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An advanced approach to predicting optimal material compositions for graphene/carbon black reinforced PP/PVC nanocomposites focusing mechanical and economic performance

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ABSTRACT

The growing need for enhanced materials has led to the development of nanocomposites, which have shown great potential in various industries. However, optimizing the composition of these materials to achieve the best mechanical performance and cost-effectiveness remains a challenge. This research addresses this challenge by employing a virtual experimental approach, utilizing Digimat for material modeling and CATIA for Design and Finite Element Analysis (FEA). This approach allows for the simulation and analysis of different nanocomposite compositions without the need for costly and time-consuming physical experiments. The study focuses on Polypropylene (PP) and Polyvinyl Chloride (PVC) based nanocomposites with graphene and carbon black reinforcements. The research investigates the impact of varying the weight percentages of these nanofillers on the mechanical properties of the composites. The PP/PVC blends are created in different weight ratios to provide further compositional control. The material preparation is carried out in Digimat, where the properties of the composites are defined using a micromechanical model. The FEA is then conducted in CATIA, where a standard ASTM D638 tensile specimen is simulated under controlled conditions. The results are validated by varying mesh sizes to optimize deflection and Von Mises stress predictions. Furthermore, an economic analysis is conducted to evaluate the cost-effectiveness of the different nanocomposite compositions. The study highlights the importance of virtual experimentation in material science, as it allows for efficient exploration of various material compositions and reduces the need for physical prototyping. This approach accelerates the material development process and enables the optimization of material design for specific applications. The virtual trials explored alternatives to PVC using PP-based composites reinforced with graphene/carbon black. PP/PVC 40/60 reinforced with 1.5% wt. graphene (P4V6G15) and reinforced with 7.5% wt. carbon black (P4V6C75) showed 31.6% and 31.2% deflection reductions compared to pure PP, respectively. These results show that P4V6 blends, especially those with graphene or high carbon black concentrations, serve as promising alternatives to conventional PVC. Among them, P4V6C75 stands out by offering the best overall mechanical performance. It also provides the lowest production cost. In terms of economic favorability, P4V6C75 is approximately 2.55 times more cost-effective than the graphene-based blend P4V6G15. This combination of high performance and low cost makes P4V6C75 the most suitable candidate for PVC replacement.

Keywords: Nanocomposites, Polypropylene (PP), Polyvinyl Chloride (PVC), Graphene, Carbon Black

INTRODUCTION

The development of composite materials has revolutionized various industries, offering enhanced mechanical properties, durability, and cost efficiency. Nanocomposites—materials reinforced with nanoparticles such as graphene and carbon black—have gained significant attention due to their superior strength, electrical conductivity, and thermal stability. Combining polypropylene (PP) and polyvinyl chloride (PVC) with nanofillers provides a versatile material with potential applications in agriculture and construction industries. However, optimizing the composition of these nanocomposites to achieve mechanical performance as an alternative to PVC remains a challenge. Simulation and virtual testing have become essential tools in material science, significantly reducing the need for costly and time-consuming physical experiments. Finite Element Analysis (FEA) and multiscale modeling allow researchers to predict material behavior under different loading conditions, ensuring performance evaluation before real-world implementation. Digimat software is employed in this research to create a homogeneous mixture of nanocomposites, providing critical material properties such as density, Poisson’s ratio, and Young’s modulus. These parameters are then used in CATIA to simulate and analyze standard tensile specimens (D638) under controlled conditions. By varying mesh sizes in the analysis, the study ensures accuracy in validation of deflection and Von Mises stress predictions.

The significance of this approach lies in its cost-effectiveness and efficiency. Traditional material testing involves expensive fabrication and extensive laboratory experiments, whereas simulation driven research minimizes waste, optimizes resources, and accelerates the development cycle. By virtually identifying the best-performing material composition, this study aims to provide a practical, data-driven method for selecting nanocomposites tailored to specific applications, ultimately advancing material innovation without needing physical prototyping.

PVC, a widely used synthetic polymer, presents significant environmental and health concerns due to the release of toxic chemicals like phthalates and dioxins during its lifecycle, coupled with recycling challenges [1]. This necessitates the exploration of sustainable alternatives. While materials like PE, PP, and PET offer potential replacements [2], polymer blending has emerged as a promising strategy to create materials with tailored properties. Furthermore, incorporating nanoparticles, such as Graphene, MWNTs, into these polymer matrices to form nanocomposites has shown significant potential for enhancing mechanical, thermal, and other properties [3]. These advancements in polymer blends and nanocomposites offer promising avenues for replacing PVC in various applications.

Polymer blends offer a versatile platform for tailoring material properties, but challenges arise from phase separation and poor interfacial adhesion. This literature review explores the use of nano-scale reinforcements, particularly graphene and carbon black, to enhance the mechanical performance of polypropylene (PP) and polyvinyl chloride (PVC) blends. Furthermore, it examines the application of computational modeling, specifically using Digimat software, to optimize blend composition and predict material behavior, minimizing the need for extensive experimental testing. Nano- and micro-scale reinforcements offer a promising route to enhance PVC polymer composites' mechanical performance and thermal stability. Incorporating nano-fillers such as carbon nanotubes (CNTs), graphene, and carbon black (CB) can significantly improve tensile strength, stiffness, and durability compared to traditional micro-scale reinforcements. However, optimizing the filler composition for PP-PVC blends presents a considerable challenge. Computational methods offer a powerful tool to address this challenge. Micromechanical modeling and virtual testing, using software like Digimat, can predict optimal blend compositions, reducing the need for extensive experimental trials. This approach enables accurate simulation of stress-strain behavior, failure mechanisms, and phase interactions, facilitating the development of high-performance polymer composites.[4]

