | <u>29</u> | 2,556.66    | 6,002.53      |
| 14  | 2,518.54    | 5,943.18      | <u>30</u> | 2,589.24    | 6,117.12      |
| 15  | 2,174.17    | 5,111.13      | <u>31</u> | 2,267.86    | 5,331.65      |
| 16  | 2,376.74    | 5,599.96      | <u>32</u> | 2,684.96    | 6,363.91      |

## 4.2. In-plane mechanical response of tensile samples

Here, the in-plane mechanical properties infer to the properties obtained for the tensile test samples fabricated along the 1<sup>st</sup> principal axis, as shown in Fig. 4.1, under the sets of material extrusion parameters determine based on the CCSR design of experiments. The following diagrams and charts have been developed using the regression models, obtained using AI modeling, and coding in MATLAB.

### 4.2.1. In-plane modulus of elasticity, $E_1$

The bar-charts in Figs. 4.2 – 4.7, represent the variation of modulus of elasticity of 3D printed ABS/PVC/CNF blend polymer nanocomposites, containing different fractions of PVS polymer in the matrix, along the 1<sup>st</sup> principal axis ( $E_1$ ) versus the material extrusion parameters. Comparing the results in Figs. 4.2 and 4.3 shows that the addition of PVC in the ABS matrix can be effective in improving the  $E_1$  of fabricated samples, especially at lower extrusion rate (*printing speeds*) and printing orientation (*raster angle*) of 0°. Considering the amorphous

nature of ABS and PVC polymers, increasing the extrusion rate makes no significant difference on the microstructure, but reduces the stiffness of fabricated sample by increasing the cooling rate and inducing tensile residual stresses in the matrix (Fig. 4.2.a). The overlap of induced stresses and quasi-static loading during tensile experiments decreases by changing the raster orientation from cross  $[0/90^\circ]$  to  $[\pm 35^\circ]$ . Changing the raster orientation, resulting in a slight improvement of modulus of elasticity of samples along the 1<sup>st</sup> axis (Fig. 4.3.a).

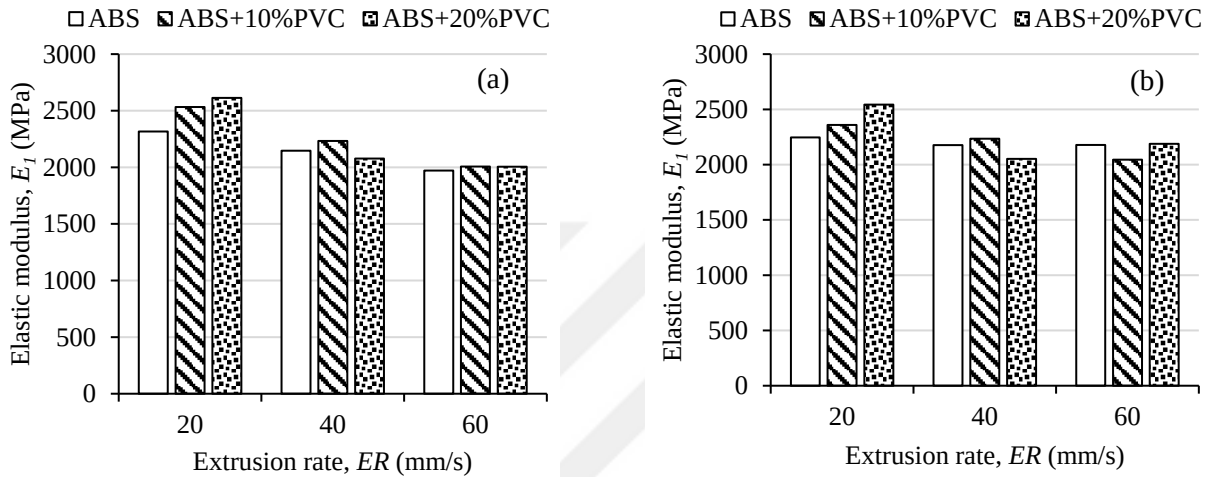


**Figure 4.2.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the extrusion rate at printing orientation of  $0^\circ$ ; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

On the other hand, the addition of carbon nanofiber (CNF) has led to a slight improvement of  $E_1$  for the samples fabricated at raster angle of  $0^\circ$  (Fig. 4.2), while there is no improvement for samples printing at a different reorientation of internal architecture with respect to the principal axis (Fig. 4.3). This behavior could show the dependency of the CNFs in formation of load carrying network and acting as a reinforcing filler to the material extrusion parameters and compatibility of the CNF with the material as the base polymers.

The variations of the modulus of elasticity ( $E_1$ ) with the printing orientation (raster angle) for different composites of ABS/PVC/CNF blend polymer nanocomposites are depicted in Figs. 4.4 and 4.5. At a lower extrusion rate of 20 mm/s, changing the printing orientation from  $[0/90^\circ]$  to  $[\pm 70^\circ]$  does not have a significant impact on the  $E_1$  of the fabricated samples. However, the addition of PVC improves the in-plane stiffness of the 3D printed samples to some extent. Conversely, increasing the extrusion rate to 60 mm/s (Figure 4.5) leads to a greater reduction in the stiffness of samples fabricated at a printing orientation of  $0^\circ$ . This reduction could be attributed to the higher level of residual strains along the loading direction induced by the higher extrusion rate.

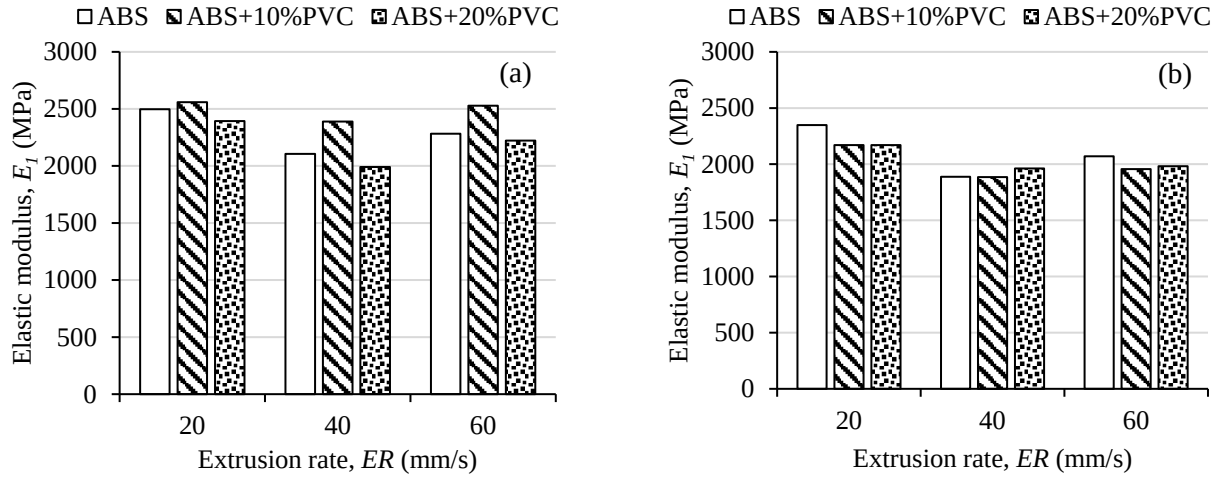


**Figure 4.3.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the extrusion rate at printing orientation of 35°; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

The presence of CNF in the matrix has a lesser effect on the  $E_1$  for samples printed at an extrusion rate of 20 mm/s (Figure 4.4.b). However, it results in a reduction in stiffness at a higher extrusion rate of 60 mm/s (Figure 4.5.b). This phenomenon may be attributed to the enhanced cooling rate facilitated by the presence of CNF. CNFs are known for their excellent heat conductivity, which reduces the impact of the creation of a load carrying network in the matrix due to the presence of CNF nanoadditives. This reduction in the load carrying network can contribute to the observed decrease in stiffness.

In summary, the presence of PVC improves the in-plane stiffness of the 3D printed samples, while the addition of untreated CNF in the matrix can lead to a reduction in stiffness, especially at higher extrusion rates. The cooling rate enhancement associated with CNFs plays a role in reducing the effects of the load carrying network, impacting the stiffness of the fabricated samples.

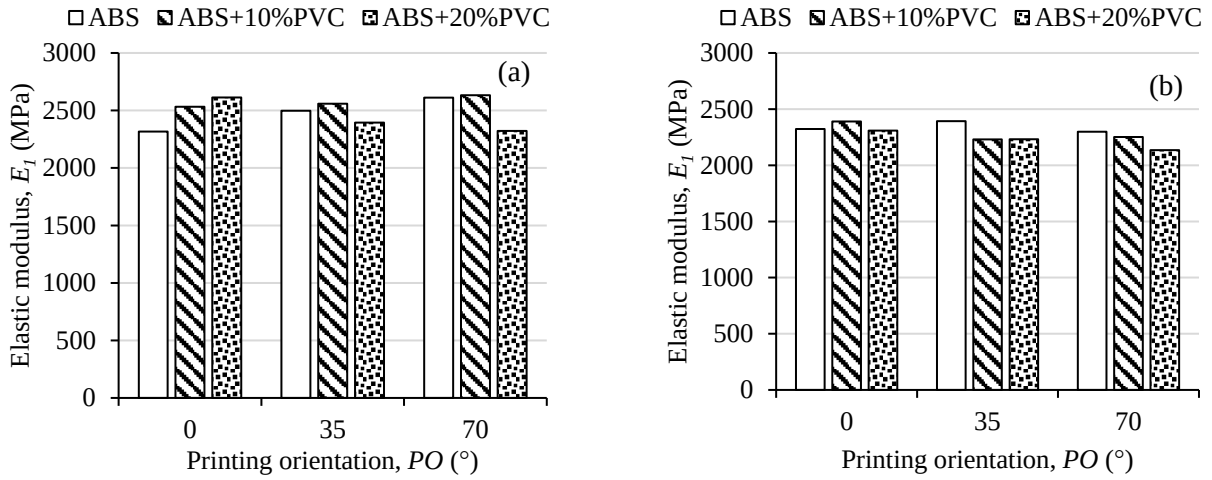


**Figure 4.4.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the printing orientation at extrusion rate of 20 mm/s; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.1\text{wt}\%$ .

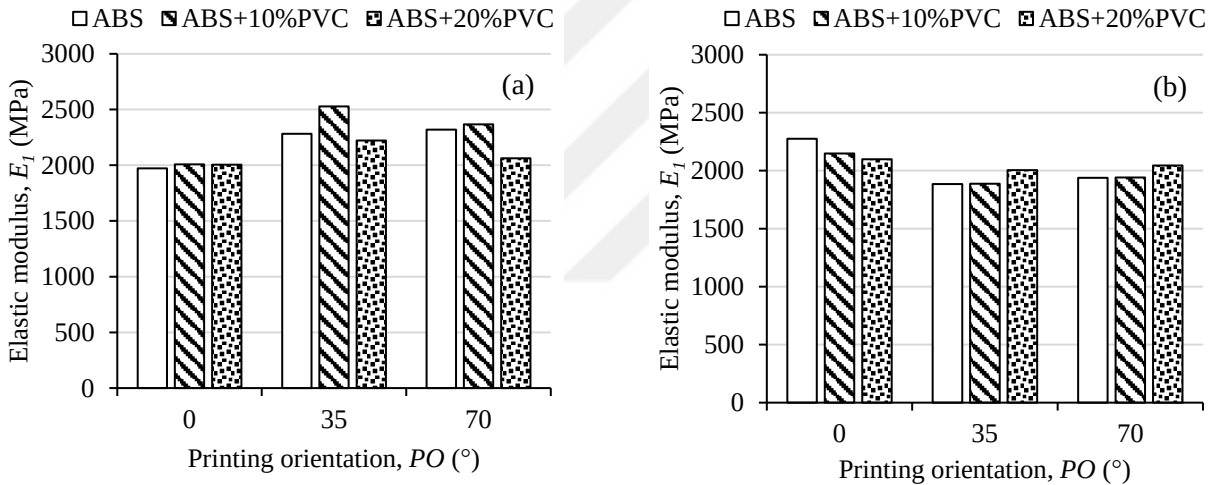


**Figure 4.5.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the printing orientation at extrusion rate of 60 mm/s; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.1\text{wt}\%$ .

The variation of  $E_1$  versus the CNF concentration in the matrix under different material extrusion parameters are shown in Figs. 4.6 and 4.7. Here, the most important observation is that, for the sample printed with raster orientation of  $[0/90^\circ]$ , while the presence of CNF results in negligible difference in the stiffness of the structure at  $ER$  of 20 mm/s (Fig. 4.6.a), there is a slight improvement of  $E_1$  at higher extrusion rate of 60 mm/s. this could be due to the fact that, at higher extrusion rates, the effects of formation of load carrying network of CNFs overcomes its heat transfer effects, rendering in an improvement in the mechanical response of the 3D printing samples. This effect, however, becomes less significant at  $PO$  angle of  $70^\circ$ , as the

polymer orientation and CNF reinforcement network do not overlap with the loading direction, enhancing the effects of cooling rate of CNF on the stiffness of the 3D printed samples (Fig. 4.7).

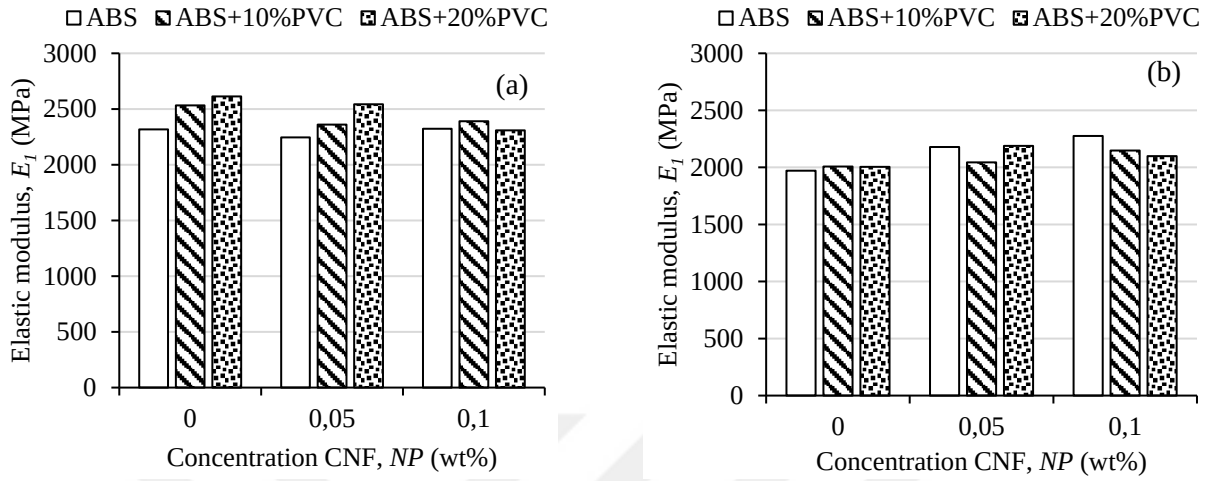


**Figure 4.6.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the concentration of CNF as printing orientation of  $0^\circ$ ; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

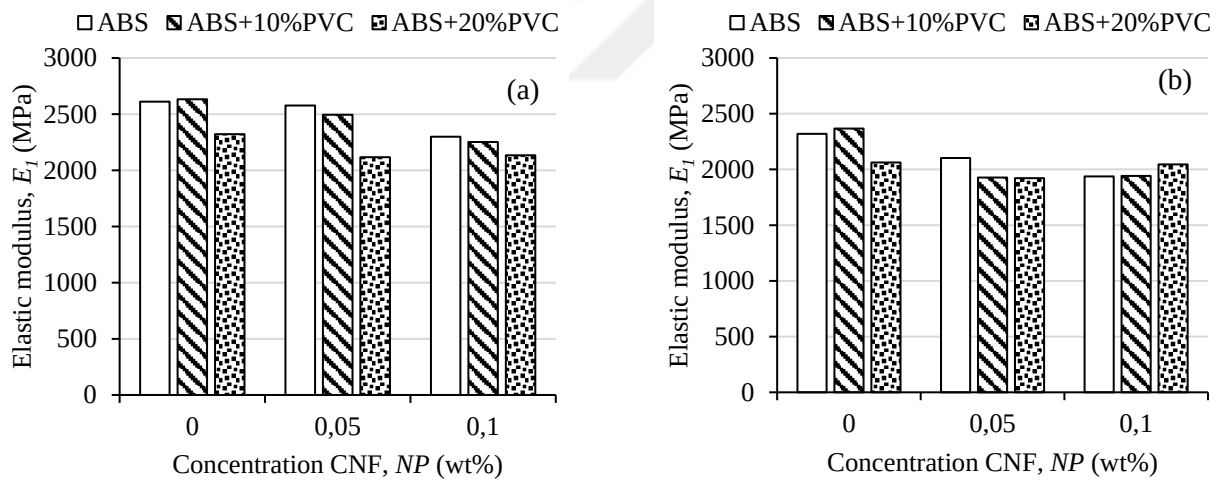


**Figure 4.7.** Modulus of elasticity along the 1<sup>st</sup> principal axis versus the concentration of CNF as printing orientation of  $70^\circ$ ; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

The response surface of  $E_1$  versus the CNF concentration and extrusion rate of 3D printed tensile samples are shown in Fig. 4.8 for various concentrations of PVC in the matrix as printing orientation of  $0^\circ$ . As shown in Fig. 4.8.a, the presence of CNF makes no significant difference on the  $E_1$  of ABS sample fabricated at  $ER$  of 20 mm/s. However, by increase in the extrusion rate up to 60 mm/s, there is a consistent reduction in the in-plane stiffness of the specimens,

probably due to increase in the cooling rate that induces higher residual stresses along the printing orientation. The addition of CNF, on the other hand, can reduce the negative influence of residual stresses through creation of load carrying network on the matrix. By addition of PVC in the matrix, Fig. 4.8.b-c, the effects of CNFs become negligible and the maximum stiffness appears at lower extrusion rate of 20 mm/s.

