COMPUTATIONAL MODELING AND ANALYSIS OF NANOFIBER COMPOSITES FOR MARITIME APPLICATIONS

Kolluri Padma
Research Scholar
University of Technology
Jaipur.

Dr.Sudhir Ojha
Research Supervisor
University of Technology
Jaipur.

Dr. S. Chakradhar Goud
Research Co-Supervisor
University of Technology
Jaipur.

ABSTRACT

This study investigates the drug release performance of electrospun composite nanofiber mats, which hold significant promise as drug carriers for site-specific delivery in therapeutic applications such as cancer therapy. Predicting drug release rates from poly nanofibers produced via emulsion electrospinning is challenging due to the system's inherent complexity. Computational modeling was employed to evaluate the continuous drug release from these nanofibers. The carbon nanotubes/nanofibers reinforced composites show great mechanical properties. There are several methods to simulate the mechanical properties of composites. In the last few decades nanofibers have been developed and introduced in a vast number of industrial and research applications. One of their most effective use is as interleaved reinforcement for composite laminate materials against delamination. Nanofibrous mats have the ideal morphology to be embedded between two plies of a laminate, and a vast and deep research has been carried out investigating their effect on the global behaviour of a composite laminate. This review is the first of its kind to date which presents a detailed state-of the-art on the effect of nanofibrous interleaves into composite laminates with focus on the mechanical performances and behaviours of nano modified materials. A detailed description of the working mechanisms of the nano interleave under different load cases is presented, and a comparative analysis between papers in literature will provide readers with a powerful tool to understand and use nanofibers for reinforcing purposes.

***Keywords**: Nanofibers, Composite Materials, Nano composite, carbon nanofibers, Computational modeling*

INTRODUCTION

Additionally, these electrospun nanofibers possess the ability to interconnect and create intricate networks of highly porous mesh structures, making them versatile candidates for numerous applications. The remarkable attributes of electrospun nanofibers include their exceptional extensibility, high mechanical strength, substantial porosity, large surface area, as well as the capacity for adjusting fiber diameter. Furthermore, they exhibit thin layering, high permeability, low basis weight, customizable wettability, retention of electrostatic charges, and mechanical flexibility. In addition to these characteristics, electrospinning possesses the added advantage of a user-friendly application. An essential aspect of electrospun nanofibers is their diameter, which directly governs their mechanical and functional attributes. Through meticulous manipulation of electrospinning process parameters, the precise control of nanofiber diameter and morphology can be achieved, thereby tailoring their properties to suit specific applications across diverse fields. Recently, many electrospun nanofibers have been successfully employed to reinforce the polymer matrix. Many processes have been reported for the fabrication of nanofiber-reinforced composites, including solution impregnation, layer-by-layer coating, dip-coating, melt mixing with short electrospun nanofibers, in situ fabrication, casting, draining, and subsequent stacking by hotpress. However, to fabricate electrospun nanofiber-reinforced composites, it is necessary to achieve an effective impregnation of the polymer matrix with the nanofibers, in order to establish intimate contact and strong interfacial bonding between the two, which then enables good mechanical interlocking with the surrounding polymer chains. Electrospun nanofiber-reinforced composites are widely used in human motion detection, self-healing electronic skins, sensors, fuel cells, epidermal electronics, microfluidic devices, biomedical applications, and so on. It would be beneficial to predict the mechanical properties of these composites with analytical and numerical modeling. Polymer nanocomposites reveal significant high-performance properties using small fractions of nanofillers in the polymer matrices. The excellent properties of nanocomposites have attracted extensive attention in distinct technologies such as automobiles, energy, sensors, fuel cells, agriculture, and biotechnology. One of the attractive characteristics of polymer nanocomposites is their mechanical properties. However, the mechanical characteristics of composites cannot be predicted properly due to the small fractions and novel characteristics of the polymer nanocomposites, compared to traditional composites. The mechanical characteristics of polymer nanocomposites have been estimated with many proposed models