Graphene and CNTs offer exceptional mechanical properties, making them attractive reinforcements for polymers, metals, and ceramics. However, achieving uniform dispersion in polymer matrices is a key challenge significantly affecting composite performance [5]. Studies show that graphene nanoplatelet (GNP) size influences mechanical properties—smaller GNPs (5 µm) enhance tensile strength and modulus, while larger GNPs (25 µm) improve impact resistance due to different reinforcement mechanisms. Additionally, graphene acts as a nucleating agent, increasing polypropylene (PP) crystallinity and thermal stability [6]. Carbon black (CB) is another widely used reinforcement, offering cost-effective mechanical and electrical properties improvements. However, when compared to graphene-reinforced composites, CB exhibits lower reinforcement efficiency. Studies in nitrile butadiene rubber (NBR) show that GNPs outperform CB by providing higher tensile and tear strength, faster curing times, and improved durability [7]. Additionally, increasing CB content in natural rubber leads to a transition from amorphous to semicrystalline structures, as confirmed by X-ray Diffraction **(**XRD) and Scanning Electron Microscope (SEM). Differential Scanning Calorimetry (DSC) analysis reveals that CB enhances thermal resistance, while maintaining a homogeneous rubber matrix [8].

PP and PVC immiscibility leads to poor mechanical properties, improved by compatibilizers [9]. PVC-PMMA blends show better interaction than PVC-PP [10]. Nanoparticle-reinforced PVC-PP enhances strength and toughness, with 1% EPDM showing optimal performance [11]. ABS increases flexural strength but reduces toughness, and 3% TiO_2 improves properties, but higher loadings cause agglomeration [11]. SEBS/PP blends are explored as safer alternatives to PVC-DEHP in medical bags [12]. Stabilizers significantly impact PVC composite mechanical properties, with specific types and concentrations yielding varied results [13]. Computational modeling via Digimat offers a data-driven approach to optimize material composition by simulating nano-filler dispersion and predicting mechanical behavior, validated across diverse materials like $BaTiO_3$ composites and graphene-reinforced alloys [14, 15, 16]. This study leverages Digimat to model PP-PVC blends with graphene and carbon black, aiming to identify optimal filler ratios and reduce experimental trials, thereby bridging the gap between simulation and experimental materials science [17, 18]. Additionally, accurate Finite Element Analysis (FEA) necessitates mesh refinement, particularly in high-stress regions, to ensure result reliability and consistency across software and element types [19, 20, 21]. Another study confirms the efficacy of graphene and carbon black as reinforcing agents [22, 26], and validates computational modeling for predicting mechanical behavior [23, 24]. Research also highlights the impact of nanofiller reinforcement on polymer blends [25, 27]. Specifically, FEM simulation assesses tensile properties [22], RVE modeling evaluates mechanical properties [23], numerical models test composite vessels [24], and studies demonstrate nanofiller enhancement of polymer matrix composites [25, 27], all emphasizing the value of virtual experimentation in material optimization.

This study explores PP/PVC-based nanocomposites reinforced with graphene and carbon black, analyzing their mechanical properties. Using Digimat for material modeling and CATIA for FEA simulations on ASTM D638 specimens, it optimizes deflection and stress predictions. An economic analysis assesses cost-effectiveness, emphasizing virtual experimentation to reduce physical prototyping needs.

EXPERIMENTAL

A virtual experimental approach was adopted to optimize nanocomposite material's mechanical performance and cost-effectiveness. The study involved the creation of a homogeneous mixture of graphene, carbon black, PP and PVC using Digimat for material modeling. The obtained material properties—density, Poisson’s ratio, and Young’s modulus—were then used in CATIA to conduct a Finite Element Analysis (FEA) on a standard ASTM D638 tensile specimen. The results were validated by varying mesh sizes to optimize deflection and Von Mises stress. The goal was to determine the best material composition for specific applications without physical experimentation.

Experimental Design

This experiment details the composition of various polymer nanocomposites. It explores three different material systems: polypropylene with graphene (PP/G), blends of polypropylene and polyvinyl chloride with graphene (PP/PVC/G), and blends of polypropylene and polyvinyl chloride with carbon black (PP/PVC/CB). The table 1, systematically varies the weight percentages of the nanofillers (graphene or carbon black) within each polymer matrix, allowing for the study of how these additions affect the material properties. The PP/PVC blends are created in 60/40, 50/50, and 40/60 weight ratios, providing further compositional control. Each unique composition is assigned a specific code for easy identification. The letter "G" denotes graphene, and "CB" denotes carbon black. The number following "G" or "CB" indicates the nanomaterial content in weight percent (wt%), multiplied by 10 to keep the code concise. In this experiment the code P6V4G05 signifies a nanocomposite made of a 60/40 blend of PP and PVC with 0.5 wt% graphene added as a nanofiller and code P4V6-C75 signifies a nanocomposite made of a 40/60 blend of PP and PVC with 7.5 wt% carbon black added as a nanofiller. The selection of 60/40, 50/50, and 40/60 PP/PVC blend ratios was driven by the need to explore the effect of compositional variations on the final nanocomposite properties. These ratios were chosen to systematically observe changes in the relative amounts of PP and PVC influence on the mechanical behaviour especially when combined with nanofiller incorporation.

Table 1. Design of Experiments with variation in wt.% of polymer blend and nanocomposite.