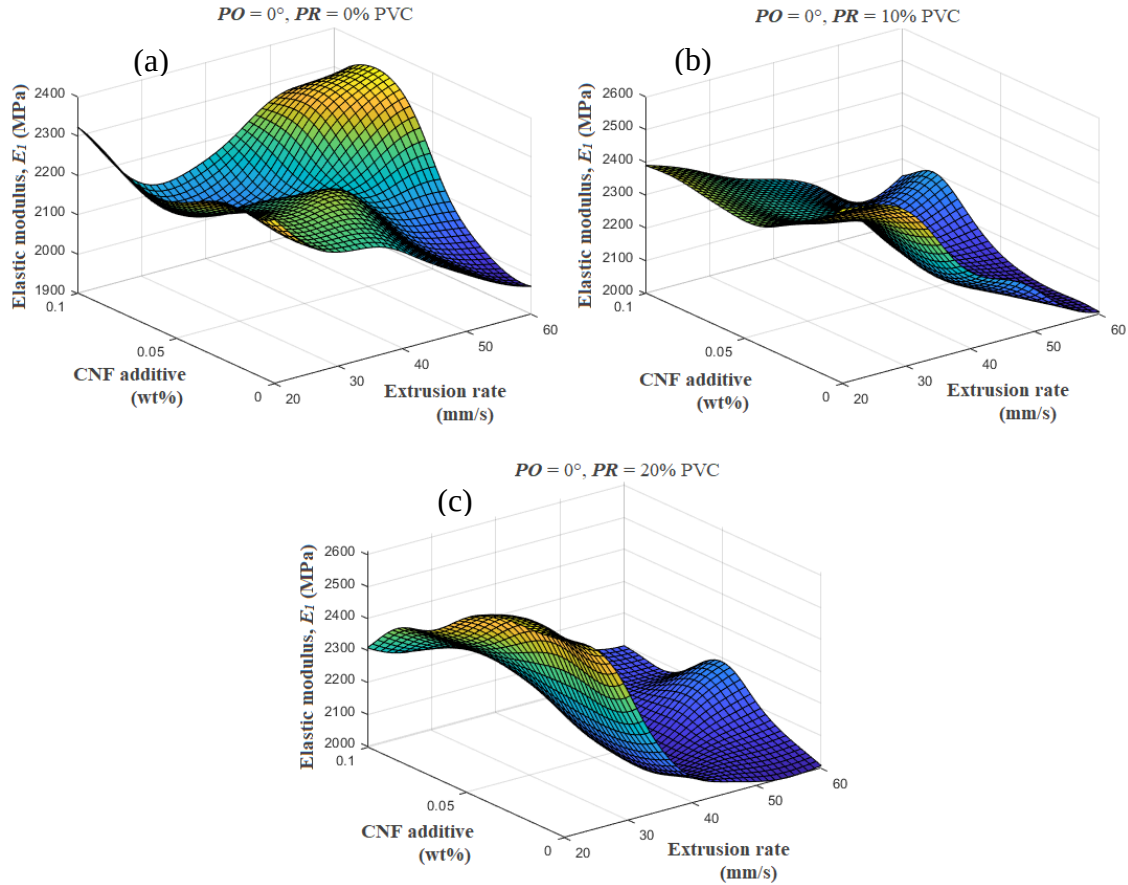


**Figure 4.8.** Response surface of modulus of elasticity along the 1<sup>st</sup> principal axis versus the concentration of CNF and extrusion rate at printing orientation of  $0^\circ$ ; a)  $PR = 0\text{wt}\%$ , b)  $PR = 10\text{wt}\%$  and c)  $PR = 20\text{wt}\%$  of PVC.

The effects of PVC polymers as a blend with the ABS matrix on the in-plane stiffness of the fabricated sampled could be further explored using the response surface graphs of  $E_1$  represented in Figs. 4.9 and 4.10. As shown in Fig. 4.9, regardless of the presence of CNFs in the matrix, the maximum stiffness takes place for the samples containing PVC polymer and fabricated at lower extrusion rate. This reflects the effectiveness of long/flexible PVC molecules elongated at the printing direction in enhancing the stiffness of 3D printed specimens. Additionally, as shown in Fig. 4.10.a, the presence of CNF makes no difference at low ER in

which the enhancement in the heat transfer and therefore, the cooling rate of the sample reduces the effect of reinforcing network created by the mechanical CNFs in the matrix. As the CNFs received no special surface treatments, as surface oxidation by chemical treatments or activation by the plasma treatment, prior to the filament fabrication and material extrusion processes, the possible mechanism in formation of reinforcing network is the mechanical interlocking and Vander Wales forces between the carbon nanofibers and polymer molecules. The effectiveness of this mechanism in enhancing the stiffness of fabricated samples is more significant at higher extrusion rates and for the raster orientation of  $[0/90^\circ]$ .

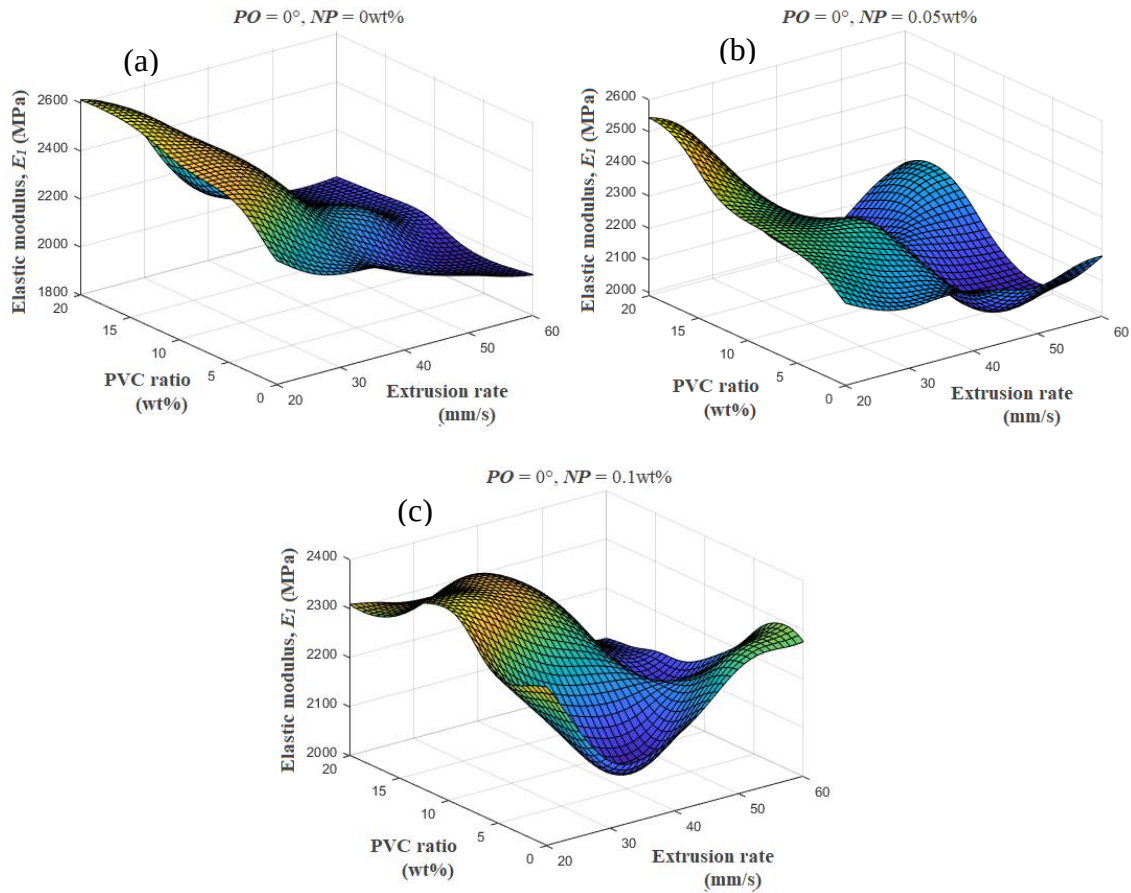


**Figure 4.9.** Response surface of modulus of elasticity along the 1<sup>st</sup> principal axis versus the concentration of PVC polymer and extrusion rate at printing orientation of  $0^\circ$ ; a)  $NP = 0\text{wt}\%$ , b)  $NP = 0.05\text{wt}\%$  and c)  $NP = 0.1\text{wt}\%$  of CNF.

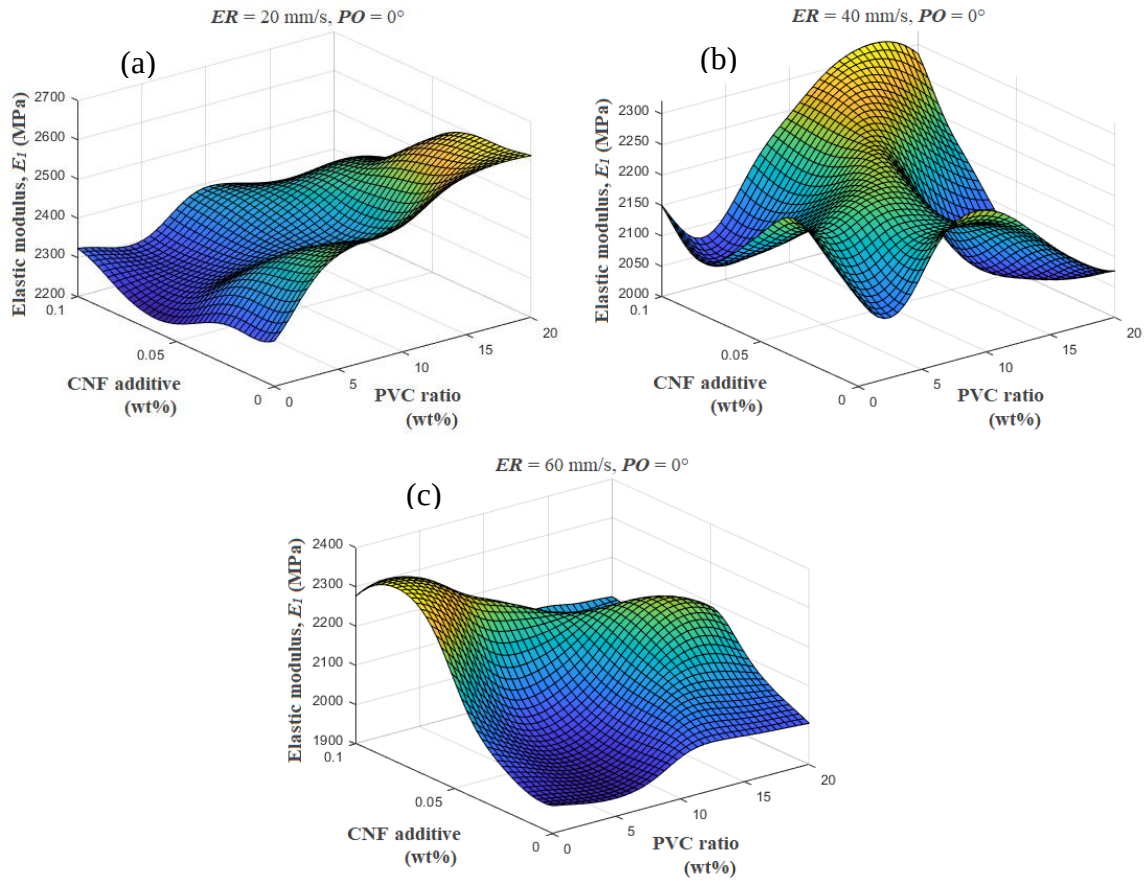


**Figure 4.10.** Response surface of modulus of elasticity along the 1<sup>st</sup> principal axis versus the concentration of carbon nanofiber and PVC polymer at printing orientation of  $0^\circ$ ; a)  $ER = 20$  mm/s, b)  $ER = 40$  mm/s and c)  $ER = 60$  mm/s.

#### 4.2.2. In-plane ultimate strength, $S_{u1}$

The bar-charts in Figs. 4.11 to 4.16 illustrate the variations in ultimate strength ( $S_{u1}$ ) observed in 3D printed ABS/PVC/CNF blend polymer nanocomposites. These composites contain different proportions of PVS polymer and carbon nanofibers in the matrix, and the analysis focuses on the 1<sup>st</sup> principal axis in relation to the material extrusion parameters.

A comparison between the results in Figs 4.11 and 4.12 reveals that the addition of PVC in the ABS matrix does not effectively enhance the  $S_{u1}$  of the fabricated samples, especially at higher extrusion rates (printing speeds) and printing orientations (raster angle) of  $70^\circ$ . Regarding the amorphous nature of ABS and PVC polymers, increasing the extrusion rate has minimal impact on the microstructure but leads to reduced ultimate strength due to increased cooling rates and induced tensile residual stresses in the matrix. The absence of a compatibilizer during the processing of ABS/PVC blend filaments results in only mechanical interlocking as the adhesion

mechanism between ABS and PVC molecules, occurring during the melt blending process. However, as PVC has a lower ultimate strength than ABS, its presence in the blend and weak interfacial adhesion between their molecules cause a reduction in the ultimate strength of ABS/PVC blend polymer specimens. These findings underscore the significance of utilizing compatibilizers, such as methyl methacrylate and butyl acrylate copolymers, which act as intermediaries at the ABS/PVC interface, bridging the gap between the PVC and ABS molecules.

On the other hand, the addition of CNF in the matrix, as depicted in Figs. 4.11b and 4.12.b, significantly counteracts the reduction in  $S_{ul}$  caused by an increase in extrusion rate for samples with a raster orientation of  $[0/90^\circ]$ . However, for samples with a printing orientation of  $70^\circ$ , the presence of CNF in the matrix does not have a notable impact on the ultimate strength of the fabricated samples.

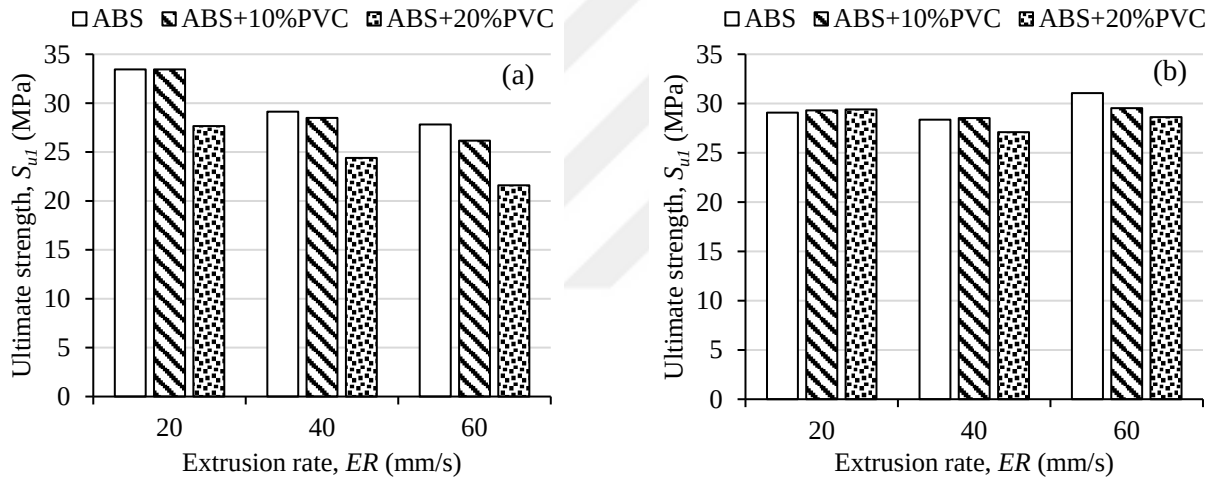


**Figure 4.11.** Ultimate strength along the 1<sup>st</sup> principal axis versus the extrusion rate at printing orientation of  $0^\circ$ ; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

Figures 4.13 and 4.14 present the variations in ultimate strength ( $S_{ul}$ ) of various ABS/PVC/CNF blend polymer nanocomposites with respect to the printing orientation (*raster angle*). A comparison between Figs. 4.13.a and 4.14.a shows that increasing the extrusion rate (ER) to 60 mm/s results in reduced strength of samples fabricated at a raster orientation of  $0^\circ$ . This reduction can be attributed to the higher level of residual strains induced along the loading direction. In contrast, at an extrusion rate of 20 mm/s (Fig. 4.13.a), the raster orientation has negligible effects on the in-plane strength of fabricated samples. However, when the orientation changes from  $[0/90^\circ]$  to  $[\pm 70^\circ]$ , it prevents the reduction in the load-carrying capacity of the specimens by shifting the angle between the tensile sample's loading direction and the orientation of induced residual strain.

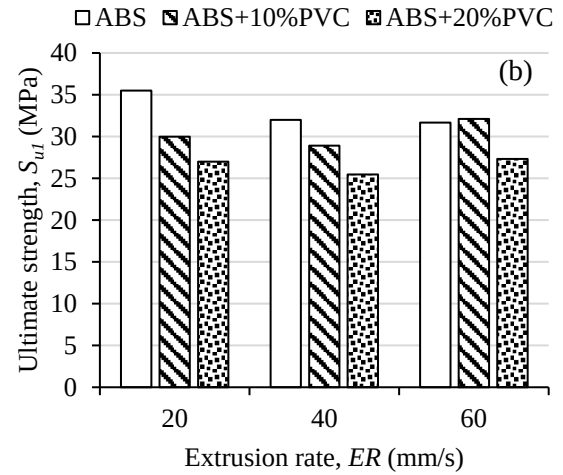
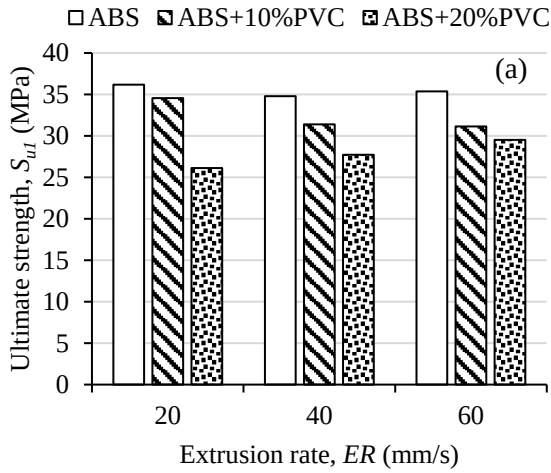


**Figure 4.12.** Ultimate strength along the 1<sup>st</sup> principal axis versus the extrusion rate at printing orientation of 70°; a) NP = 0wt% and b) NP = 0.05wt%.