LITERATURE REVIEW

Yasser Zare (2025) Herein, the dimensions of the interphase and tunneling zones are utilized to develop a model for the conductivity of polymer composites with carbon nanofiber (CNF) named as PCNFs. The effective CNF concentration and percolation onset depend on the interphase depth to estimate the concentration of the CNF/interphase network. Additionally, the length and diameter of tunnels are considered to account for tunneling resistance in the developed model. Accordingly, the current model assumes simple, measurable, and effective factors to estimate the conductivity of PCNF. Parametric analyses and experimental data of conductivity for real examples are used to validate the developed model. Additionally, the minimum tunneling distance (λ = 1 nm) and maximum contact diameter (d = 40 nm) yield the maximum output of 0.045 S/m. Therefore, a deeper interphase, lower onset of percolation, and narrower and wider tunnels are essential to improve the nanocomposite conductivity.

Balakrishnan Subeshan (2024) Electrospun nanofibers have gained prominence as a versatile material, with applications spanning tissue engineering, drug delivery, energy storage, filtration, sensors, and textiles. Their unique properties, including high surface area, permeability, tunable porosity, low basic weight, and mechanical flexibility, alongside adjustable fiber diameter distribution and modifiable wettability, make them highly desirable across diverse fields. However, optimizing the properties of electrospun nanofibers to meet specific requirements has proven to be a challenging endeavor. The electrospinning process is inherently complex and influenced by numerous variables, including applied voltage, polymer concentration, solution concentration, solution flow rate, molecular weight of the polymer, and needle-to-collector distance. This complexity often results in variations in the properties of electrospun nanofibers, making it difficult to achieve the desired characteristics consistently. Traditional trial-and-error approaches to parameter optimization have been time-consuming and costly, and they lack the precision necessary to address these challenges effectively.

Ramkumar Vanaraj (2023) The present review article discusses the elementary concepts of the sensor mechanism and various types of materials used for sensor applications. The electrospinning method is the most comfortable method to prepare the device-like structure by means of forming from the fiber structure. Though there are various materials available for sensors, the important factor is to incorporate the functional group on the surface of the materials. The post-modification sanction enhances the efficiency of the sensor materials. This article also describes the various types of materials applied to chemical and biosensor applications. The chemical sensor parts include acetone, ethanol, ammonia, and CO2, H2O2, and NO2 molecules; meanwhile, the biosensor takes on glucose, uric acid, and cholesterol molecules. The above materials have to be sensed for a healthier lifestyle for humans and other living organisms. The prescribed review articles give a detailed report on the Electrospun materials for sensor applications.

Vishal Gavande (2022) In this study, a simple approach was described to investigate the theoretical models for electrospun polymer nanofiber-reinforced nanocomposites. For predicting the tensile strength of the electrospun nylon 6 nanofiber-reinforced polyurethane acrylate composites, conventional Pukanszky, Nicolais–Narkis, Halpin–Tsai, and Neilson models were used, while for Young's modulus, Halpin–Tsai, modified Halpin–Tsai, and Hui–Shia models were used. As per the Pukanszky model, composite films showed better interaction since the values of the interaction parameter, B, were more than. Similarly, the value of an interfacial parameter, K, was less than 1.21 ($K = -5$, for the curve fitting) as per the Nicolais–Narkis model, which indicated better interfacial interaction. For composite films, the modified Halpin–Tsai model was revised again by introducing the orientation factor, α, which was 0.333 for the randomly oriented continuous nanofiber-reinforced composites, and the exponential shape factor, which showed the best agreement with the experimental Young's modulus results. Based on mentioned remarks, these models would be applicable for estimating the tensile strength and Young's modulus of electrospun nanofiber-reinforced polymer composite films.