Composition	Polymer Composition (wt. %)	Variation (Nanocomposite wt.%)	Experiment Code
PP/G	Neat PP	Graphene 0.5,1,1.5 %	PP-G05, PP-G10, PP-G15
PP/PVC/G	PP/PVC 60/40, 50/50, 40/60 wt./wt. %	Graphene 0.5,1,1.5 %	P6V4-G05, P6V4-G10, P6V4-G15, P5V5-G05, P5V5-G10, P5V5-G15, P4V6-G05, P4V6-G10, P4V6-G15
PP/PVC/CB	PP/PVC 60/40, 50/50, 40/60 wt/wt %	Carbon Black 2.5,5,7.5 %	P6V4-C25, P6V4-C50, P6V4-C75, P5V5-C25, P5V5-C50, P5V5-C75, P4V6-C25, P4V6-C50, P4V6-C75

Material Preparation in Digimat

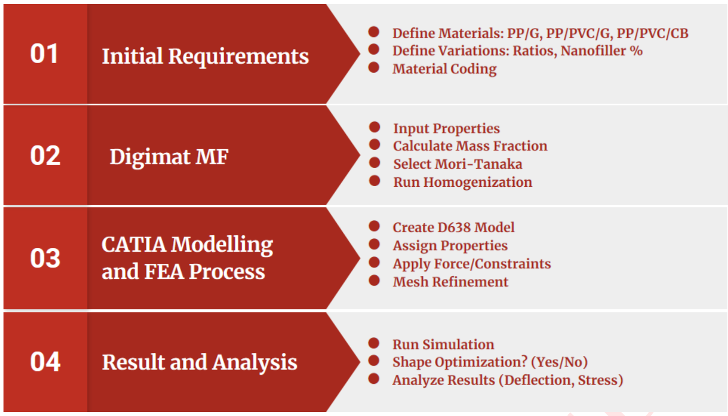

Figure 1. Workflow for virtual design and FEA of a D638 tensile specimen, including material selection, composite modeling, meshing, and simulation to assess mechanical performance.

The process of material characterization using Digimat MF involved a detailed, multi-step approach to predict the effective properties of the composite materials as shown in figure 1. For each distinct composite formulation and the neat PP and PVC, specific input parameters were defined within Digimat Mean Field (MF) Homogenization. For the matrix polymers (PP and PVC), the elastic properties, namely Young's modulus and Poisson's ratio, were specified, along with their respective densities. These values were obtained from material datasheets. Similar properties were input for the nanofillers, graphene, and carbon black, as well as Young's modulus, Poisson's ratio, and density. These values were also taken from material datasheets. Crucially, the geometry of the fillers was also defined. The morphology of the composite was then characterized by defining the filler mass fraction, which was directly calculated from the weight percentages used in the experimental formulations. Assumptions regarding filler orientation were made. Once all constituent and morphological parameters were defined, an appropriate micromechanical model within Digimat MF was selected. The choice of model ‘Mori-Tanaka’ depended on the specific composite system and the desired level of accuracy. The selected model then calculated the homogenized, or effective, properties of the composite material, including Young's modulus, Poisson's ratio, and density. These output values, representing the overall mechanical behavior of the composite, were then used as input parameters for the subsequent finite element analysis.

Finite Element Analysis (FEA) in CATIA

Finite Element Analysis (FEA) was conducted to simulate the tensile behavior of a D638 tensile test specimen. Material properties, including density, Poisson's ratio, and Young's modulus, were obtained using Digimat, a software tool for composite material characterization. A virtual model of the D638 test specimen was created in CATIA, conforming to the standard's specifications. These material properties were then assigned to the virtual specimen within CATIA's material library. A tensile force of 1 kN was applied along the longitudinal axis of the specimen to simulate a tensile test. One end of the specimen was fully constrained, while the opposite end experienced the applied force. CATIA's FEA solver was employed to calculate the deflection and Von Mises stress distribution within the specimen under the 1 kN load. The resulting deflection and Von Mises stress contours were analyzed to identify potential failure points and assess the overall deformation. This simulation enabled the prediction of the specimen's mechanical response under the defined loading conditions, providing insights into its structural integrity and informing design optimization.

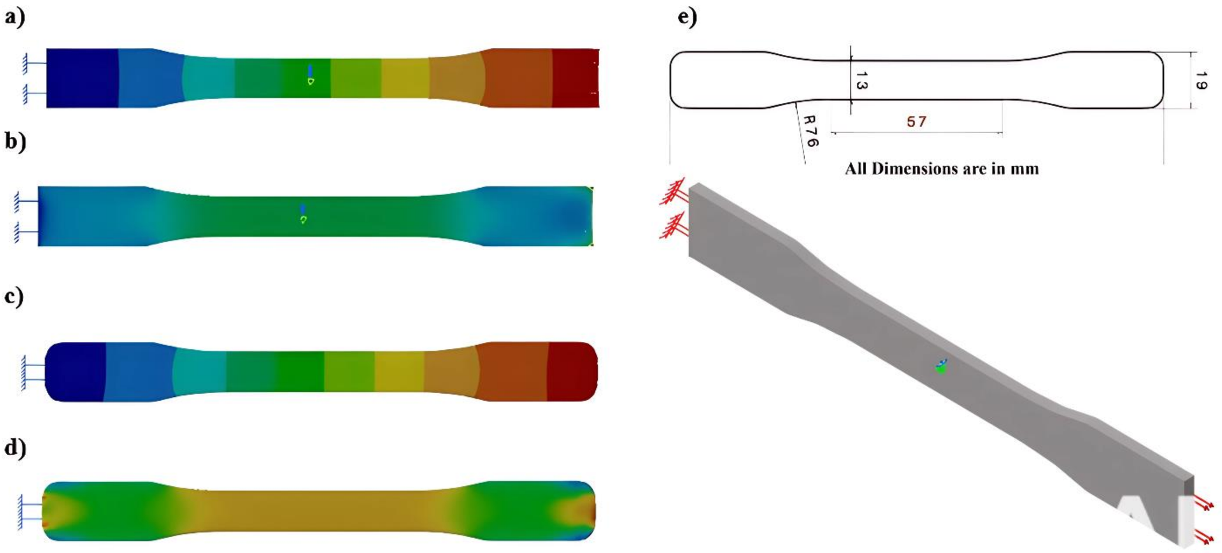

Figure 2. Comparison of D638 tensile test specimen performance under 1kN load (a-b) Normal Shape: Deflection and Von Mises stress. (c-d) Optimized Shape: Deflection and Von Mises stress. (e) Specimen Details: Dimensions and loading condition.