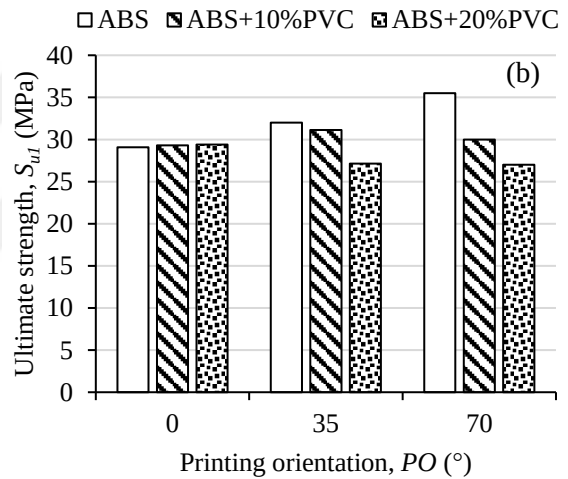
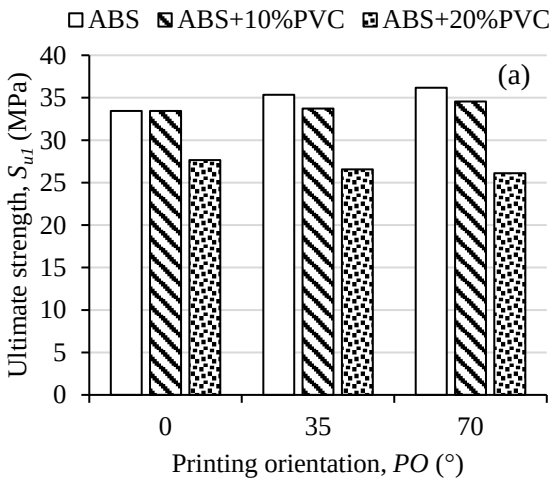


**Figure 4.13.** Ultimate strength along the 1<sup>st</sup> principal axis versus the printing orientation at extrusion rate of 20 mm/s; a) NP = 0wt% and b) NP = 0.05wt%.

The presence of CNF in the matrix has a lesser impact on  $S_{u1}$  at a low extrusion rate of 20 mm/s (Fig. 4.13.b). This might be due to enhanced heat transfer from the sample caused by CNFs in the matrix, leading to increased residual stresses at the printing orientation and reducing the reinforcing effect of the CNF-ABS/PVC network on the strength of specimens. This phenomenon is likely related to the CNFs' excellent heat conductivity, which diminishes the effects of raster orientation on the distribution of residual stresses in the fabricated samples. However, at a higher extrusion rate of 60 mm/s, the reinforcing effect of CNFs in the matrix becomes more significant due to limited time for heat transfer, resulting in an improvement in  $S_{u1}$  of samples with a raster orientation of 0° (see Fig. 4.14). Under the same conditions,

increasing the raster orientation does not significantly affect the ultimate strength of the samples with CNFs in the matrix. This could be attributed to limitations in the reinforcing network of nanofibers, primarily developed by mechanical interlocking between the nanofibers and the ABS/PVC blend polymer, without the presence of functionalized groups on the surface of CNFs before the filament extrusion process.

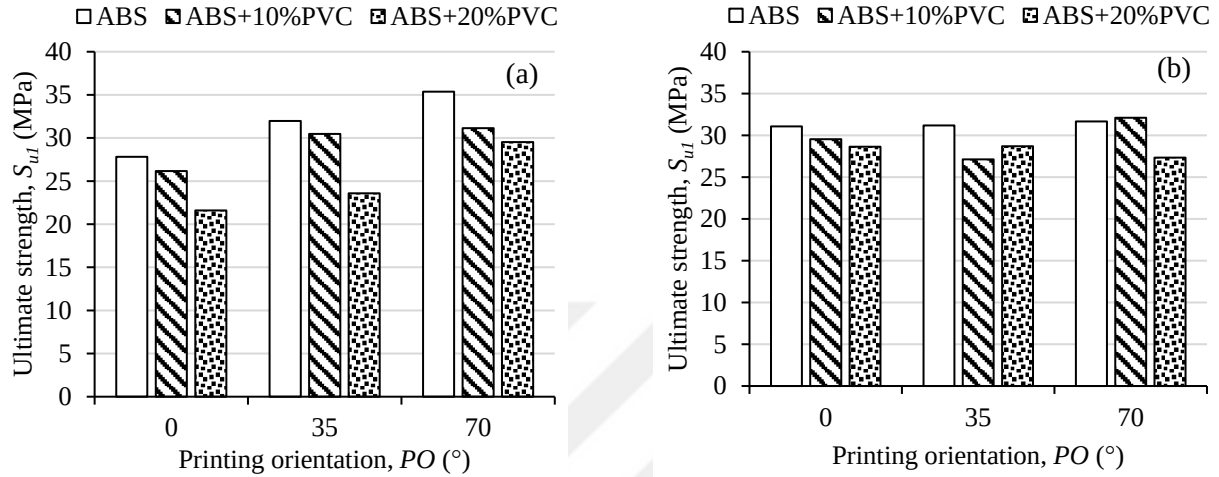


**Figure 4.14.** Ultimate strength along the 1<sup>st</sup> principal axis versus the printing orientation at extrusion rate of 60 mm/s; a) NP = 0wt% and b) NP = 0.05wt%.

The variation of  $S_{u1}$  versus the CNF concentration in the matrix under different material extrusion parameters are shown in Figs. 4.15 and 4.16. Here, the most important observation is that, the addition of CNF in the matrix doesn't appear to be effective in enhancing the ultimate strength of fabricated samples, but rather it results in reduction of the load carrying capacity of the specimens, except for the samples that have been fabricated at higher extrusion rate of 60 mm/s and at raster orientation of 0°. These improvements were also more significant for the samples containing PVC polymer, showing that the untreated CNFs were more compatible with PVC molecules as they create stronger mechanical interlocking with the simpler PVC molecules (Fig. 4.15.b).

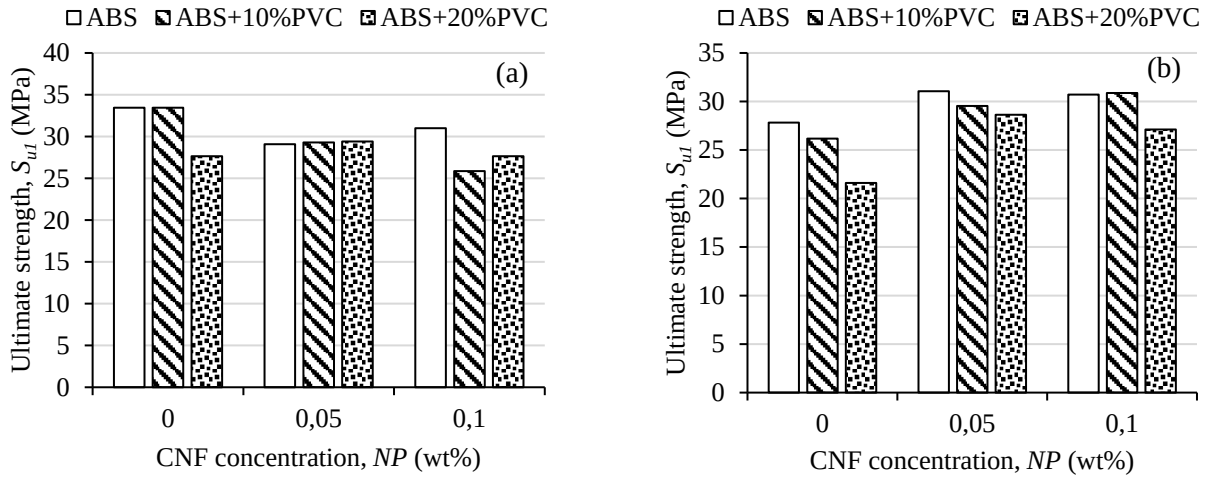


**Figure 4.15.** Ultimate strength along the 1<sup>st</sup> principal axis versus the concentration of CNF at printing orientation of 0°; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

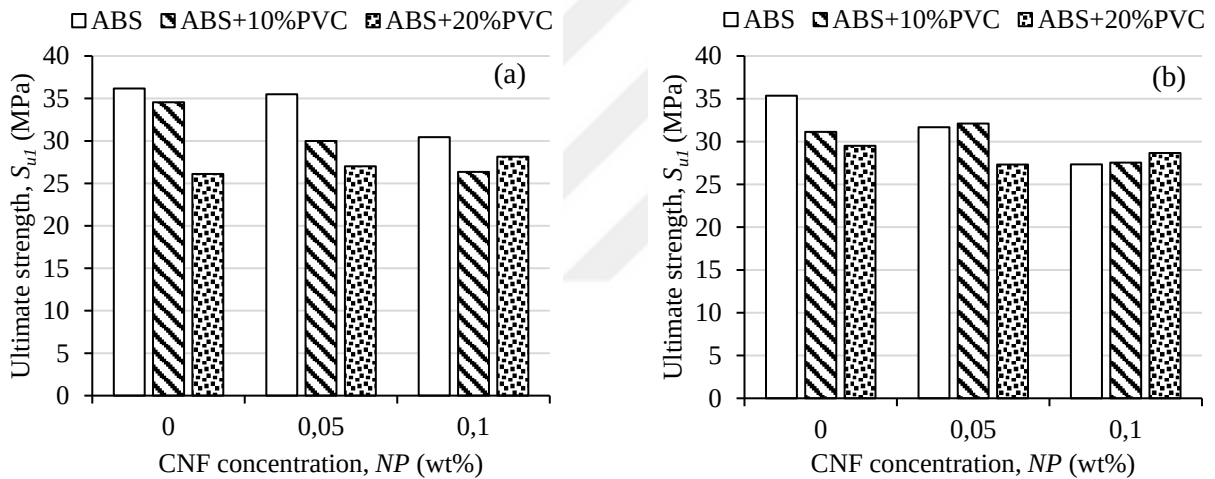


**Figure 4.16.** Ultimate strength along the 1<sup>st</sup> principal axis versus the concentration of CNF at printing orientation of 70°; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

However, the most important observation is that although the addition of untreated CNFs is useful in improving the mechanical characteristics of 3D printed samples to some extent with respect to the printing parameters, they are generally less compatible with PVC (polyvinyl chloride) compared to functionalized CNFs. The surface of untreated CNFs is typically hydrophobic and lacks specific functional groups that can strongly interact with the PVC polymer matrix. As a result, untreated CNFs may have limited interfacial adhesion with the PVC molecules, leading to poor stress transfer and load-bearing capabilities. This results in lower mechanical properties such as tensile strength, modulus, and toughness in the nanocomposite. As a solution to follow in future studies, the CNFs can have various functional groups on their surface as they are typically composed of graphene layers arranged in a

cylindrical structure. To improve the compatibility of CNF nanoparticles with PVC, surface functionalization is often performed. By attaching certain functional groups (such as carboxyl, hydroxyl, or amine groups) to the surface of CNFs, it becomes easier for them to interact with the PVC polymer matrix. These functional groups can also create active sites on the CNF surface that can form covalent bonds with the ABS polymer. Nevertheless, the following steps could also be followed for raising the interfacial bonding of CNFs with the ABS/PVC polymer:

1. Surface activation: The first step is to activate the surface of the CNFs to make it more reactive and capable of forming chemical bonds with the base polymer. This can be achieved by various methods, including chemical oxidation, plasma treatment, or UV/ozone treatment.
2. Introduction of functional groups: After surface activation, functional groups are introduced onto the CNF surface. Common functional groups used for this purpose include carboxylic acids, hydroxyl groups, or amine groups. These functional groups create active sites on the CNF surface that can form covalent bonds with the ABS polymer.
3. Chemical treatment: The CNFs are then treated with specific chemicals that can react with the activated surface and attach the desired functional groups. For example, oxidation with nitric acid or sulfuric acid is commonly used to introduce carboxylic acid groups.
4. Washing and drying: After the chemical treatment, the functionalized CNFs are thoroughly washed to remove any residual chemicals. Then, they are dried to remove moisture and any solvent used during the process.
5. Mixing with polymer: The functionalized CNFs are then mixed with ABS resin during the melt compounding process. The mixture is typically heated to a temperature above the melting point of base polymer, and the functionalized CNFs disperse uniformly within the matrix.

Figure 4.17 illustrates the response surface of ultimate strength ( $S_{ul}$ ) concerning the concentration of CNF and extrusion rate in 3D printed tensile samples with a printing orientation of  $0^\circ$ . In Fig. 4.17.a, a nonlinear relationship is observed between the CNF concentration in the pure ABS matrix and the extrusion rate at a printing orientation of  $0^\circ$ . At a lower extrusion rate of 20 mm/s, the effect of CNF on the load carrying capacity of 3D printed ABS specimens is insignificant, while an increase in the extrusion rate up to 60 mm/s results in higher  $S_{ul}$  values. This improvement is attributed to the formation of a load carrying network through mechanical locking between the polymer molecules and CNFs, which counteracts the

adverse effects of increased cooling rate and induced residual stresses due to higher extrusion rates.

The same trend is observed for samples containing 10 wt% of PVC in the matrix, as shown in Fig. 4.17.b. However, in Fig. 4.17.c, where the PVC ratio in the matrix is further increased to 20 wt%, the influence of CNF on the ultimate strength of 3D printed samples becomes more pronounced. At a lower extrusion rate of 20 mm/s, the  $S_{u1}$  remains relatively constant with increasing CNF concentration in the matrix. Conversely, at a higher extrusion rate of 60 mm/s, the strength of the material increases with higher CNF content in the matrix.

These findings highlight the significance of the CNF concentration, extrusion rate, and PVC ratio in the matrix on the ultimate strength of 3D printed samples. The mechanical locking between CNFs and the polymer matrix plays a crucial role in enhancing the load carrying capacity, mitigating the impact of cooling rates, and induced residual stresses. Moreover, the interplay of these factors offers a valuable opportunity to tailor the mechanical properties of 3D printed materials for specific applications.

The response surface graphs of ultimate strength ( $S_{u1}$ ) represented in Figures 4.18 offer valuable insights into the effects of PVC polymers as a blend with the ABS matrix in response to variations in the extrusion rate ( $ER$ ) on the in-plane strength of fabricated samples containing different fractions of CNF. In Figure 4.18.a, it is evident that the maximum ultimate strength at a printing orientation of  $[0/90^\circ]$  and without the presence of CNF occurs at a lower extrusion rate for samples made of pristine ABS. Upon addition of 0.05 wt% CNF to the polymer (Fig. 4.18.b), the strength of the specimens becomes less dependent on the extrusion rate and the ratio of PVC in the matrix. This phenomenon is likely due to the mechanical interaction between CNF and polymer molecules, creating a load-carrying network that mitigates the effects of induced thermal stresses and enhances the compatibility between ABS and PVC molecules.

Furthermore, with a further increase in the CNF content in the ABS/PVC matrix (Fig. 4.18.c), the maximum  $S_{u1}$  is observed at a higher extrusion rate. This phenomenon may be attributed to limitations imposed on the heat transfer enhancements facilitated by the presence of CNF nanoparticles with high thermal conductivity. Additionally, the prevention of molecular relaxation and the release of mechanical interlocking between the polymer molecules and CNF nanoparticles contribute to the observed behavior.

These findings highlight the complex interplay between CNF concentration, extrusion rate, and the presence of PVC in the matrix, influencing the ultimate strength of 3D printed samples. The mechanical interactions and load carrying network formed by CNF and polymer molecules offer promising avenues for tailoring the mechanical properties of fabricated materials and optimizing their performance.

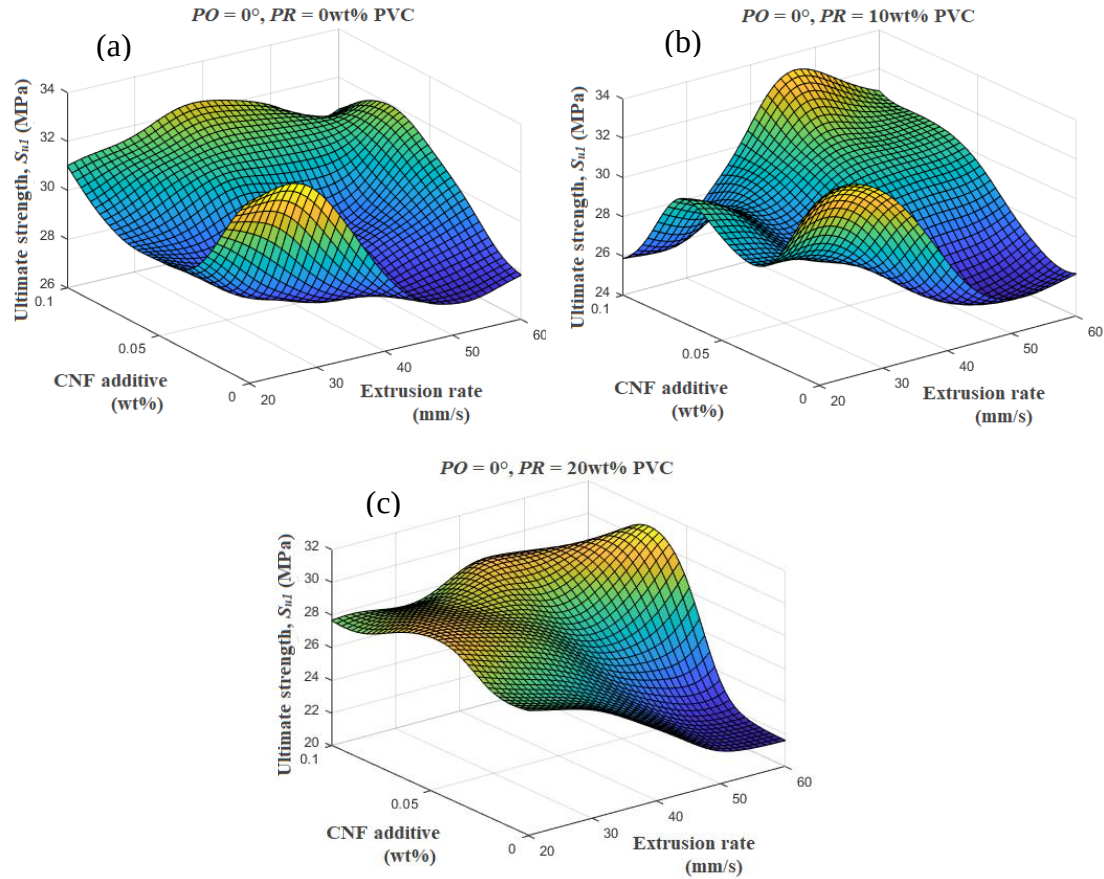


**Figure 4.17.** Response surface of ultimate strength along the 1<sup>st</sup> principal axis versus the concentration of CNF and extrusion rate at printing orientation of  $0^\circ$ ; a)  $PR = 0\text{wt\%}$ , b)  $PR = 10\text{wt\%}$  and c)  $PR = 20\text{wt\%}$  of PVC.