Computational Modeling of Polymer Composites

Polymer composites have become an indispensable class of structural and functional materials due to their high specific stiffness and strength, design flexibility, and broad applicability across aerospace, automotive, civil, and biomedical engineering. The inherently heterogeneous mechanical properties of polymer composites, arising from the coexistence of polymer matrices and reinforcing phases, pose significant challenges for experimental characterization alone, particularly in elucidating the underlying small-scale deformation and failure mechanisms. Owing to its efficiency, cost-effectiveness, and ability to capture details, computational modeling has emerged as a critical tool for understanding structure–property–performance relationships in polymer composites and for guiding their rational design. This section focuses on the computational modeling of polymer composites, with emphasis on continuum-based frameworks that have been extensively developed and applied over the past several decades and proven to be both efficient and robust.

Fundamentals of Polymer Composites and Nanocomposites

In this review, polymer composites and polymer nanocomposites are distinguished based on the characteristic length scales of their reinforcements and the resulting dominant physical mechanisms. Polymer composites typically consist of a polymer matrix reinforced with fibers or particulates whose dimensions are on the order of micro meters or larger, such that their mechanical behavior can often be described using continuum-based micromechanics, representative volume elements, and homogenization approaches. In contrast, polymer nanocomposites incorporate reinforcements with at least one characteristic dimension in the nanometer range, leading to a significantly increased interfacial area between the reinforcement and the matrix. As a result, nanoscale effects, such as interphase formation, confinement-induced changes in polymer chain dynamics, and dispersion or agglomeration of nanofillers, play a critical role in governing mechanical response. These fundamental differences in length scale and underlying physics necessitate distinct modeling assumptions and multiscale strategies, which are discussed throughout this review.

Modeling of nanofiber composites

Researches in this area are in their infancy stage. Limited publications have focused on simulation for the elastic properties of composites reinforced with random nanofibers or nanoparticulates. In these papers, micromechanics formulae, such as Halp in and Tsai equations, for random short fiber composites have been used. From a simulation viewpoint, there has been no difference between nanofiber composites and traditional (micro) fiber reinforced composites Although doubts exist on whether it is possible to use the continuum-level elastic description to predict the overall elastic constants of nanocomposites, based on their morphology, elastic constants of the pure matrix, and the elastic properties of the reinforcement nanofibers, the lack in experimental evidences (e.g. no available uni directionally nanofiber reinforced composites for which the micromechanics formulae are most applicable and the most accurate, no reliable experimental data for the elastic constants of nanofibers, etc.) makes it too early to say yes or no. However, a recent theoretical investigation seemed to suggest that the traditional micromechanics model would be still applicable to predict the overall mechanical properties of nanofiber reinforced composites.

Modeling of nanofibrous preform

The mechanical performance of nanofiber preforms is of interest in applications such as semi-permeable membranes, filters, protective clothing, and tissue engineering. For instance, the nanofiber scaffold template should be designed to be structurally biocompatible with the host tissue. This will be possible when the structure–property relationship of the scaffolds has been clearly understood. Challenges in the modeling of mechanical properties of nanoscale nonwoven scaffolds (films) include the determination of the nano-fiber orientation distributions in the scaffolds, the measurement of the coefficient of friction of the nanofibers, and the specification of the condition under which the fiber slippage occurs. In addition to the mechanical behavior, the geometric properties of nanofibrous preforms such as pore shape, pore size and pore size distribution, free volume or voidage and surface area are also important for applications. In tissue engineering, for instance, these properties influence to a great extent the cell seeding and growth efficiency.

Composite application

This is because nanofibers can have even better mechanical properties than micro fibers of the same materials, and hence the superior structural properties of nanocomposites can be anticipated. Moreover, nanofiber reinforced composites may possess some additional merits which cannot be shared by traditional (microfiber) composites. For instance, if there is a difference in refractive indices between fiber and matrix, the resulting composite becomes opaque or non-transparent due to light scattering. This limitation, however, can be circumvented when the fiber diameters become significantly smaller than the wavelength of visible ligh Perhaps the majority work in the current literature on nanofiber composites is concerned with carbon nanofiber or nanotube reinforcements. These nanofibers or nanotubes are generally not obtained through electrospinning. Several comprehensive reviews have summarized the researches done until very recently on these composites. On the other hand, so far polymer nanofibers made from electrospinning have been much less used as composite reinforcements. Only limited researchers have tried to make nanocomposites reinforced with electrospun polymer nanofibers. Information on the fabrication and structure-property relationship characterization of such nanocomposites is