Figure 2, illustrates the impact of shape optimization on stress concentration in a D638 tensile test specimen. The normal specimen shape (a-b) exhibits sharp corners which induce significant stress concentrations and lead to inaccurate Von Mises stress calculations. This is contrasted with the optimized specimen shape (c-d), where sharp corners have been removed, effectively reducing stress concentration and resulting in more accurate Von Mises stress readings. Figure 1(e) shows that the specimen is fixed at one end and subjected to a 1kN load at the other. Also it provides detailed dimensions and loading conditions optimized specimen shape. The shape optimization, specifically the removal of sharp corners, demonstrably improves the accuracy of stress analysis.

Mesh Refinement Study

A mesh refinement study was conducted to assess the convergence of the Finite Element Analysis (FEA) solution for the tensile test specimen, both with and without shape optimization. The study aimed to determine an appropriate mesh density that would provide accurate results while minimizing computational cost. Six different mesh sizes were evaluated (Table 2 and 3), characterized by the Octree Tetrahedron element size, ranging from a coarse mesh of 10.325 to a fine mesh of 0.313.

For each mesh size, the maximum Von Mises stress (measured in N/m²) and deflection (measured in mm) were recorded for both the baseline geometry (without shape optimization) and the optimized geometry. The relative error in both Von Mises stress and deflection was calculated, presumably with respect to the finest mesh solution (0.313), to quantify the convergence behavior.

Table 2. Mesh Refinement Results for Baseline Geometry (with normal shape).

Sample Number	Octree Tetrahedron mesh size	Max. Von Mises stress (N/m2)	Deflection (mm)	Relative error in Von Mises stress (%)	Relative error in deflection (%)
1	10.325	23189030	2.31	11.63985729	-1.298701299
2	5	25888200	2.34	88.73965745	-1.188034188
3	2.5	48861300	2.3678	14.2040838	0.302390405
4	1.25	55801600	2.36064	13.61896433	2.077402738
5	0.625	63401200	2.3116	112.8619017	-0.85308877
6	0.313	134957000	2.33132	N/A	N/A

Table 3. Mesh Refinement Results for Optimized Geometry (with optimized shape).

Sample Number	**Octree Tetrahedron mesh size**	**Max. Von Mises stress(N/m2)**	**Deflection (mm)**	**Relative error in Von Mises stress (%)**	**Relative error in deflection (%)**
1	10.325	38628100	2.433732	-3.522824058	0.048156494
2	5	37267300	2.43256	3.387956734	-0.284885059
3	2.5	38529900	2.43949	-3.054510912	-0.017626635
4	1.25	37353000	2.43992	46.22761224	-0.349191777
5	0.625	54620400	2.44844	62.03872546	0.015111663
6	0.313	88506200	2.44807	N/A	N/A

Table 4. Mesh Size, nodes and Elements for Optimized shape.

Sample Number	**Mesh Size**	**Nodes**	**Element**
1	10.325	2943	9819
2	5	3511	12512
3	2.5	3648	13044
4	1.25	9020	35490
5	0.625	198239	917543

As shown in table 4, mesh size decreases, nodes and elements increase, improving accuracy but raising computational costs. A 2.5 mesh size (3648 nodes, 13,044 elements) offers the best balance of detail and efficiency. Larger meshes reduce accuracy, while smaller ones demand excessive processing. Automatic mesh optimization ensures efficient simulations by adjusting density based on shape complexity.Octree Tetrahedron meshing in CATIA is an automated, flexible method for complex 3D geometries, optimizing accuracy while reducing preprocessing steps. Unlike structured hex meshing, it directly generates volume meshes, efficiently handling real-world imperfections. A 2.5 mesh size offers the best balance between accuracy and computational efficiency—finer meshes improve precision but increase processing demands, while coarser meshes reduce accuracy. Automatic mesh optimization further refines mesh density based on geometry. Compared to other CATIA meshing methods, Delaunay meshing provides better element quality but lacks automation, while advancing front meshing offers smoother transitions but struggles with irregular shapes. Octree remains superior for its adaptability and efficiency.

The optimized design consistently outperformed the normal design, exhibiting significantly lower error in both Von Mises stress and deflection across all mesh refinements (Figure 3). Specifically, at the 2.5mm mesh size, the normal shape showed 14.2% error in Von Mises stress and 0.3% in deflection, while the optimized shape had errors of -3.1% and -0.02%, respectively. Although finer meshes were explored, the 2.5mm mesh provided a suitable compromise for both shapes, with the optimized design demonstrating superior accuracy throughout the study.