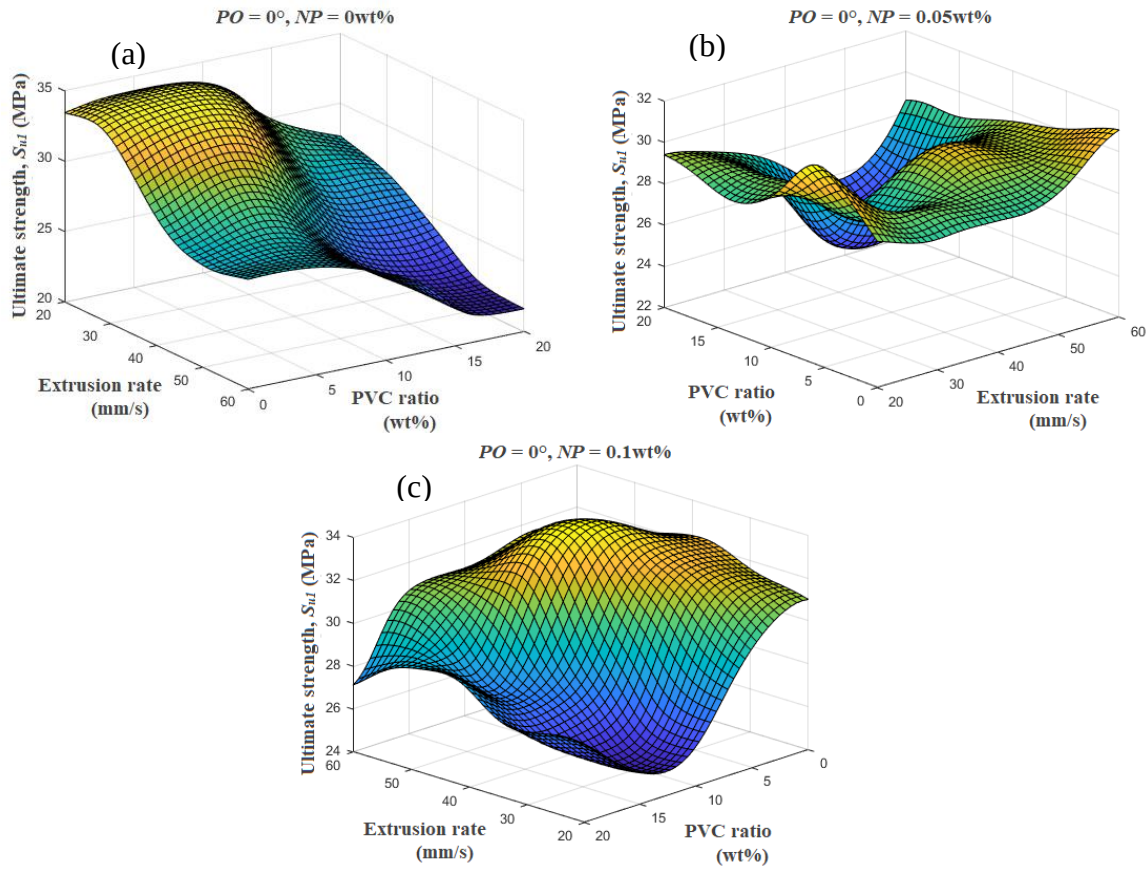


**Figure 4.18.** Response surface of ultimate strength along the 1<sup>st</sup> principal axis versus the concentration of PVC polymer and extrusion rate at printing orientation of 0°; a)  $NP = 0\text{wt}\%$ , b)  $NP = 0.05\text{wt}\%$  and c)  $NP = 0.1\text{wt}\%$  of CNF.

Figure 4.19 provides an additional representation of the results presented in Figure 4.18, allowing us to explore the variations in ultimate strength ( $S_{u1}$ ) concerning the concentration of CNF and the ratio of PVC in the matrix at various extrusion rates ( $ER$ ) during the material extrusion process. In Figure 4.19.a, it is evident that at a lower extrusion rate of 20 mm/s, the presence of CNF and PVC does not lead to any notable improvement in the mechanical strength of the samples. However, as the extrusion rate is increased to 40 mm/s (Fig. 4.19.b), the presence of CNFs becomes crucial in enhancing the  $S_{u1}$  of the fabricated samples. This can be attributed to the increased solidification and cooling rate of the extruded material, which limits the enhancement of heat transfer facilitated by the high thermally conductive CNFs in the matrix and restrains the relaxation of mechanical interlocking between CNFs and the matrix.

With a further increase in the extrusion rate, up to 60 mm/s, the presence of CNF in the matrix, regardless of the composition of the ABS/PVC blend polymer, makes a significant difference in the load carrying capacity and strength of the 3D printed samples. This highlights the

importance of CNFs in reinforcing the matrix and enhancing the overall mechanical performance of the printed materials under higher extrusion rates.

Overall, the response surface shown in Figure 4.19 demonstrates the intricate relationship between CNF concentration, PVC ratio in the matrix, and extrusion rate, which jointly influence the ultimate strength of the 3D printed samples. These insights are valuable for optimizing the printing parameters and material composition to achieve desired mechanical properties in the final products.

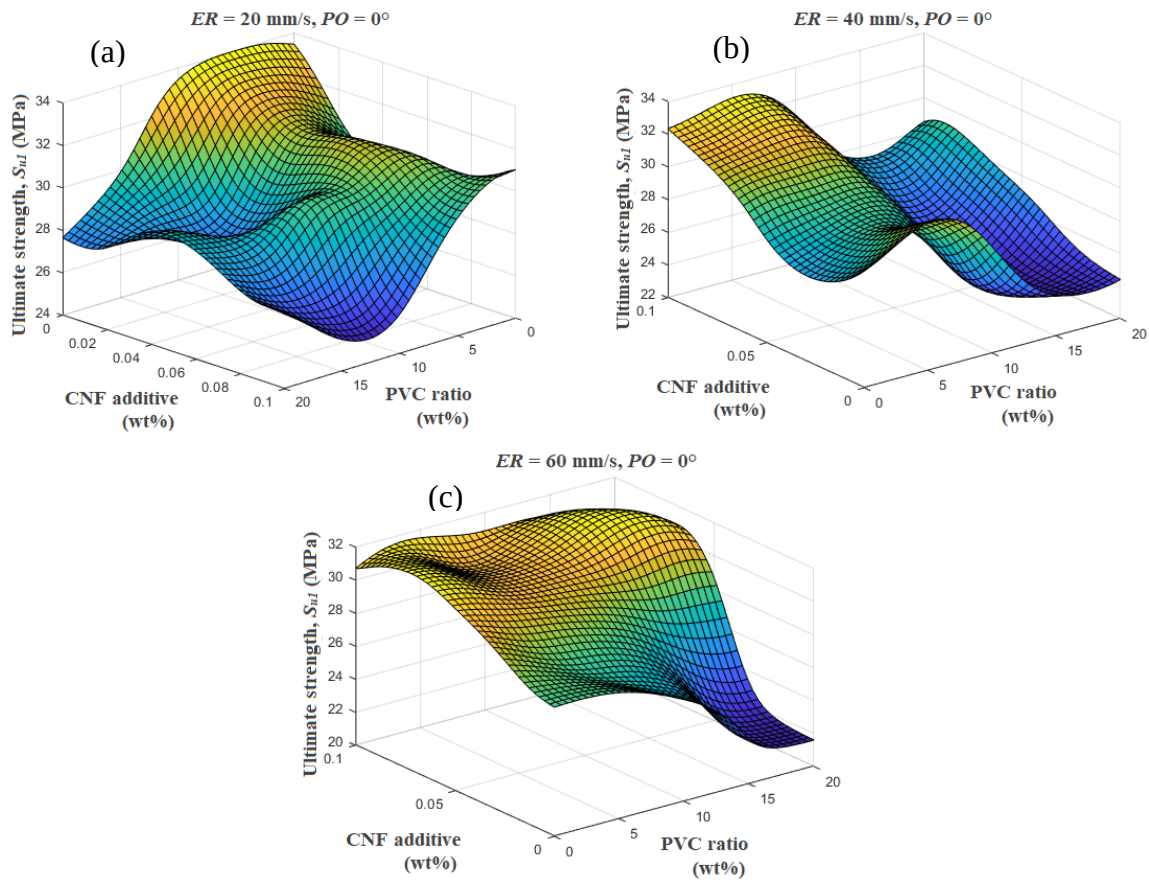


**Figure 4.19.** Response surface of ultimate strength along the 1<sup>st</sup> principal axis versus the concentration of carbon nanofiber and PVC polymer at printing orientation of  $0^\circ$ ; a)  $ER = 20 \text{ mm/s}$ , b)  $ER = 40 \text{ mm/s}$  and c)  $ER = 60 \text{ mm/s}$ .

### 4.3. Flexural response of composite core shell panels

Here, the flexural behavior of composite core shell sandwich panels (CCSSP) obtained from finite element analysis of panels with hybrid circular/triangular corrugated core (HCTC) structure are represented as flexural modulus ( $E_f$ ) and maximum flexural loading ( $F_{max}$ ) for 5 mm displacement of the loading pin. The response variables have been developed based on the hybrid ANN/Bayesian modeling algorithm, in which the input variable included the set of parameters determined by central composite surface response (CCSR) design of experiments in fabrication of tensile test sample. The results of tensile tests of samples fabricated along 3 main axes under the parameters determined by CCSR method have been introduced as engineering constant of HCTC core structure in analyses. A flowchart of this process is represented in Fig. 4.20. The following diagrams and charts have been developed using the regression models, obtained using AI modeling, and coding in MATLAB.

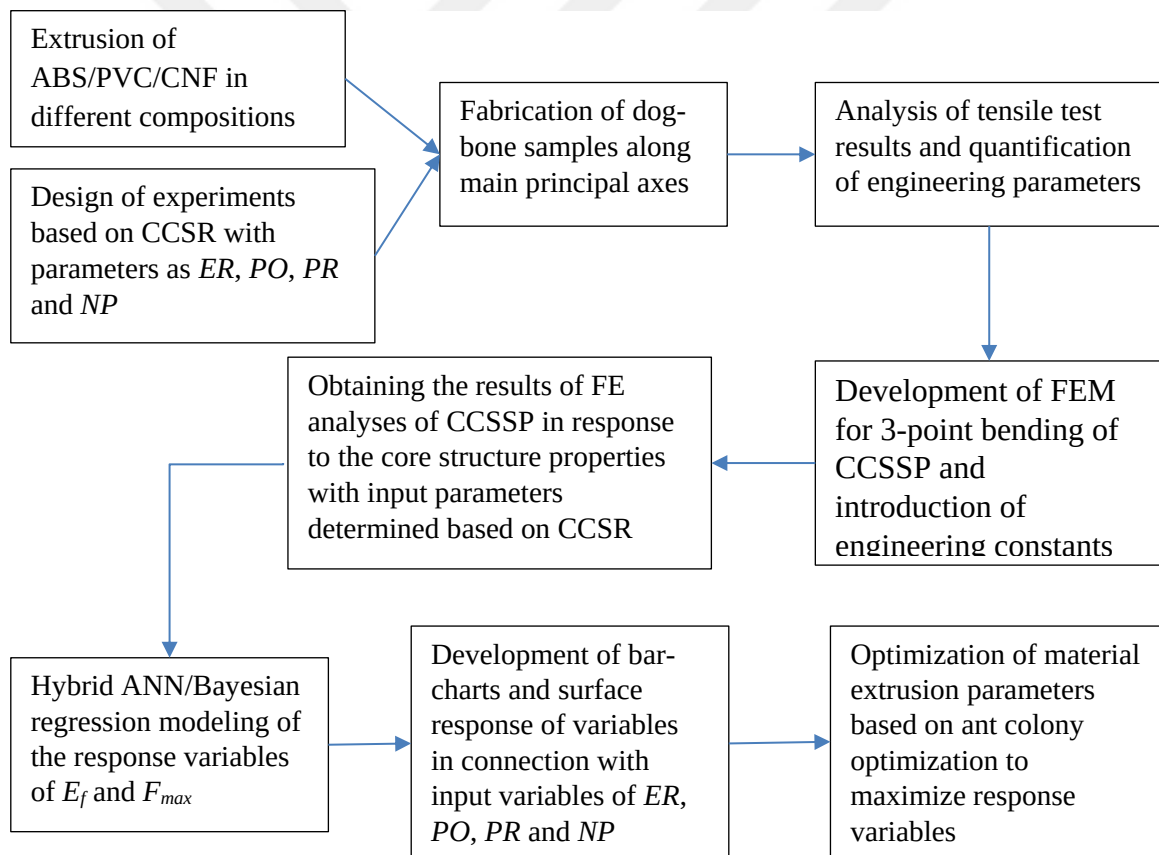


**Figure 4.20.** Flowchart representing the steps of analysis and optimization of flexural response of composite core shell sandwich panels.

#### 4.3.1. Flexural modulus, $E_f$

The variations of flexural modulus ( $E_f$ ) in composite core shell sandwich panels (CCSSP) with a 3D printed hybrid circular/triangular corrugated core (HCTC) structure are represented in bar-charts in Figures 4.21 to 4.26, highlighting the influence of material extrusion parameters. A comparison between Figs. 4.21 and 4.22 reveals that the addition of PVC in the ABS matrix can effectively improve the  $E_f$  of CCSSPs under specific fabrication parameters of the core structure, particularly when using a  $[0/90^\circ]$  raster orientation for 3D printing the core. In this configuration, the alignment of PVC polymer chains along the direction of bending stresses applied in 3-point bending loadings contributes to enhancement of  $E_f$  (Fig. 4.21). However, at higher printing orientations (PO) of  $[\pm 35^\circ]$ , the effects of PVC molecule alignment along the raster orientation become less effective in improving the  $E_f$  of CCSSPs as interfacial bonding between ABS and PVC molecules becomes more significant. Without a compatibilizer between ABS and PVC, the only bonding mechanism between them is mechanical interlocking.

With the addition of extrusion rate, a consistent reduction in  $E_f$  is observed for all core structure compositions, except for the one containing 0.05 wt% CNF and fabricated at a PO of  $0^\circ$  (Figure 4.21.b). Increasing the extrusion rate affects the microstructure minimally but reduces the stiffness of the fabricated samples due to increased cooling rates and induced tensile residual stresses in the matrix. Changing the raster orientation from  $[0/90^\circ]$  to  $[\pm 35^\circ]$  results in a slight improvement in the flexural stiffness of CCSSPs, as the overlap of induced stresses and quasi-static loading during 3-point bending experiments decreases (compare Figs 4.21.a and 4.22.a).

The addition of carbon nanofiber (CNF) leads to a slight improvement in  $E_f$  for core structures fabricated at a raster angle of  $0^\circ$  and higher extrusion rates of 60 mm/s (Fig. 4.21.b), while no improvement is observed for samples printed at higher orientations of the internal architecture with respect to the principal axis (Fig. 4.22.b). Since no surface treatment was applied to the CNFs, this behavior indicates that at higher extrusion rates, the enhancement of cooling rate by incorporating CNFs in the matrix becomes less significant compared to the mechanical interlocking between the polymer molecules and the CNFs. The load carrying network created by the mechanical interlocking becomes more effective in improving the flexural stiffness of CCSSP as relaxation becomes less likely at higher cooling rates. At higher raster orientations, where the effects of residual stresses are less significant due to their angle with the main bending stress orientations, the influence of CNFs on the flexural stiffness of the core shell structures becomes less pronounced.

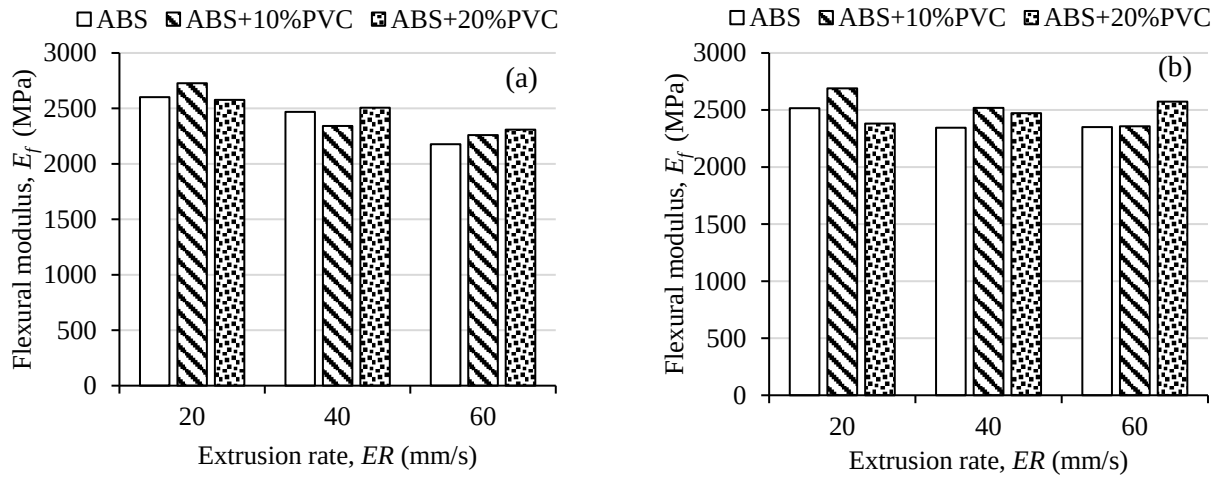


**Figure 4.21.** Flexural modulus of composite core shell sandwich panels versus the extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

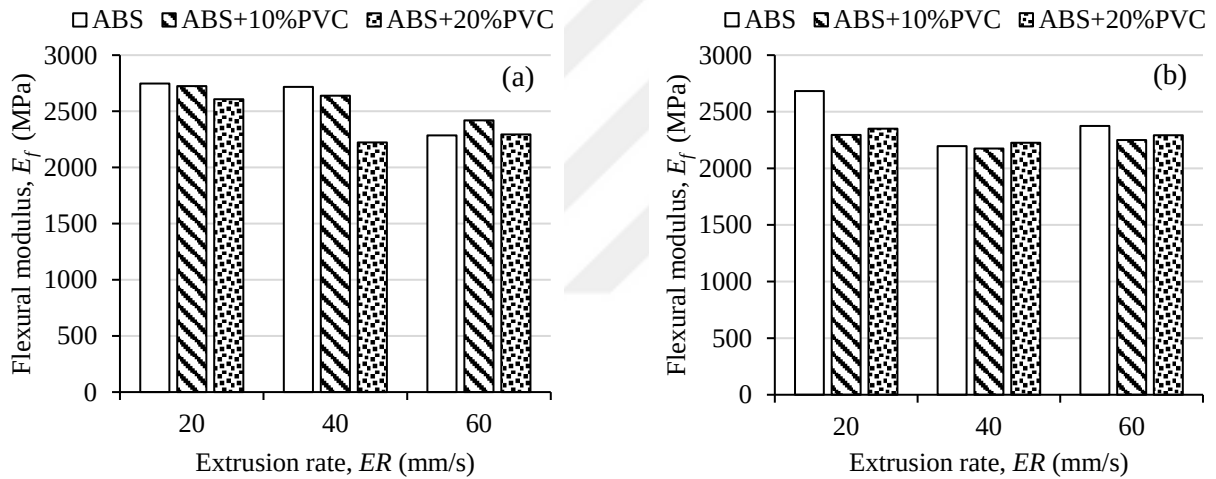


**Figure 4.22.** Flexural modulus of composite core shell sandwich panels versus the extrusion rate at printing orientation of  $35^\circ$  of core structure; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

The variations of the flexural modulus ( $E_f$ ) with the printing orientation (raster angle) for different composites of ABS/PVC/CNF blend polymer nanocomposites are shown in Figs. 4.23 and 4.24. At a lower extrusion rate of 20 mm/s, changing the printing orientation from  $[0/90^\circ]$  to  $[\pm 70^\circ]$  does not significantly impact the  $E_f$  of the CCSSPs. However, the addition of PVC enhances the flexural stiffness of core shell structures of 3D printed cores to some extent. Conversely, increasing the extrusion rate to 60 mm/s (Fig. 4.24) leads to a greater reduction in flexural stiffness of CCSSPs with core structures fabricated at lower printing orientations of  $[0/90^\circ]$  and  $[\pm 35^\circ]$ . This reduction in stiffness can be attributed to the higher level of residual strains oriented along the loading direction induced by the higher extrusion rate.