METHODOLOGY

The electrospinning unit consists of a high-voltage power source, a syringe pump, a spinneret, and a stationary collecting plate. Cover the collector plate with aluminium foil to gather nanofibers. Connect the syringe to the syringe pump and fill it with the produced polyacrylonitrile solution. Nanofibers will begin to accumulate on the collector plate as soon as the electrostatic forces counterbalance the surface tension of the polyacrylonitrile solution at critical voltage, and an electrified jet is formed and ejected from the tip. As the electrospinning period proceeds for 16 hours, the thickness of the randomly oriented fibers increases in the stationary collector. In the sliding substrate, the same technique has been for collecting nanofibers, but the sliding collector plate is designed to manually switch back and forth on each side. The nanofibers are carefully labelled and stored for strength testing. There are three kinds of modeling concepts employed for polymer nano composites according to different size effects, such as molecular-scaled, micro-scaled, and meso-/macro-scaled models. For the nanofiber-reinforced polymer composites, an applied force could be transferred from the polymer matrix to the polymeric nanofibers through shear stress at the nanofiber/polymer matrix interface

RESULTS AND DISCUSSIONS

The deviations of E_c of the N6/PUA nanocomposites with the different volume fractions are plotted in Figure 1. To further determine the effectiveness of reinforcement, we implemented the conventional Halp in–Tsai model for N6/PUA nanocomposites. The Halp in–Tsai model is apparently effective in predicting Ec of not merely unidirectional aligned fiber-reinforced composites, but also of several nanocomposites where the reinforcement phase has functionality relating to the aspect ratio in regards to CNF, CNTs, and cellulose nanofibers.

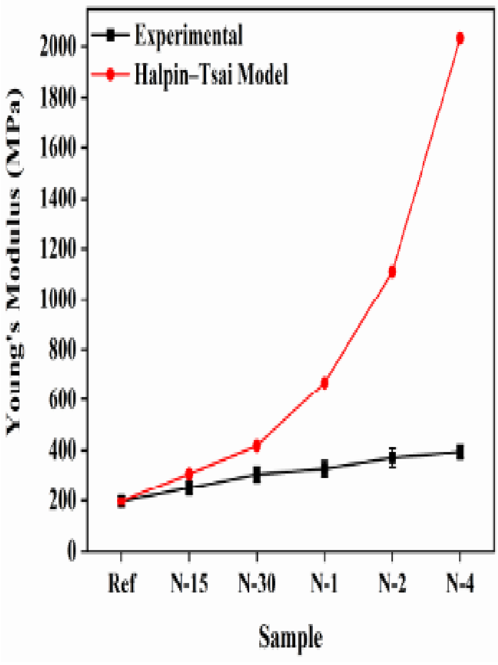

Figure 1.Comparison between the experimental E_c and theoretical E_c employing the Halp in–Tsai model.

As shown in Figure 1, the illustrated calculations show increments in Ec as the volume fraction of nanofibers is enhanced. The experimental data of relative strength and the predictions of the model did not properly follow the experimental data at numerous nanofibers concentrations because of the absence of some parameters, such as an alignment of the nanofibers, shape factor, and aggregation in the composite.