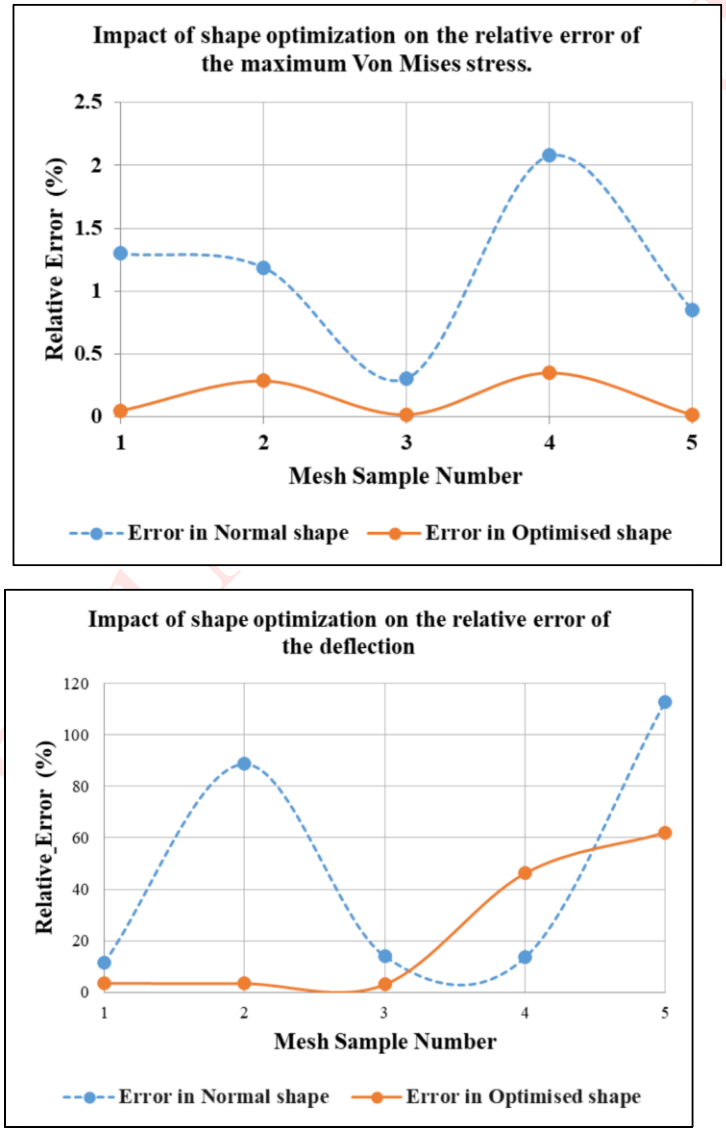

Figure 3. Comparison of mesh refinement effects on Deflection and Von Mises Stress Error for Normal and Optimized Shapes.

RESULTS AND DISCUSSION:

A combined computational and economic analysis was performed to identify viable alternatives to PVC. Various graphene and carbon black reinforced PP and PP/PVC blend composites were simulated to assess their mechanical behavior. Promising materials were further evaluated for cost effectiveness relative to PVC.

Deflection and Max. Von Mises Stress Calculation

Deflection (δ) was recorded from CATIA's simulation output. A CATIA simulation was conducted to evaluate potential replacement materials for PVC. Various plastic formulations were tested, including PP (polypropylene) based materials and variations of P4V6, P5V5, and P6V4, each reinforced with graphene ("G") or carbon black ("C") at different concentrations. The simulation measured deflection and maximum Von Mises stress under load for each material configuration. The results are displayed in table 4.

Table 5. Simulated Deflection and Von Mises Stress of Reinforced Composites.

Trial	Label	Deflection (mm)	Max Von Mises Stress (N/m2)	Trial	Label	Deflection (mm)	Max Von Mises Stress (N/m2)
1	PP-G05	2.42935	37362700	**14**	P6V4 C50	1.93463	37234500
2	PP-G10	2.41886	37372900	**15**	P6V4 C75	1.92462	37267800
3	PP-G15	2.40829	37382600	**16**	P5V5 C25	1.8183	37117000
4	P6V4G05	1.94452	37182400	**17**	P5V5 C50	1.81041	37146800
5	P6V4G10	1.93461	37193700	**18**	P5V5 C75	1.80241	37182900
6	P6V4G15	1.92481	37205500	**19**	P4V6 C25	1.68928	36990000
7	P5V5G05	1.81645	37089800	**20**	P4V6 C50	1.68355	37028500
8	P5V5G10	1.80694	37101800	**21**	P4V6 C75	1.6777	37068000
9	P5V5G15	1.79735	37114200	**22**	P4V6	1.69488	36952300
10	P4V6G05	1.6856	36965400	**23**	P5V5	1.82606	37077400
11	P4V6G10	1.67626	36977900	**24**	P6V4	1.9543	37170600
12	P4V6G15	1.66702	36991000	**25**	PP	2.43992	37353000
13	P6V4 C25	1.94453	37202100	**26**	PVC	1.13808	35788000

The table 5 presents the deflection (mm) and maximum Von Mises stress (N/m²) for various composite materials under testing. Deflection values indicate the material's flexibility, with lower values suggesting greater stiffness and structural integrity. Among the tested materials, PVC exhibits the lowest deflection (1.13808 mm), indicating its superior rigidity, whereas PP-G05 and PP variants have the highest deflection values (above 2.4 mm), making them less rigid. Notably, composites such as P4V6G15 (1.66702 mm), P5V5G15 (1.79735 mm), and P6V4G15 (1.92481 mm) show improved stiffness compared to polypropylene-based variants, making them potential alternatives to PVC in structural applications. The Carbon Black -series composites P6V4 C25, P5V5 C50, P4V6 C75) also demonstrate competitive deflection characteristics, further indicating their feasibility for cost-effective material substitution. This analysis helps in assessing the structural efficiency of different composite formulations for PVC replacement.