The presence of CNF in the matrix has a lesser effect on the  $E_f$  for CCSSPs with core structures printed at an extrusion rate of 20 mm/s (Fig. 4.23.b). However, it results in a reduction in stiffness at a higher extrusion rate of 60 mm/s (Fig. 4.24.b). This phenomenon can be associated with the enhanced cooling rate facilitated by the presence of CNF. The carbon nanofibers exhibit excellent heat conductivity, which reduces the impact of the load carrying network created through mechanical interlocking between the CNF and the matrix. This reduction in the load carrying network contributes to the observed decrease in stiffness.

In summary, the addition of PVC improves the flexural stiffness of CCSSPs with core structures fabricated using the material extrusion process. However, the presence of CNF in the matrix can lead to a reduction in stiffness, particularly at higher extrusion rates. The enhanced cooling rate associated with CNFs plays a role in mitigating the effects of the load carrying network, influencing the flexural stiffness of the fabricated samples.

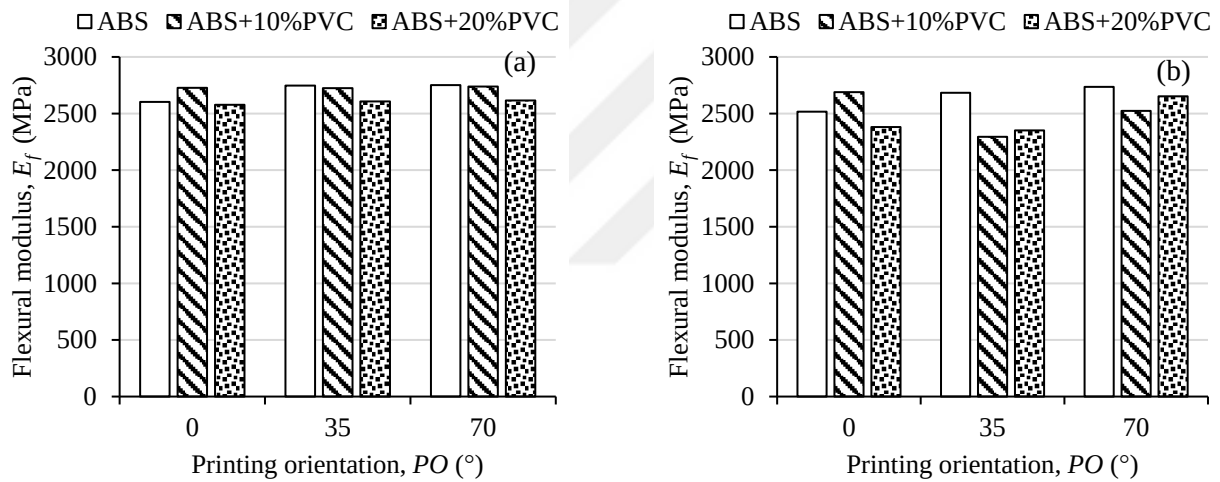


**Figure 4.23.** Flexural modulus of composite core shell sandwich panels versus the printing orientation at extrusion rate of 20 mm/s of core structure; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

The variations of the flexural modulus ( $E_f$ ) of CCSSPs with the concentration of CNF in the matrix under different material extrusion parameters are presented in Figs. 4.25 and 4.26. The key observation is that for the sample printed with a raster orientation of  $[0/90^\circ]$ , the presence of CNF results in minimal changes in the flexural stiffness of the CCSSP structure at an extrusion rate ( $ER$ ) of 20 mm/s (Fig. 4.25.a). However, there is a slight improvement in  $E_f$  at a higher extrusion rate of 60 mm/s. This improvement can be attributed to the formation of a load carrying network of CNFs, which outweighs their heat transfer effects and leads to an enhancement in the mechanical response of the 3D printed cores.

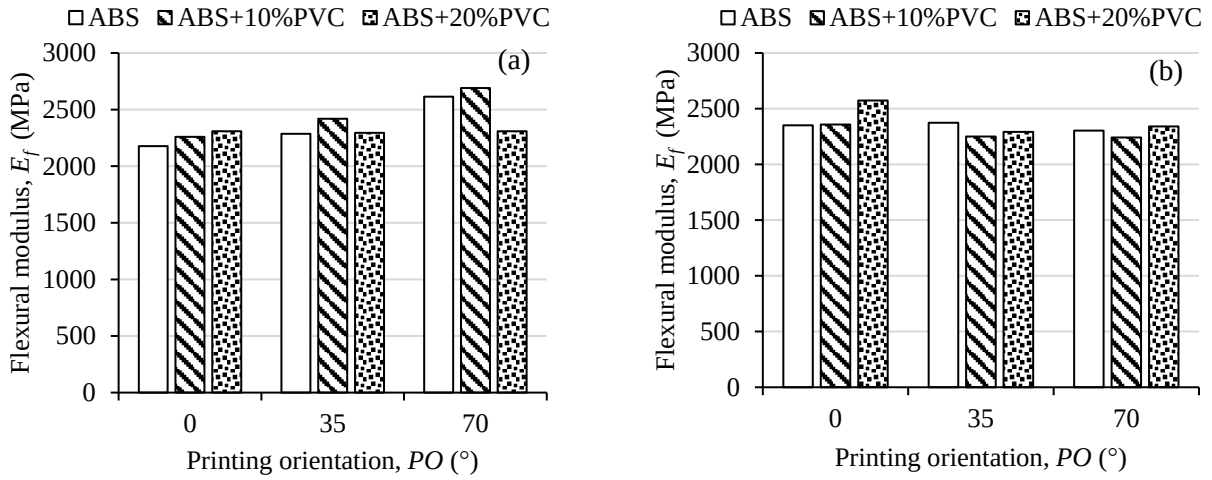


**Figure 4.24.** Flexural modulus of composite core shell sandwich panels versus the printing orientation at extrusion rate of 60 mm/s of core structure; a)  $NP = 0\text{wt}\%$  and b)  $NP = 0.05\text{wt}\%$ .

On the other hand, at a printing orientation ( $PO$ ) angle of  $70^\circ$ , where the polymer orientation and CNF reinforcement network do not align with the loading direction, the impact of CNF cooling rate becomes less significant. This enhances the effects of the CNF's cooling rate on the stiffness of the 3D printed samples and results in a reduction of the flexural stiffness of the core shell structure (Fig. 4.26). The influence of higher cooling rates and induced residual stresses on the flexural stiffness of 3D printed core structures, and consequently on the flexural modulus of CCSSPs, becomes more pronounced at higher extrusion rates of 60 mm/s (Fig. 4.26.b).

These findings suggest that the concentration of CNF, extrusion rate, and printing orientation all play significant roles in the flexural modulus of CCSSPs. The presence of CNF can lead to improvements in flexural stiffness, especially at higher extrusion rates, where the load carrying network dominates. However, the effects of CNF cooling rate and residual stresses become more influential at certain printing orientations, resulting in reduced flexural stiffness of the core shell structure. It highlights the importance of optimizing these parameters to achieve the desired mechanical properties in 3D printed CCSSPs.

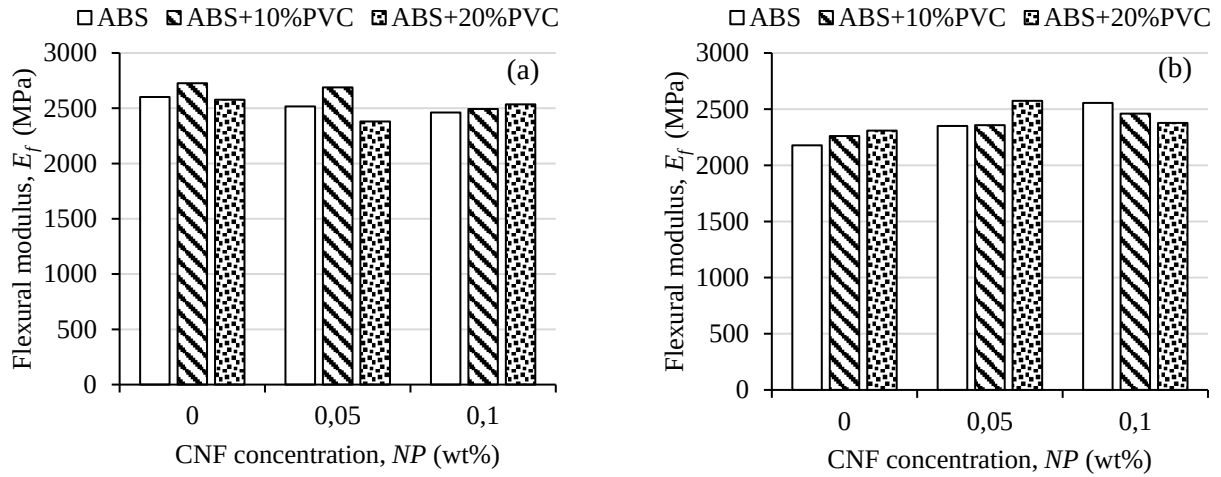


**Figure 4.25.** Flexural modulus of composite core shell sandwich panels versus the concentration of CNF at printing orientation of  $0^\circ$  of core structure; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

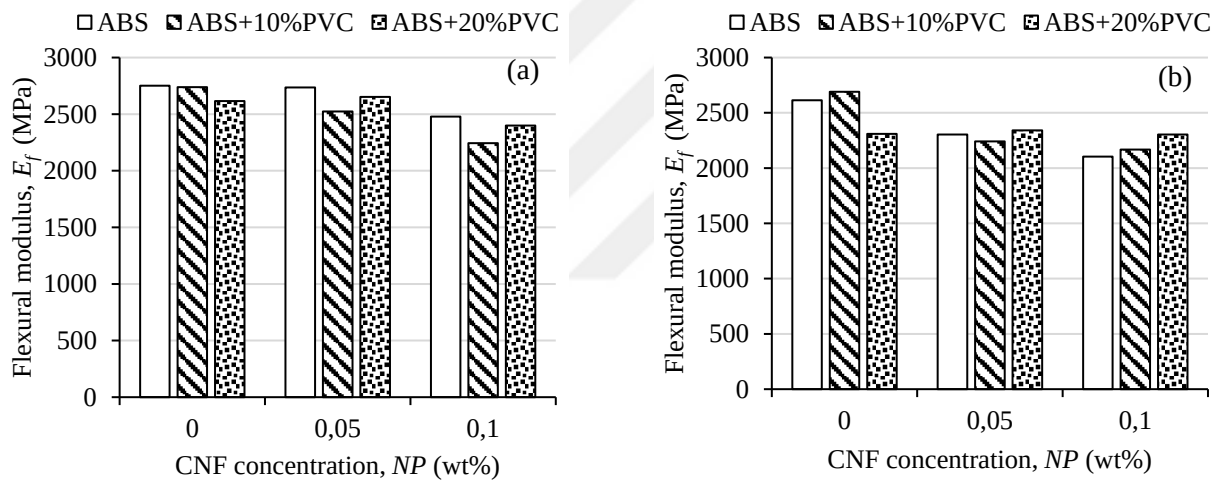


**Figure 4.26.** Flexural modulus of composite core shell sandwich panels versus the concentration of CNF at printing orientation of  $70^\circ$  of core structure; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

The response surface analysis of the flexural modulus ( $E_f$ ) of CCSSPs, in relation to the CNF concentration and extrusion rate during the fabrication of 3D printed core structures, is presented in Fig. 4.27. These structures were printed with a  $0^\circ$  orientation and different concentrations of PVC in the matrix. In Fig. 4.27.a, the presence of CNF does not have a significant impact on the flexural modulus of ABS samples fabricated at an extrusion rate of 20 mm/s. However, as the extrusion rate increases to 60 mm/s, the inclusion of CNF in the matrix enhances the flexural stiffness of CCSSPs. This enhancement can be attributed to the mechanical interlocking between the CNFs and the matrix molecules, as well as a reduction in relaxation due to the higher extrusion rate.

Furthermore, the addition of PVC to the ABS matrix reduces the influence of the extrusion rate on the flexural stiffness of the core shell structure when CNFs are present in the matrix (Fig. 4.27.b and c). Moreover, CNFs have a positive impact on the flexural modulus of CCSSPs, particularly when the matrix contains 20% PVC (Fig. 4.27.c). This suggests a stronger mechanical bonding between the untreated CNFs and PVC, which has a simpler molecular structure compared to ABS.

These findings highlight the combined effects of CNF concentration, extrusion rate, and PVC addition on the flexural modulus of CCSSPs. The presence of CNFs enhances the flexural stiffness, especially at higher extrusion rates, due to improved mechanical interlocking and reduced relaxation. Additionally, the incorporation of PVC in the matrix further enhances the mechanical bonding between CNFs and the matrix, resulting in an improved flexural modulus in CCSSPs.

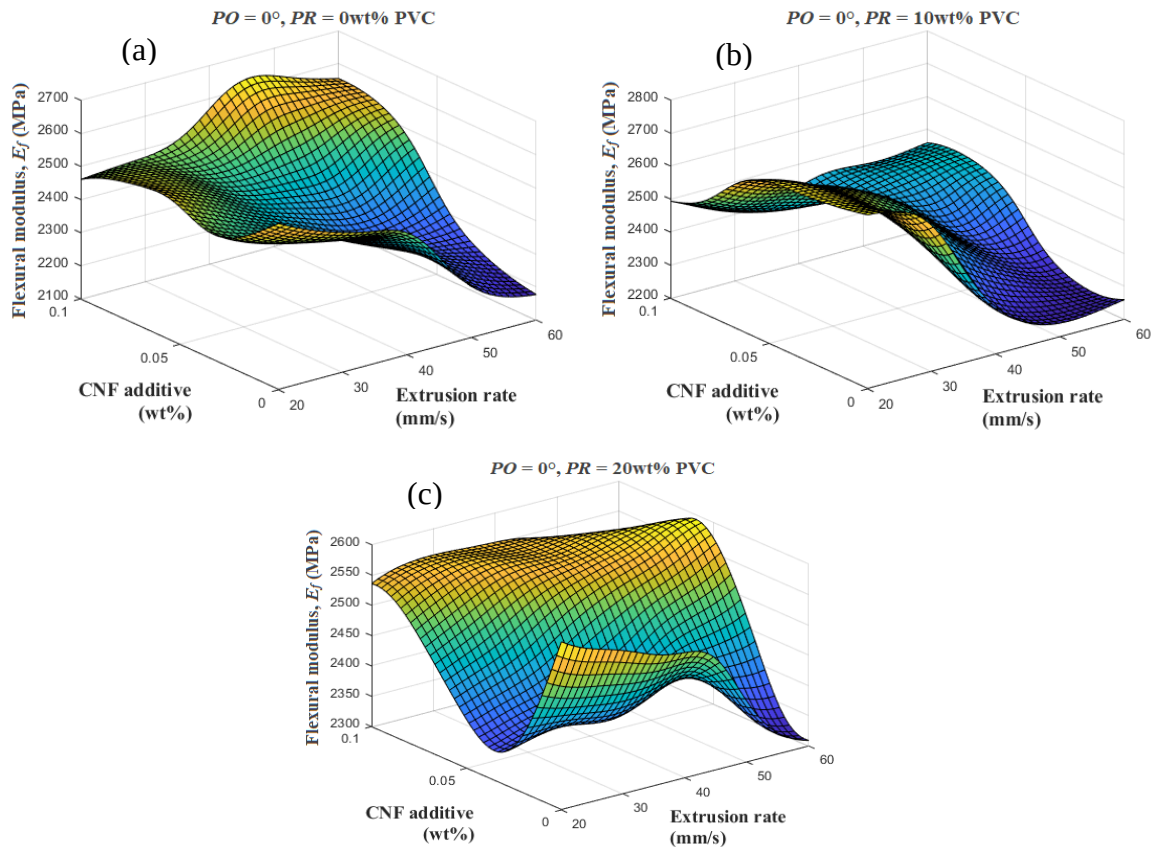


**Figure 4.27.** Response surface of flexural modulus of composite core shell sandwich panels versus the concentration of CNF and extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $PR = 0\text{wt\%}$ , b)  $PR = 10\text{wt\%}$  and c)  $PR = 20\text{wt\%}$  of PVC.