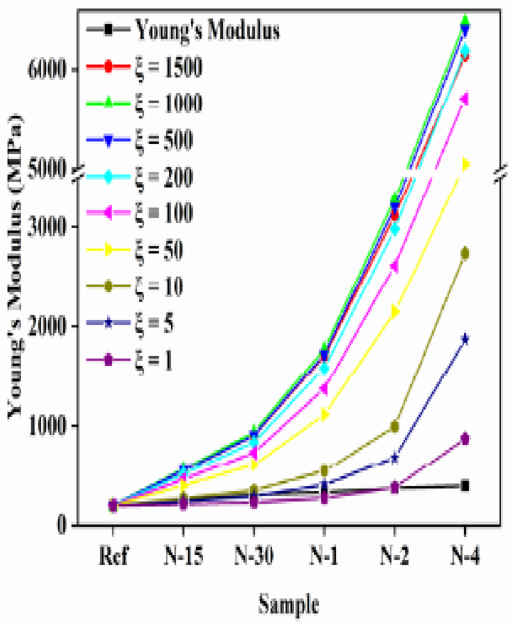

Figure 2.Effect of the exponential shape factor on E_c of the nylon 6 nanofiber-reinforced PUA composites

For the Halpin–Tsai equation, shape factor and orientation factorαwere introduced, and modified the model as shown in Equations (12) and (13). In this research, values were assumed and the graph was plotted for nanofiber-reinforced composites, as shown in Figure 2. However, this model usually unpredicted the E_c of nanofiber-reinforced nanocomposites, and it was clearly found that the calculations were above the experimental data as volume fractions of the nanofibers increased in the composites.

The effect of aggregation-related coefficient a nurtured to relent the fitted curves of Ec of the nanofiber-reinforced composites at a high % of nanofibers, which demonstrated more aggregation established with multiplying nanofiber content. The aggregation-related coefficient bon the model curve for Ec of the nanofiber-reinforced composites is depicted in Figure 3. The Ec of composites was further adapted to trend lower for higher values of bat a high-volume fraction of nylon 6 nanofibers.

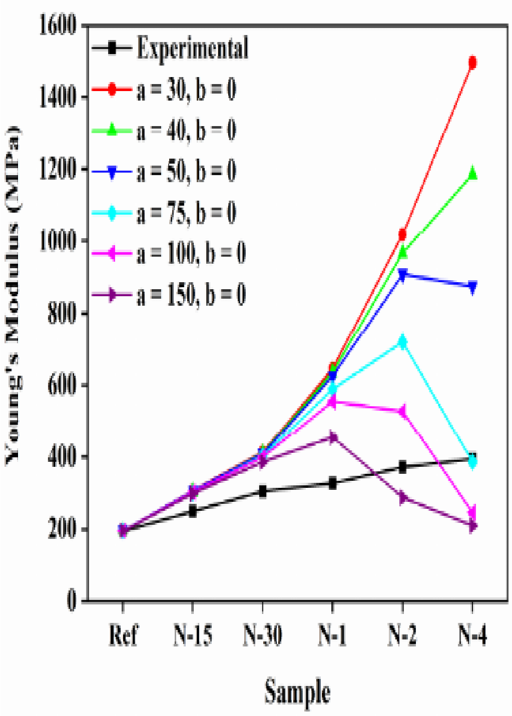

Figure 3. Effect of the aggregation/agglomeration coefficients a on Ec of the nylon 6 nanofiber-reinforced PUA composites

CONCLUSION

This work provides an overview of numerical strategies based on the finite element method for analyzing drug diffusion from nanofiber-based delivery systems. Two approaches— detailed and smeared models—were developed, incorporating partitioning and degradation effects, which are critical factors in drug delivery from nanofibers commonly used in implant design. On the other hand, the smeared model utilizing CSFE for axial diffusion transport and connectivity elements for radial exchange, offers a computationally efficient and user-friendly alternative. The models were validated through experiments using electrospun PLGA nanofiber mats with varying compositions. These models serve as effective tools for analyzing drug transport within polymer fiber networks and release into the surrounding porous medium. The combination of advanced fabrication techniques, such as emulsion electrospinning, with computational modeling provides a robust framework for designing next-generation drug delivery systems. Future research should focus on optimizing polymer compositions, exploring novel biodegradable materials, and refining predictive models to achieve precise control over drug release kinetics. Additionally, developing multifunctional nanofiber mats that integrate drug delivery with other therapeutic properties, such as antimicrobial or anti-inflammatory effects, could further expand their applications in tissue engineering and regenerative medicine

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