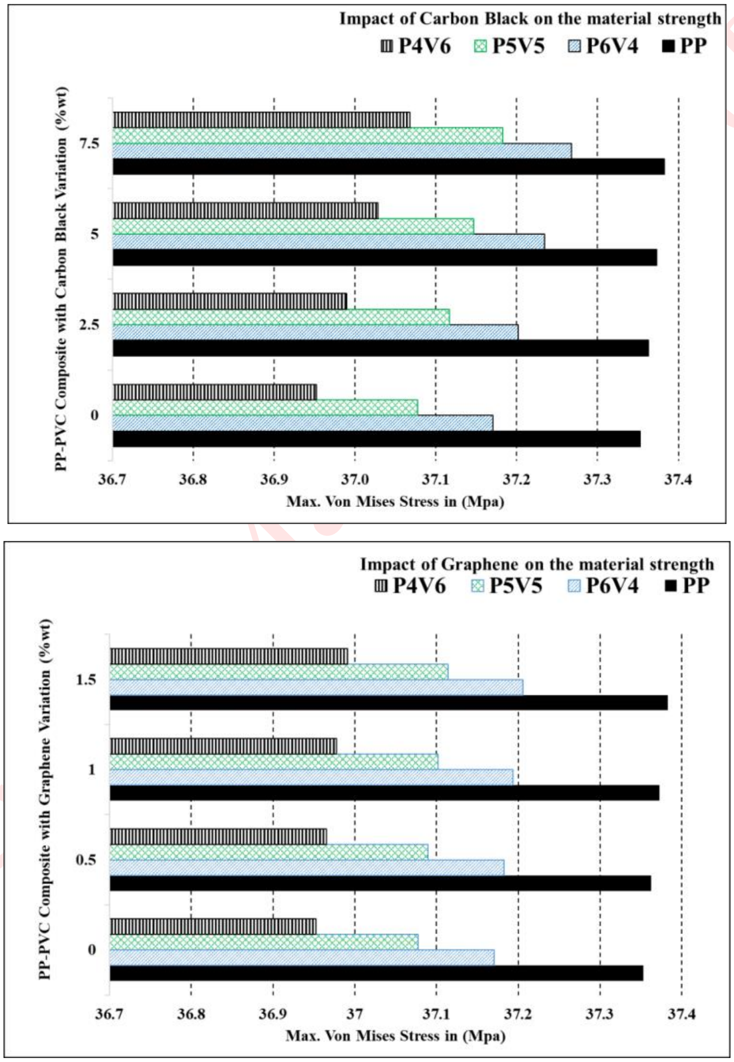

Figure 4. Variations in maximum Von Mises stress observed in PP/PVC blended nanocomposites with different weight percentages of carbon black and graphene.

As shown in figure 4, two bar graphs compare the maximum Von Mises stress of four material groups (PP, P4V6, P5V5, and P6V4) with varying amounts of graphene and carbon black reinforcement. Across both, PP consistently exhibits the highest stress, indicating the lowest resistance to stress. Conversely, P4V6 consistently demonstrates the lowest stress, suggesting superior stress management. P5V5 and P6V4 fall between these two extremes. Graphene reinforcement generally reduces stress more effectively than carbon black across the tested materials. While both reinforcements tend to lower stress, the impact of graphene is more consistent and pronounced. P4V6 exhibits the lowest stress regardless of reinforcement type or concentration, suggesting superior inherent stress resistance.

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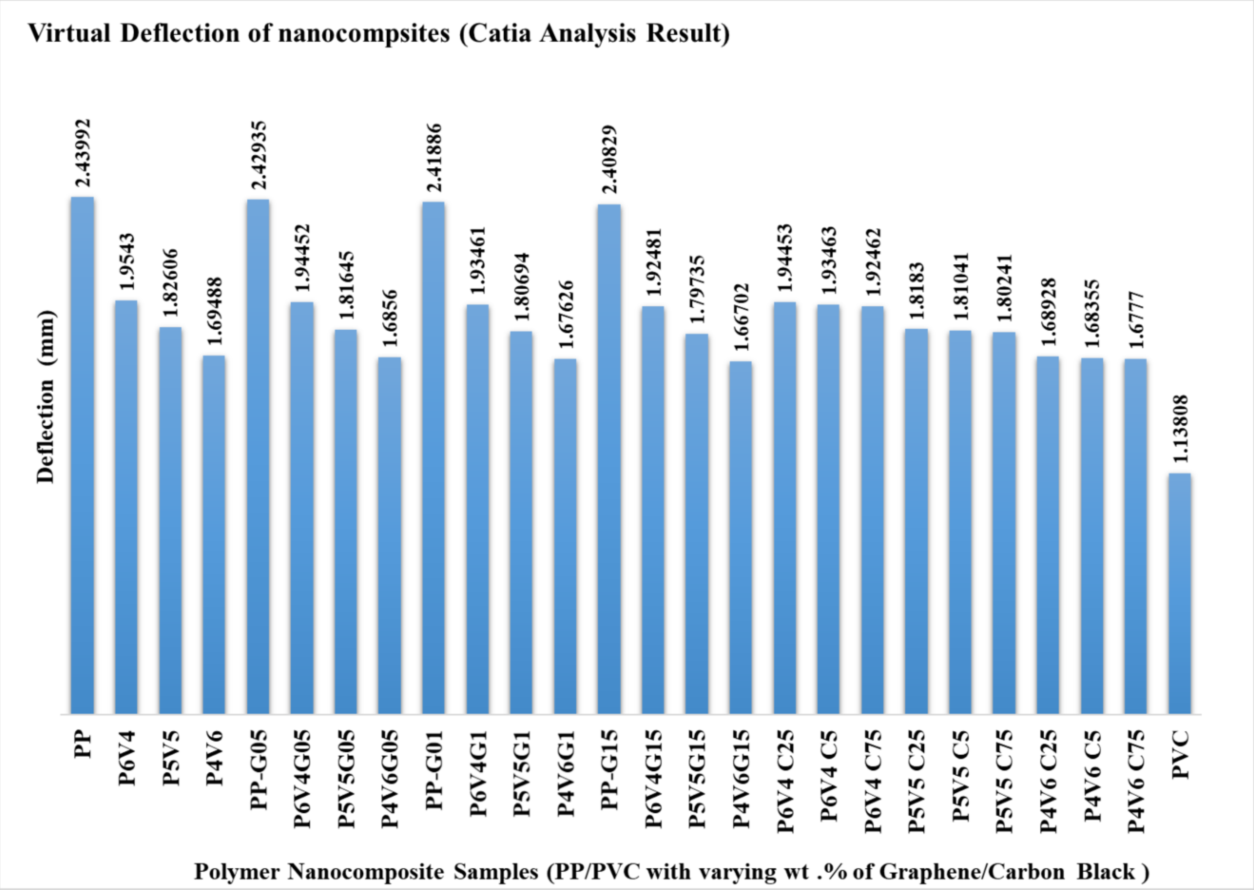