The effects of PVC polymers blended with the ABS matrix on the flexural stiffness of the fabricated core shell structures can be further investigated using the response surface graphs of the flexural modulus ( $E_f$ ) presented in Figs. 4.28 and 4.29. In Fig. 4.28.a, it is observed that in the absence of CNFs in the matrix, the samples containing PVC exhibit maximum stiffness when fabricated at lower extrusion rates. This behavior is also reflected in the response surface depicted in Fig. 4.29.a, highlighting the effectiveness of elongated long/flexible PVC molecules in enhancing the stiffness of 3D printed core structures. Since the CNFs were not subjected to any special surface treatments, such as chemical oxidation or plasma activation, prior to filament fabrication and material extrusion processes, the primary mechanism for the formation of a reinforcing network involves mechanical interlocking and van der Waals forces between the carbon nanofibers and polymer molecules. This mechanism's effectiveness in enhancing the stiffness of the fabricated samples becomes more significant at higher extrusion rates and for the raster orientation of  $[0/90^\circ]$ .

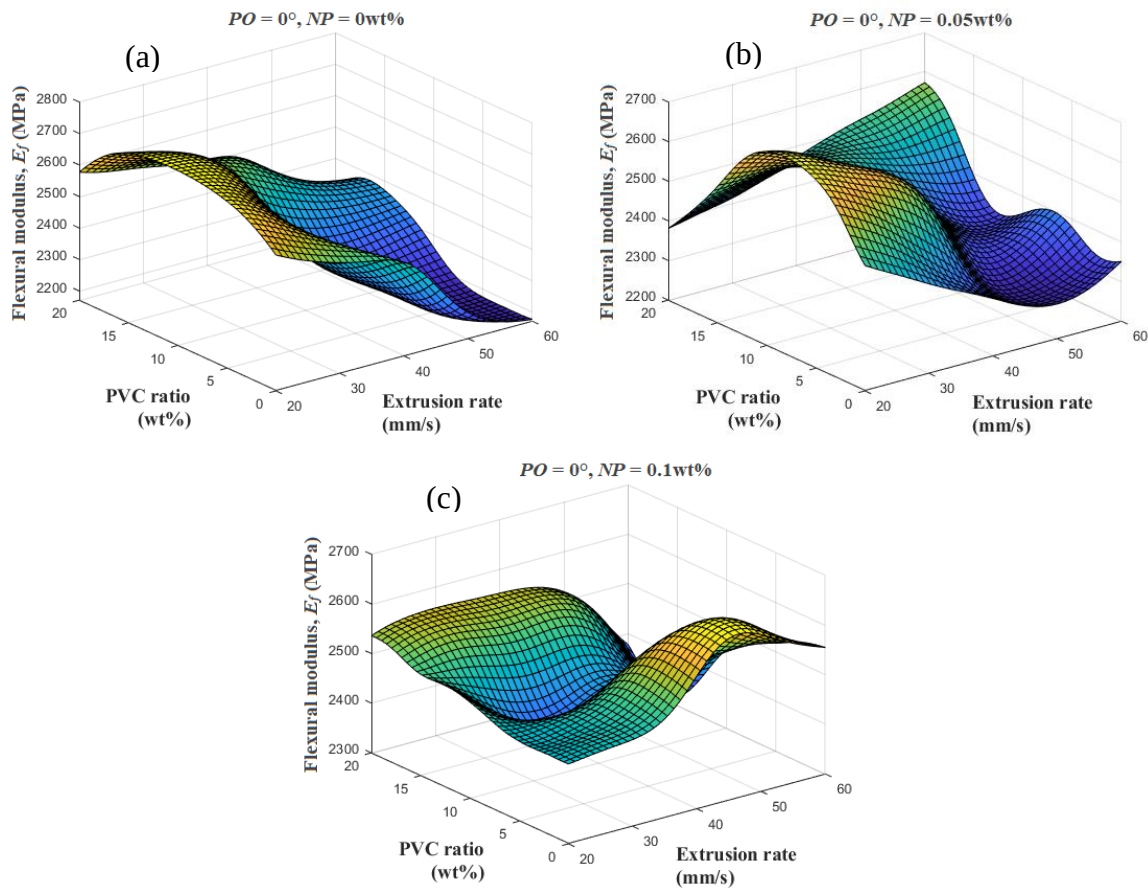


**Figure 4.28.** Response surface of flexural modulus of composite core shell sandwich panels versus the concentration of PVC polymer and extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $NP = 0\text{wt}\%$ , b)  $NP = 0.05\text{wt}\%$  and c)  $NP = 0.1\text{wt}\%$  of CNF.

With the addition of CNFs at a concentration of 0.05wt%, as shown in Fig. 4.28.b, the presence of PVC in the ABS matrix leads to an improvement in  $E_f$ , even at high extrusion rates of 60 mm/s. This phenomenon suggests a better mechanical interlocking between the CNFs and PVC molecules, as well as a reduction in the relaxation rate of the mechanical bonding created between the CNFs and the matrix due to the higher cooling rate. However, as the CNF concentration in the matrix increases further, the positive impact of PVC on  $E_f$  is observed only at low extrusion rates (Fig. 4.28.c). This could be attributed to the ability of the cooling rate of CNFs to overcome the effects of the load carrying network created by the mechanical interlocking between the polymer molecules and the carbon nanofibers. The surface responses shown in Figs. 4.29.b and 4.29.c provide a better representation of the interaction between CNF and PVC at higher extrusion rates of 40 and 60 mm/s, respectively.

Overall, the results highlight the complex interplay between the CNF concentration, PVC addition, and extrusion rate on the flexural stiffness of core shell structures. The presence of PVC enhances the stiffness, especially at lower extrusion rates, while the incorporation of CNFs further strengthens the mechanical interlocking and bonding, leading to improved flexural modulus. These findings emphasize the potential for tailoring the mechanical properties of 3D printed core structures by optimizing the CNF concentration, PVC content, and extrusion parameters.

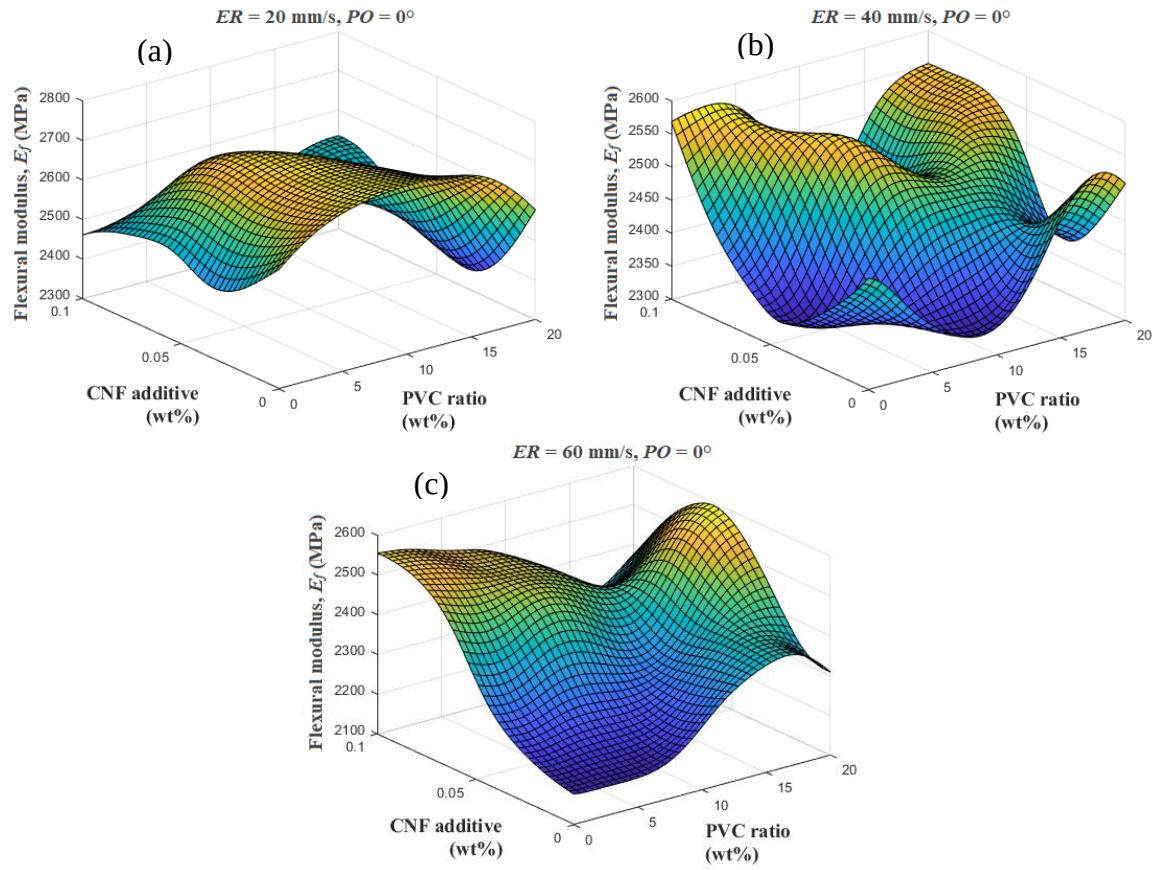


**Figure 4.29.** Response surface of flexural modulus of composite core shell sandwich panels versus the concentration of carbon nanofiber and PVC polymer at printing orientation of  $0^\circ$  of core structure; a)  $ER = 20$  mm/s, b)  $ER = 40$  mm/s and c)  $ER = 60$  mm/s.

#### 4.3.2. Maximum flexural loading, $F_{\max}$

The bar-charts presented in Figs. 4.30 to 4.31 provide insights into the variations in maximum flexural loading ( $F_{\max}$ ) observed during 3-point bending analyses of CCSSPs with 3D printed core structures of ABS/PVC/CNF blend polymer nanocomposites. A comparison between the results in Figs. 4.30 and 4.31 reveals that the addition of PVC in the ABS matrix has a slight positive effect on enhancing the  $F_{\max}$  of the core shell structures, particularly for structures fabricated at higher extrusion rates (printing speeds) and printing orientations (raster angles) of  $0^\circ$ . While ABS and PVC are both amorphous polymers, increasing the extrusion rate has minimal impact on the microstructure but leads to a reduction in the loading carrying capacity of the structure due to increased cooling rates and induced tensile residual stresses in the matrix. The lack of a compatibilizer during the processing of ABS/PVC blend filaments results in only mechanical interlocking and van der Waals forces as the adhesion mechanisms between ABS and PVC molecules. However, due to PVC's lower ultimate strength compared to ABS, its presence in the blend and weak interfacial adhesion between the molecules lead to a decrease in the maximum loading capacity of ABS/PVC blend polymer specimens. These findings emphasize the importance of using compatibilizers, such as methyl methacrylate and butyl acrylate copolymers, which act as intermediaries at the ABS/PVC interface, bridging the gap between the PVC and ABS molecules.

On the other hand, the addition of CNF in the matrix, as depicted in Fig. 4.30.b, slightly counteracts the reduction in  $F_{\max}$  of core structures fabricated at an extrusion rate of 60 mm/s with a raster orientation of  $[0/90^\circ]$ . This can be attributed to the formation of a load carrying network through mechanical interlocking between CNFs and matrix polymers, as well as a reduction in the relaxation of this mechanical bonding due to enhanced cooling rates. However, for samples with a printing orientation of  $70^\circ$ , the presence of CNF in the matrix has a negative impact on the  $F_{\max}$  of the fabricated core structures. This is likely due to an increase in the cooling rate, leading to higher residual stresses induced in the structure (Fig. 4.31.b).

These findings highlight the complex interplay between PVC, CNF, and extrusion parameters in determining the maximum loading capacity of the 3D printed core shell structures. The presence of PVC can enhance the  $F_{\max}$ , while the addition of CNF can provide some reinforcement, albeit with varying effects depending on the printing orientation and extrusion rate. It is crucial to consider the proper selection of materials and processing conditions to optimize the mechanical performance of CCSSPs.

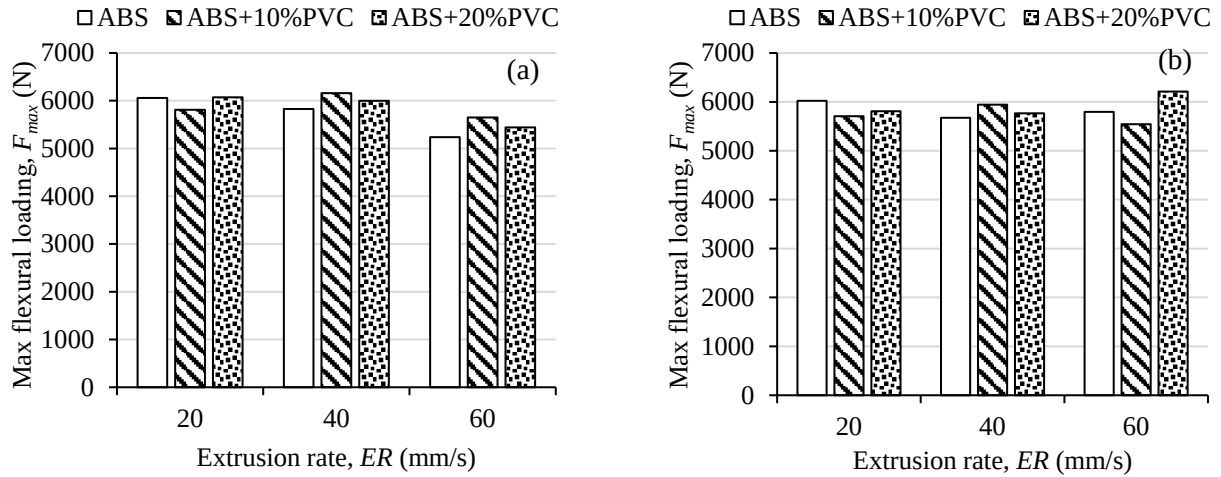


**Figure 4.30.** Maximum flexural loading of composite core shell sandwich panels versus the extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $NP = 0wt\%$  and b)  $NP = 0.05wt\%$ .

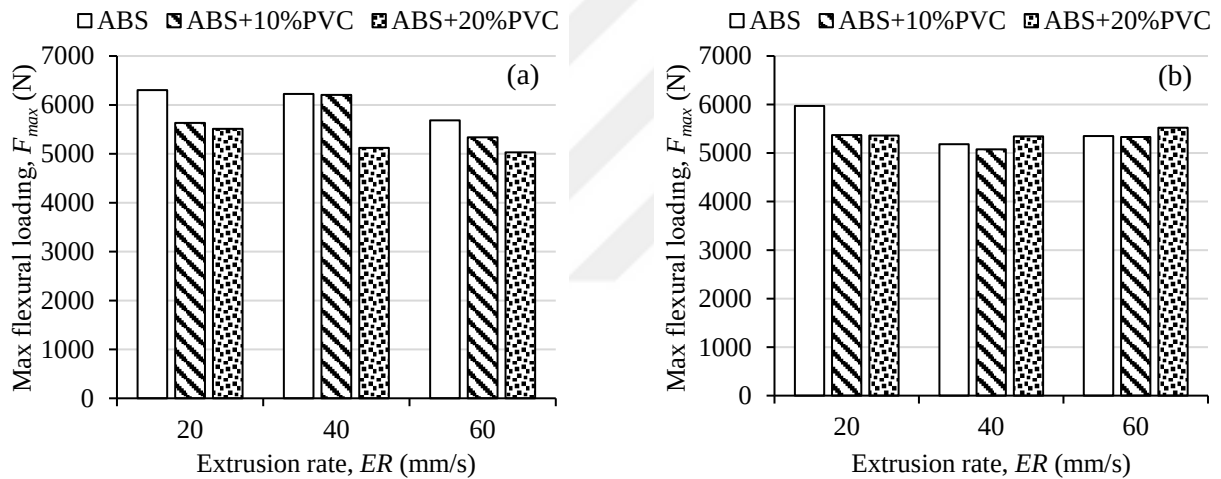


**Figure 4.31.** Maximum flexural loading of composite core shell sandwich panels versus the extrusion rate at printing orientation of  $35^\circ$  of core structure; a)  $NP = 0wt\%$  and b)  $NP = 0.05wt\%$ .

Figures 4.32 and 4.33 provide insightful data on the variations in maximum flexural loading ( $F_{max}$ ) of CCSSPs as a function of the CNF concentration in the matrix. Upon comparing Figs. 4.13.a and 4.13.b, a notable trend emerges: increasing the extrusion rate ( $ER$ ) to 60 mm/s leads to a reduction in  $F_{max}$  for core structures fabricated with a raster orientation of  $0^\circ$  and no CNF present in the matrix ( $NP$  of 0wt%). This reduction in  $F_{max}$  can be attributed to the higher levels of residual strains induced along the loading direction. However, the incorporation of CNF in the matrix effectively mitigates this reduction by creating a load carrying network through mechanical interlocking with the matrix. The interlocking mechanism between the CNFs and

the matrix enhances the overall strength and load-bearing capacity of the CCSSPs, effectively counteracting the adverse effects of increased extrusion rates.

In contrast, as demonstrated in Fig. 4.33, the addition of CNF in the matrix has an unexpected adverse effect on the load carrying capacity under flexural loading, particularly due to the shifting angle between the load carrying network and the bending stresses within the core structure. This adverse effect becomes more pronounced when the extrusion rate is raised to 60 mm/s, exacerbating the levels of residual stresses. This enhancement in residual stresses can be attributed to the improved heat transfer capabilities of CNFs, which accelerate the cooling rates within the CCSSPs (Fig. 4.33.b). The heightened residual stresses ultimately diminish the load carrying capacity, resulting in a reduction in  $F_{max}$ .

Overall, these findings emphasize the intricate relationship between the CNF concentration, extrusion rate, and mechanical performance of CCSSPs. While the addition of CNFs can effectively strengthen the load carrying network and counteract the negative effects of increased extrusion rates, their influence on the load carrying capacity under flexural loading must be carefully considered. The shifting angle between the load carrying network and bending stresses, along with the accompanying increase in residual stresses, can impact the overall mechanical performance of the core structures. Thus, optimization of CNF concentration, extrusion rate, and structural design parameters is crucial to maximize the load carrying capacity and enhance the flexural properties of CCSSPs.

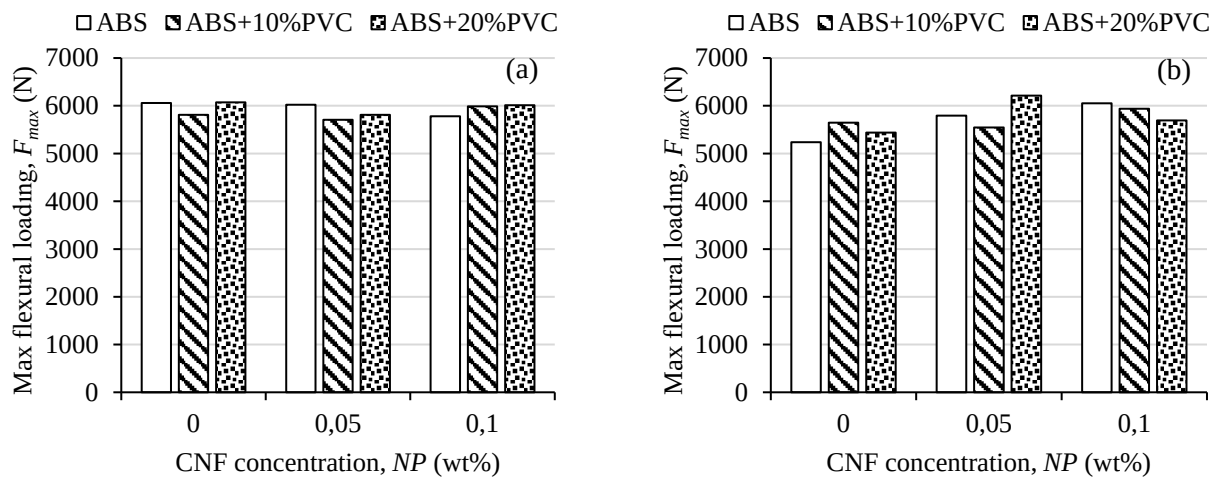


**Figure 4.32.** Maximum flexural loading of composite core shell sandwich panels versus the concentration of CNF at printing orientation of  $0^\circ$  of core structure; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

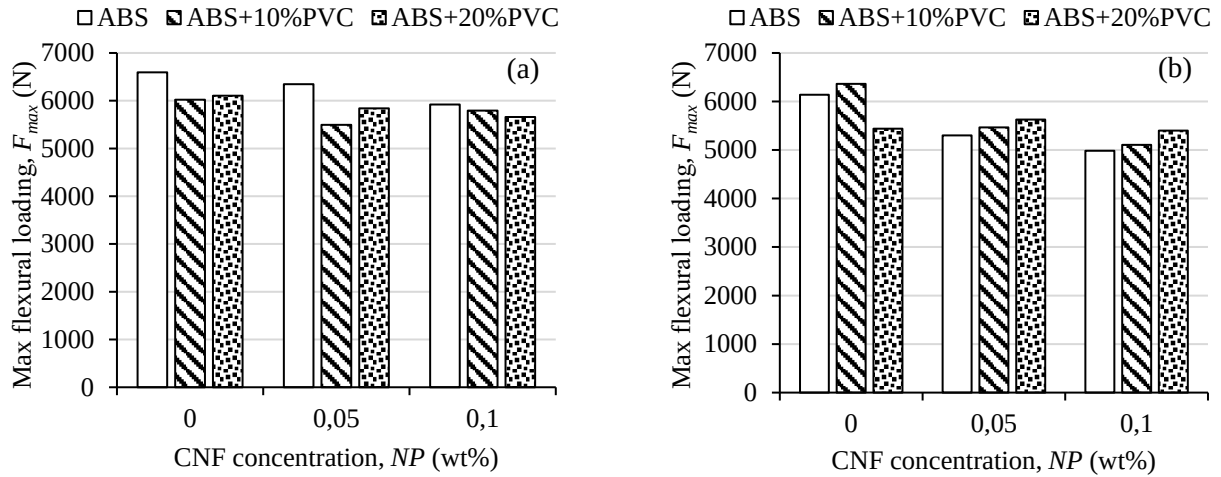


**Figure 4.33.** Maximum flexural loading of composite core shell sandwich panels versus the concentration of CNF at printing orientation of  $70^\circ$  of core structure; a)  $ER = 20$  mm/s and b)  $ER = 60$  mm/s.

The response surfaces depicted in Fig. 4.34 provide valuable insights into the variations in maximum flexural loading ( $F_{max}$ ) of CCSSPs with respect to the CNF concentration and extrusion rate during the material extrusion process of core structures. Examining Fig. 4.34.a, it is evident that there exists a nonlinear relationship between the concentration of CNF in the pure ABS matrix and the extrusion rate at a printing orientation of  $0^\circ$ . At a lower extrusion rate of 20 mm/s, the influence of CNF on the load carrying capacity of 3D printed ABS specimens is negligible. However, as the extrusion rate is increased up to 60 mm/s, the presence of CNFs results in higher  $F_{max}$  values for the fabricated core structures. This enhancement can be attributed to the formation of a load carrying network through mechanical interlocking between the polymer molecules and the CNFs, which effectively mitigates the adverse effects of higher cooling rates and induced residual stresses associated with increased extrusion rates.

The introduction of PVC into the matrix alters the flexural response of the CCSSPs, as illustrated in Figs. 4.34.b and 4.34.c. Specifically, the peak  $F_{max}$  occurs at a midrange extrusion rate of 40 mm/s when CNFs are absent from the matrix. An interesting exception arises with the core structure containing 20wt% PVC in the matrix, fabricated at an extrusion rate of 60 mm/s. In this case, the  $F_{max}$  peaks at a CNF concentration of 0.5 wt% (Fig. 4.34.c). As previously discussed, the higher extrusion rate limits the relaxation of the mechanical interlocking between the polymer molecules and the CNFs. The developed load carrying network effectively counteracts the negative effects of higher cooling rates, especially

facilitated by the presence of highly conductive CNFs in the matrix, thereby mitigating the induced residual stresses along the raster orientation of the fabricated core structure.

These findings highlight the intricate interplay between CNF concentration, extrusion rate, and the presence of PVC in the matrix, all of which significantly influence the  $F_{max}$  of CCSSPs. The formation of a load carrying network through mechanical interlocking mechanisms and the ability to counteract the detrimental effects of cooling rates and induced residual stresses are crucial for optimizing the flexural performance of core structures.

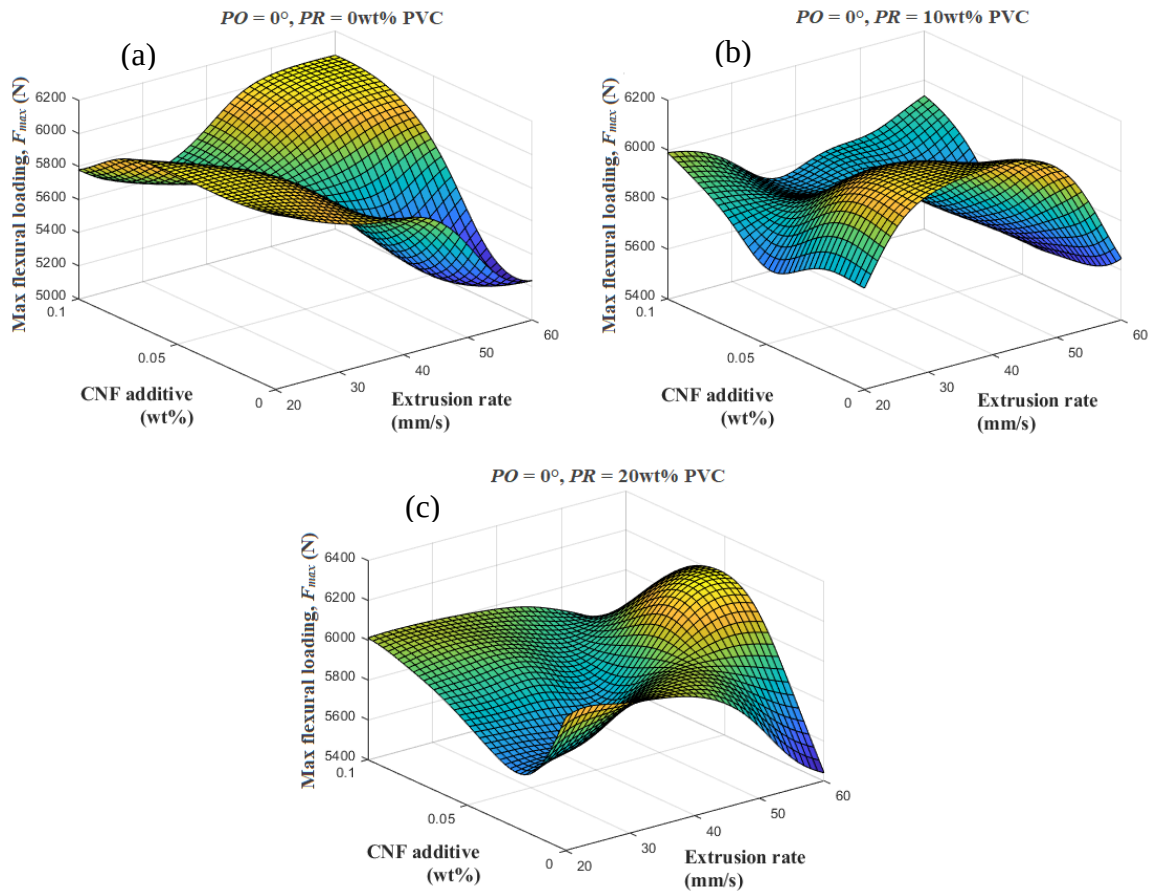


**Figure 4.34.** Response surface of maximum flexural loading of composite core shell sandwich panels versus the concentration of CNF and extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $PR = 0\text{wt\%}$ , b)  $PR = 10\text{wt\%}$  and c)  $PR = 20\text{wt\%}$  of PVC.

The effects of blending PVC polymers with the ABS matrix in core structures, along with different concentrations of CNF, on the maximum flexural loading of CCSSPs can be further examined using the response surface graphs depicted in Figs. 4.35. Figure 4.35.a shows that, without the presence of CNF, the highest  $F_{max}$  occurs at a midrange extrusion rate of

approximately 40 mm/s for the composition containing around 10wt% PVC in the matrix of the core structure, with a printing orientation of  $[0/90^\circ]$ . This enhancement in flexural loading can be attributed to the alignment of long PVC molecular chains along the printing orientation, along with the mechanical locking between ABS and PVC polymers, and a reduction in relaxation due to increased cooling rates during the core structure's extrusion process. However, with further increases in the extrusion rate and the resulting elevated level of residual stresses, there is a reduction in  $F_{max}$  (Fig. 4.35.a).

On the other hand, the addition of 0.05wt% CNF in the matrix, as illustrated in Fig. 4.35.b, shows that the presence of PVC in the matrix only increases the  $F_{max}$  at high extrusion rates, approximately 60 mm/s. This can be attributed to the load carrying network created through mechanical locking and Vander Waals forces between the CNFs and the polymer molecules, particularly those of PVC. This network effectively counters the higher cooling rate associated with high extrusion rates and the enhanced thermal conductivity resulting from the presence of highly conductive carbon nanofibers in the matrix. However, with further increases in the fraction of CNFs in the matrix, as depicted in Fig. 4.35.c, the addition of PVC becomes effective in enhancing the flexural strength of CCSSPs only at low extrusion rates of the core structure. This is because the induced residual stresses do not surpass the lower mechanical strength of PVC molecules compared to ABS. This phenomenon is also evident in Fig. 4.35.c, where the higher  $F_{max}$  in the presence of 0.1wt% CNFs and an extrusion rate of 60 mm/s is observed for the core structure without or with very low levels of PVC in the matrix.

Figure 4.36 provides additional insights into the variations of  $F_{max}$  in relation to the concentration of CNF and the ratio of PVC in the matrix of the core structure, considering different levels of extrusion rate during the material extrusion process. In Fig. 4.36.a, at an extrusion rate of 20 mm/s, the presence of PVC in the matrix effectively enhances the  $F_{max}$  of CCSSPs only when combined with a concentration of 0.1wt% CNF. This combination facilitates the creation of an efficient load carrying network within the core structure. Conversely, the addition of CNFs to the pristine ABS has minimal impact on  $F_{max}$ , indicating the superior mechanical bonding between carbon nanofibers and PVC polymer compared to ABS at low extrusion rates.

Furthermore, when the extrusion rate is increased to 40 mm/s (Fig. 4.36.b) during the fabrication process of the core structure, the  $F_{max}$  tends to occur in compositions without CNFs. This can be attributed to the enhanced cooling rate facilitated by the presence of highly

conductive CNFs in the matrix, which increases the level of induced residual stresses. However, with a further increase in the extrusion rate to 60 mm/s (Fig. 4.36.c), the presence of CNFs becomes crucial in enhancing the  $F_{max}$  for core structures containing a high level of PVC. In this case, the accelerated solidification and cooling rate of the extruded material limit the enhancement of heat transfer induced by the presence of highly thermally conductive CNFs in the matrix and the relaxation of mechanical interlocking between CNFs and the matrix. Conversely, for the core structures of pristine ABS, the presence of CNFs significantly influences the load carrying capacity and flexural response of CCSSPs.

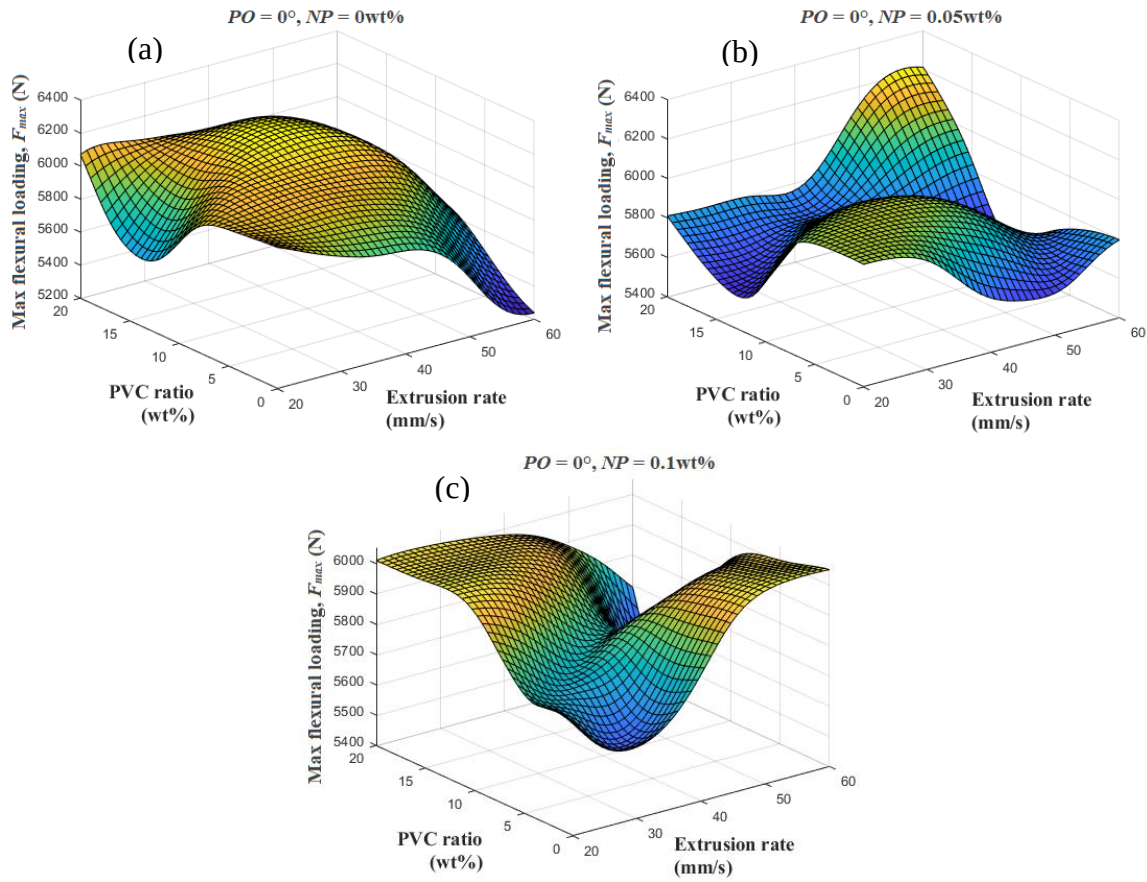


**Figure 4.35.** Response surface of maximum flexural loading of composite core shell sandwich panels versus the concentration of PVC polymer and extrusion rate at printing orientation of  $0^\circ$  of core structure; a)  $NP = 0\text{wt}\%$ , b)  $NP = 0.05\text{wt}\%$  and c)  $NP = 0.1\text{wt}\%$  of CNF.

These observations highlight the complex interactions between CNF concentration, PVC ratio in the matrix, and the extrusion rate, which impact the  $F_{max}$  of CCSSPs. The mechanical interlocking, heat transfer effects, and load carrying network formation facilitated by the combination of ABS, PVC, and CNFs play crucial roles in determining the maximum flexural

loading and performance of the fabricated core structures. It is essential to further explore and optimize these parameters to achieve desired mechanical properties and tailor the performance of CCSSPs for specific applications.

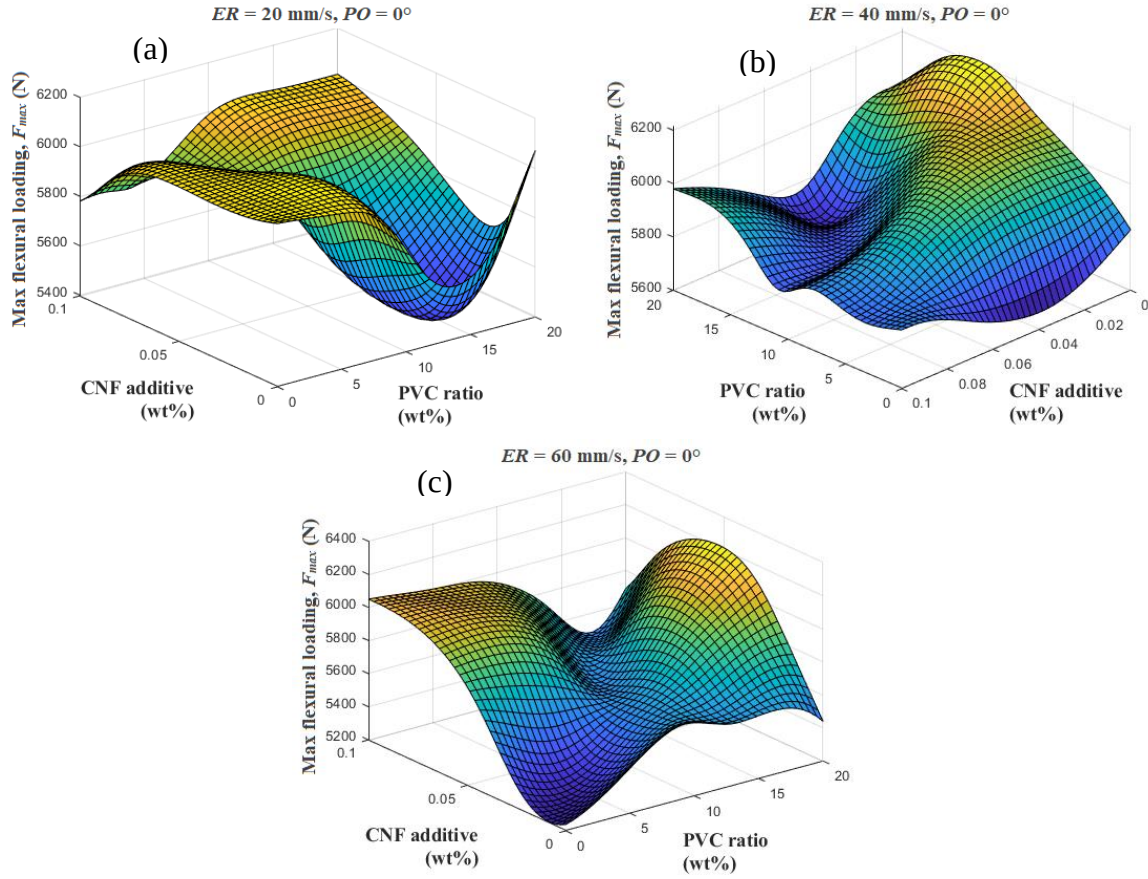


**Figure 4.36.** Response surface of maximum flexural loading of composite core shell sandwich panels versus the concentration of carbon nanofiber and PVC polymer at printing orientation of  $0^\circ$  of core structure; a)  $ER = 20$  mm/s, b)  $ER = 40$  mm/s and c)  $ER = 60$  mm/s.

#### 4.4. Optimum material extrusion parameters and polymer composition

To determine the optimal levels of input parameters in the material extrusion process and the composition of ABS/PVC blend polymer with CNF nanoadditives for achieving maximum mechanical characteristics of tensile samples and flexural response of CCSSPs with HCTC core structures, a hybrid ANN/Bayesian regression modeling and ant colony optimization (ACO) algorithm were utilized, as described in section 3.3. The hybrid ANN/Bayesian regression models were employed as functions within the ACO optimization algorithm to represent the response of 3D printed samples and CCSSPs. The Bayesian algorithm was utilized to obtain the training parameters of the AI network, minimizing the root mean square error (RMSE) and maximizing the adjusted- $R^2$  during the training, testing, and validation of the neural network-based models.

The ACO algorithm employed a swarm of ants to search the optimization space by iteratively communicating and depositing pheromone levels on the edges between starting and target points. The convergence of the ants' efforts on the search area and the best objective curve over the number of iterations of the search algorithm can be observed in Fig. 37. To ensure consistency in the levels of input parameters, all the input parameters and objective levels were normalized within the range of [-1, 1].

The optimized process parameters for various response variables of the fabricated ABS/PVC/CNF nanocomposite 3D printed tensile specimens and core shell structures were summarized in Tables (4.4) to (4.6) for the individual scheme of optimization. Additionally, the results of the accumulative scheme of optimization, considering the optimum levels of material extrusion parameters to maximize the in-plane, out-of-plane, and flexural response of 3D printed structures, were summarized in Table (4.7). These tables provide valuable insights into the recommended parameter settings to achieve the desired mechanical characteristics for the fabricated structures based on the employed optimization approach.

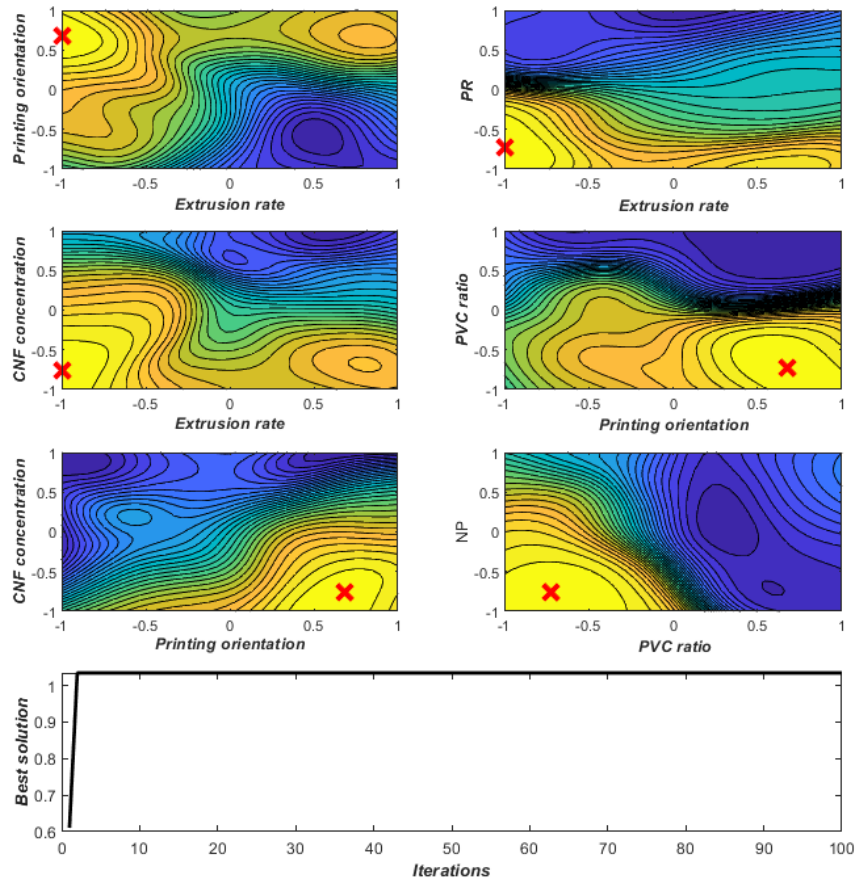


**Figure 4.37.** The final optimal position of ants on the screening space of the problem and *best objective* level of the response value with normalized axes parameters.

**Table 4.4.** Optimum levels of material extrusion parameters to obtain the best individual response of 3D printed tensile samples along the 1<sup>st</sup> principal axis (in-plane properties).

| Response variable | Solution strategy | Parameters       |               |                 |                 | Best solution |
|-------------------|-------------------|------------------|---------------|-----------------|-----------------|---------------|
|                   |                   | <i>ER</i> (mm/s) | <i>PO</i> (°) | <i>PR</i> (wt%) | <i>NP</i> (wt%) |               |
| $E_1$ (MPa)       | Best solution     | 20               | 63            | 11.2            | 0               | <u>2630.8</u> |
|                   | Maximum speed     | <b>60</b>        | 42            | 7.6             | 0               | 2603.8        |
|                   | Maximum PVC ratio | 20               | 0             | <b>20</b>       | 0               | 2612.7        |
| $S_{u1}$ (MPa)    | Best solution     | 20               | 58.8          | 2.8             | 0.01            | <u>36.42</u>  |
|                   | Maximum speed     | <b>60</b>        | 63            | 0               | 0               | 35.42         |
|                   | Maximum PVC ratio | 53.6             | 42            | <b>20</b>       | 0.08            | 32.97         |

**Table 4.5.** Optimum levels of material extrusion parameters to obtain the best individual response of 3D printed tensile samples along the 3<sup>rd</sup> principal axis (out-of-plane properties).

| Response variable | Solution strategy | Parameters          |                  |                    |                    | Best solution |
|-------------------|-------------------|---------------------|------------------|--------------------|--------------------|---------------|
|                   |                   | <i>ER</i><br>(mm/s) | <i>PO</i><br>(°) | <i>PR</i><br>(wt%) | <i>NP</i><br>(wt%) |               |
| $E_3$ (MPa)       | Best solution     | 43.2                | 49               | 6.4                | 0                  | <u>2905.4</u> |
|                   | Maximum speed     | <b>60</b>           | 70               | 7.6                | 0                  | 2901.6        |
|                   | Maximum PVC ratio | 20                  | 0                | <b>20</b>          | 0                  | 2342.2        |
| $S_{u3}$ (MPa)    | Best solution     | 20.8                | 8.4              | 1.6                | 0                  | <u>14.8</u>   |
|                   | Maximum speed     | <b>60</b>           | 53.2             | 0                  | 0                  | 13.63         |
|                   | Maximum PVC ratio | 60                  | 54.4             | <b>20</b>          | 0.1                | 7.9           |

**Table 4.6.** Optimum levels of material extrusion parameters to obtain the best individual response of core shell structures under 3-point bending condition (flexural properties).

| Response variable | Solution strategy | Parameters          |                  |                    |                    | Best solution |
|-------------------|-------------------|---------------------|------------------|--------------------|--------------------|---------------|
|                   |                   | <i>ER</i><br>(mm/s) | <i>PO</i><br>(°) | <i>PR</i><br>(wt%) | <i>NP</i><br>(wt%) |               |
| $E_f$ (MPa)       | Best solution     | 20                  | 60.2             | 0                  | 0.01               | <u>2751.2</u> |
|                   | Maximum speed     | <b>60</b>           | 68.60            | 8                  | 0                  | 2704.2        |
|                   | Maximum PVC ratio | 20                  | 68.6             | <b>20</b>          | 0.06               | 2659          |
| $F_{max}$ (N)     | Best solution     | 27.2                | 70               | 2                  | 0                  | <u>6605.4</u> |
|                   | Maximum speed     | <b>60</b>           | 70               | 9.2                | 0                  | 6367          |
|                   | Maximum PVC ratio | 57.6                | 0                | <b>20</b>          | 0.05               | 6230.8        |

**Table 4.7.** Optimum levels of material extrusion parameters to obtain the best accumulative response of 3D printed tensile samples and core shell structure.

| Optimization strategy         | Parameters          |                  |                    |                    | Response variable | Solution      | Response variable | Solution      |
|-------------------------------|---------------------|------------------|--------------------|--------------------|-------------------|---------------|-------------------|---------------|
|                               | <i>ER</i><br>(mm/s) | <i>PO</i><br>(°) | <i>PR</i><br>(wt%) | <i>NP</i><br>(wt%) |                   |               |                   |               |
| Accumulative optimum response | 24.8                | 58.8             | 0.8                | 0                  | $E_1$             | 2598.4        | $S_{u1}$          | <u>36.04</u>  |
|                               |                     |                  |                    |                    | $E_3$             | 2634.6        | $S_{u3}$          | <u>13.63</u>  |
|                               |                     |                  |                    |                    | $E_f$             | <u>2750.6</u> | $F_{max}$         | <u>6713.3</u> |
| Maximum extrusion rate        | <u>60</u>           | 56               | 0.8                | 0                  | $E_1$             | 2478.9        | $S_{u1}$          | 35.07         |
|                               |                     |                  |                    |                    | $E_3$             | <u>2659.5</u> | $S_{u3}$          | 13.43         |
|                               |                     |                  |                    |                    | $E_f$             | 2517.2        | $F_{max}$         | 6708.6        |
| Maximum PVC concentration     | 20                  | 0                | <u>20</u>          | 0                  | $E_1$             | <u>2612.7</u> | $S_{u1}$          | 27.65         |
|                               |                     |                  |                    |                    | $E_3$             | 2342.2        | $S_{u3}$          | 4.76          |
|                               |                     |                  |                    |                    | $E_f$             | 2577.3        | $F_{max}$         | 6706          |

All the parameters of modulus of elasticity, flexural modulus and the ultimate stress values are in *Mega Pascal* (MPa). The maximum flexural loading is in *Newton* (N).

The findings presented in Tables (4.4) to (4.7) indicate that the optimal parameter combinations often involve samples without CNF in the matrix. This suggests that the mechanical interlocking or Vander Waals bonding between the untreated surface of CNFs and the polymer molecules may not be sufficiently strong to exert a significant impact on 3D printed samples, particularly those fabricated at low extrusion rates. This observation could also be attributed to the adverse effect of the enhanced cooling rate induced by the presence of highly conductive CNFs in the matrix. This increased cooling rate leads to higher levels of induced stresses in the samples, which can override the reinforcing effect of the load carrying network created by the CNFs.

However, for compositions with a higher concentration of PVC in the matrix, the addition of CNF has shown a positive effect on the mechanical and flexural response of the 3D printed samples. This suggests that CNFs exhibit better compatibility with the simpler PVC polymers compared to the more complex ABS polymers. These results highlight the importance of considering the composition of the matrix and the concentration of CNFs when aiming to optimize the mechanical properties of 3D printed samples.

## 5. CONCLUSIONS

In conclusion, this thesis aimed to investigate the effects of different core structures on the flexural response of composite core shell structures fabricated using the material extrusion process, specifically fused deposition modeling (FDM). The study considered various FDM parameters and the composition of the base matrix material to understand their influence on the mechanical properties of the structures. Through a comprehensive analysis, it was found that the selection of core structures played a crucial role in determining the flexural performance of the composite core shell structures. The study examined a range of core configurations and identified specific structures that exhibited desired mechanical properties, such as stiffness and load-carrying capacity.

The investigation utilized regression modeling with artificial neural networks (ANN) to predict the mechanical variables of the 3D printed samples, including in-plane and out-of-plane modulus of elasticity and ultimate strength. Additionally, optimization techniques employing ant colony optimization (ACO) were applied to optimize the FDM parameters and material composition, leading to improved mechanical performance. Regression models obtained through AI modeling were used to analyze the variations in mechanical properties, and the results were presented using bar-charts and surface responses. Optimization algorithms were applied to determine the material extrusion parameters that maximize the response variables individually and cumulatively.

The study provides insights into the influence of material extrusion parameters and the compatibility of additives, such as PVC and CNFs, on the mechanical characteristics of 3D printed samples and CCSSP specimens. It highlights the potential for tailoring the mechanical properties of 3D printed materials for specific applications through careful selection and optimization of material extrusion parameters.

Furthermore, the findings demonstrated the potential of FDM as a viable manufacturing technique for producing composite core shell structures with tailored mechanical properties. By optimizing the core structures and FDM parameters, it was possible to enhance the flexural response and overall performance of the fabricated structures. The outcomes of this research contribute to the advancement of additive manufacturing, specifically in the context of composite core shell structures. The findings offer valuable knowledge for engineers and

researchers in optimizing FDM processes and material compositions to achieve desired mechanical properties for specific applications.

The key findings of this study could be summarized as follows:

1. The mechanical properties of 3D printed samples fabricated at different orientations of principal axes were analyzed. Engineering constants were used as material properties for finite element modeling of 3-point bending of composite core shell sandwich panels (CCSSP). The addition of PVC in the ABS matrix improved the in-plane stiffness of the 3D printed samples, particularly at lower extrusion rates and printing orientations. However, the presence of carbon nanofibers (CNFs) had a limited effect on stiffness at different printing orientations.
2. The ultimate strength of the fabricated samples was investigated, and it was found that the addition of PVC did not effectively enhance the ultimate strength, especially at higher extrusion rates and printing orientations. However, the inclusion of CNFs counteracted the reduction in ultimate strength caused by increased extrusion rates, particularly for samples with a raster orientation of  $[0/90^\circ]$ .
3. The addition of CNF to the polymer matrix creates a load-carrying network through mechanical interlocking, enhancing the compatibility between ABS and PVC molecules and improving the ultimate strength of the samples. This offers promising avenues for optimizing the mechanical properties of the fabricated materials.
4. The response surface analysis of the flexural modulus and maximum flexural loading of CCSSPs with hybrid circular/triangular corrugated cores (HCTC) reveals the influence of material extrusion parameters and polymer composition on the flexural response. The addition of PVC improves flexural stiffness, while the presence of CNF can reduce stiffness, especially at higher extrusion rates.
5. The optimization process using hybrid ANN/Bayesian modeling and ant colony optimization algorithm suggests that optimal parameter combinations often involve samples without CNF in the matrix. However, for compositions with higher PVC concentrations, the addition of CNF can positively influence the mechanical and flexural response of 3D printed samples.

6. Considering CNF concentration, PVC ratio, and extrusion parameters is crucial for achieving desired mechanical properties and tailoring the performance of 3D printed structures. The results provide insights for optimizing printing parameters and material composition to enhance mechanical properties and performance.
7. The combination of response surface analysis, regression modeling, and optimization algorithms offers a comprehensive approach for understanding and optimizing the mechanical properties of 3D printed samples and CCSSPs with HCTC core structures. This research contributes to the advancement of additive manufacturing and the development of materials with tailored mechanical properties for various applications.



## 6. RECOMMENDATIONS

The most important observations are that the lack of compatibilizer between the ABS and PVC polymers and addition of untreated CNFs significantly affect the degree of improvements that are followed in the fabrication of nanocomposite filaments for composite core applications. The surface of untreated CNFs is typically hydrophobic and lacks specific functional groups that can strongly interact with the PVC polymer matrix. Consequently, future recommendations should primarily focus on enhancing the compatibility between the nanocomposite components to facilitate stronger bonding:

1. **Lack of Compatibilizer:** The absence of a compatibilizer between ABS and PVC polymers, along with the addition of untreated CNFs, significantly affects the degree of improvements in the fabrication of nanocomposite filaments for composite core applications. It is recommended to use compatibilizers, such as methyl methacrylate and butyl acrylate copolymers, to bridge the gap between PVC and ABS molecules and enhance the interfacial adhesion and mechanical properties of the nanocomposite.
2. **CNF Surface Functionalization:** To improve the compatibility of CNFs with PVC, it is recommended to pursue the functionalization of CNFs. The introduction of functional groups, such as carboxyl, hydroxyl, or amine groups, onto the CNF surface can enhance the interaction with the PVC polymer matrix, leading to improved interfacial adhesion and mechanical properties of the nanocomposite.
3. **CNF Surface Activation:** Activate the CNF surface to increase its reactivity and enable the formation of chemical bonds with the base polymer. Methods like chemical oxidation, plasma treatment, or UV/ozon treatment can be employed for surface activation.
4. **Comprehensive Mechanical Property Analysis:** Future work should aim to conduct a comprehensive analysis of the mechanical properties of the nanocomposite, including tensile strength, modulus, toughness, and impact resistance. This analysis should be carried out systematically by varying the type and concentration of compatibilizers, as well as the extent of CNF surface functionalization and activation. This will provide valuable insights into the effects of these factors on the overall mechanical performance of the nanocomposite.

5. **Characterization Techniques:** In future studies, the use of advanced characterization techniques, such as electron microscopy (SEM/TEM), spectroscopy (FTIR/XPS), and thermal analysis (TGA/DSC), should be employed to analyze the morphology, interfacial interactions, chemical bonding, and thermal behavior of the nanocomposite. These techniques will provide a more detailed understanding of the structural and compositional changes resulting from compatibilizer addition, CNF functionalization, and surface activation.



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