Figure 5. The virtual deflection of nanocomposites samples (Catia Analysis Result), shows the deflection of each material under a 1kN loading condition.

This figure 5 shows the deflection of various material compositions, exploring potential replacements for rigid PVC. While PVC exhibits the lowest deflection (1.138 mm), several promising alternatives emerge. Polypropylene (PP) demonstrates the highest deflection (2.440 mm), but reinforcing it with graphene leads to a reduction, indicating improved stiffness. The P4V6 blend, both with and without reinforcements, exhibits notably lower deflection than PP, suggesting inherent rigidity. Further reinforcing P4V6 with graphene or carbon black leads to even smaller deflections, with graphene showing a slightly more pronounced effect. Specifically, P4V6 with graphene reinforcement achieves the lowest deflection (1.667 mm) among the modified PPbased options. These results highlight the potential of P4V6, particularly with graphene, as a viable alternative to PVC, although it doesn't quite match PVC's stiffness. Further investigation and optimization of these blends, including exploring different reinforcement types and concentrations, could yield materials that more closely approach PVC's performance.

Validation

The validation process compares the mechanical properties of nanocomposites obtained from literature [27] with those predicted by Digimat software (Table 6). Specifically, Young's modulus values of PP-based composites with different graphene loadings (0.5%, 1%, and 1.5%) are evaluated. The actual material data from the literature and the virtual material data from Digimat show close agreement, with slight variations in Young's modulus values. For instance, PP-G05 has an actual modulus of 1184.3 MPa and a virtual modulus of 1211.3 MPa, maintaining a relative ratio of 1. The trend continues for higher graphene loadings, where the virtual predictions slightly overestimate or closely match the experimental values. This comparison demonstrates the reliability of Digimat in predicting mechanical behavior, reinforcing its utility in reducing experimental efforts while maintaining accuracy.

Table 6. Results of PP/G nanocomposites: Experimental and virtual vomparison.

Sr. No.	Nanocomposite	Physical Properties (Liturature) [27]		Virtual Properties (Digimat Softwere)	
		Young's Modulus (MPa)	Relative Young's Modulus Ratio	Young's Modulus (MPa)	Relative Young's Modulus Ratio
1	PP-G05	1184.3	1	1211.30	1
2	PP-G10	1207.2	1.0194	1218.38	1.0061
3	PP-G15	1432.2	1.2093	1225.89	1.0123

In actual material preparation and testing of nanocomposites, several influencing factors contribute to variations in experimental results, which are not considered in virtual simulations. Material properties may vary due to inherent inconsistencies, while differences in injection pressure, nanomaterial positioning within the composite, cooling time after injection, and injection temperature further impact the final material structure. Additionally, polymer compatibility, trapped gases within the sample, and potential testing errors introduce uncertainties that are unavoidable in physical experiments. These factors make it difficult to achieve an exact match between experimental and simulated data. However, despite numerical differences, virtual simulations generally capture the correct trend in strength variations**.**

Economic Analysis

A cost model was developed based on the price per unit weight of each component:

Cost Factor = [(Cg × Wg) + (Ccb × Wcb) + (Cpp × Wpp) + (Cpvc × Wpvc)]/100

Where:

Cost Factor: Represents the total cost.
Cg: Cost per unit weight of graphene.
Wg: Weight of graphene used.
Ccb: Cost per unit weight of carbon black.
Wcb: Weight of carbon black used.
Cpp: Cost per unit weight of polypropylene.
Wpp: Weight of polypropylene used.
Cpvc: Cost per unit weight of polyvinyl chloride.
Wpvc: Weight of polyvinyl chloride used.

Deflection Factor and Economic Factor Calculation

The Deflection Factor (DF) is calculated as:

DF = Deflection of tested composite / Deflection of standard PVC sample The Economic Factor (EF) is then determined using:

EF = Cost Factor × Deflection Factor

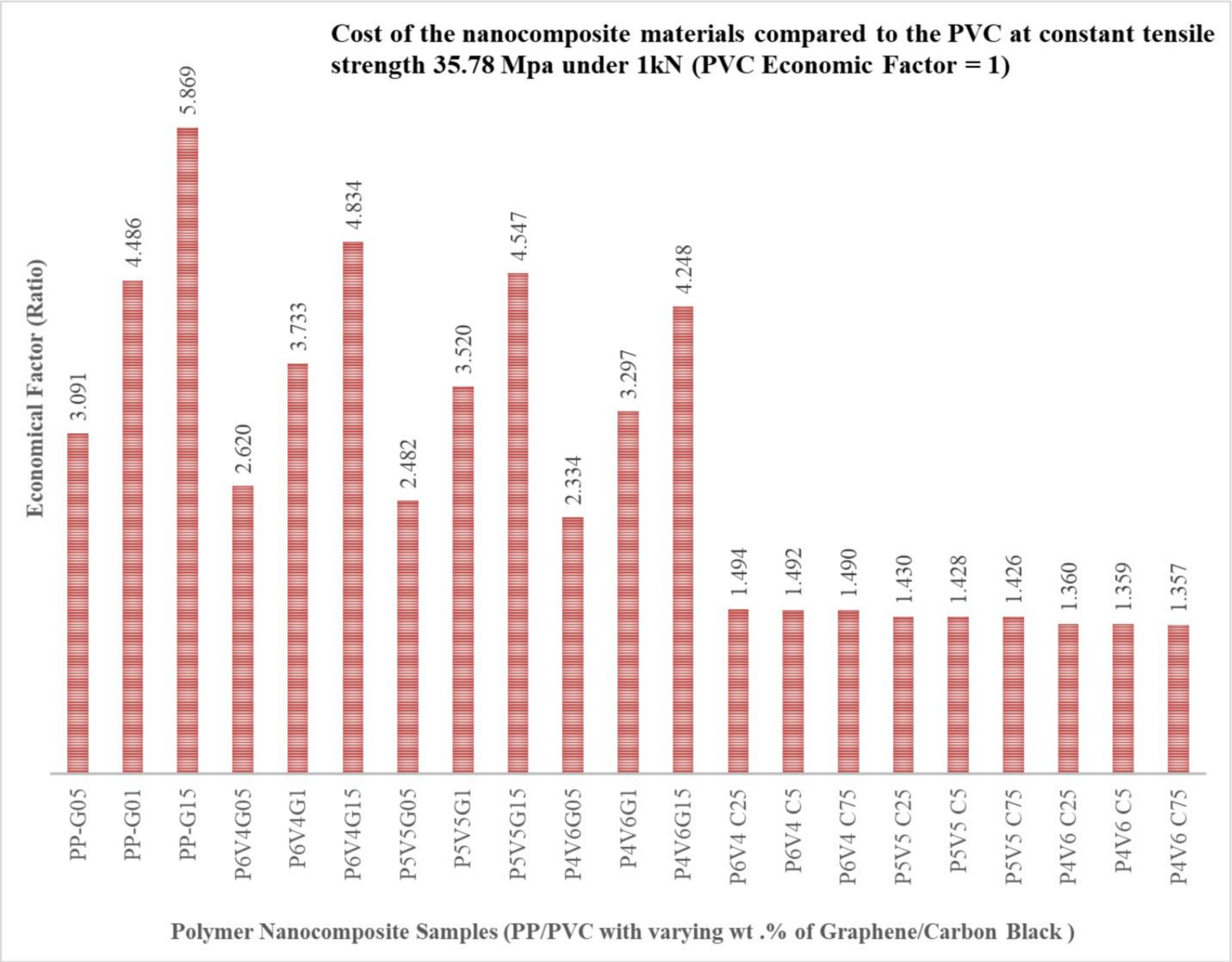

Figure 6. Economic factor of nanocomposite materials compared to PVC under a constant tensile strength of 35.78 MPa and 1kN load (PVC Economic Factor = 1).

This approach ensures a standardized comparison of composite materials based on both cost and strength performance relative to PVC. The Deflection Factor accounts for variations in composite deflection, establishing a baseline for comparison. It is calculated as the ratio of the deflection of a standard PVC sample to the deflection of the tested composite. This ensures that all materials are evaluated under a uniform reference. The Economic Factor, determined by Cost Factor Deflection Factor, assesses composites' cost-effectiveness and strength performance relative to PVC as a replacement material. The cost of materials per kilogram in USD, based on the average exchange rate of ₹83.68 per USD for FY2023–2024 in India, is as follows: Polypropylene (PP) is approximately $1.49/kg, Polyvinyl Chloride (PVC) is around $1.90/kg, Graphene stands out with a significantly higher cost of about $253.66/kg, and Carbon Black is priced at roughly $1.97/kg.

Based on the cost model and deflection factor, the economic analysis of various composites indicates (Figure 6) that lower economic factor values signify better cost-effectiveness and performance efficiency. The most economical composites are P4V6 C75, P4V6 C50, and P4V6 C25, with values 1.36, making them the most suitable alternatives to PP/PVC-based materials.

Moderately performing composites, such as P6V4 G05 (2.62), P5V5 G05 (2.48), and P4V6 G10 (2.33), offer a reasonable balance between cost and deflection performance. In contrast, PP-G15 (5.87), P6V4 G15 (4.83), and PV5V5 G15 (4.55) exhibit the highest economic factors, making them less favorable due to higher costs or suboptimal deflection performance. Overall, Series P4V6 blend with Carbon Black nanoparticles emerge as the most viable choices for cost-effective and efficient material selection.

This study employed a virtual experimentation approach, leveraging Digimat for material modeling and CATIA for FEA, to investigate the mechanical properties of PP/PVC nanocomposites with graphene and carbon black reinforcements. This methodology offers a costeffective and efficient alternative to traditional experimental methods, reducing the need for extensive physical prototyping and testing. The use of Digimat allowed for the prediction of essential material properties, including density, Poisson's ratio, and Young's modulus, which were then utilized in CATIA to simulate the tensile behavior of ASTM D638 specimens. By varying the mesh sizes, the study ensured the accuracy and convergence of the FEA results, validating the reliability of the predicted deflection and Von Mises stress values. This virtual approach accelerates the material development process and enables the exploration of a wider range of compositions and parameters, leading to optimized material design for specific applications. The successful implementation of this methodology highlights the potential of computational tools in material science to drive innovation and reduce development costs.

This economic analysis establishes a baseline for composite material comparison through a simplified cost model, focusing on direct material costs and deflection performance to derive the Economic Factor (EF). The model deliberately excludes complex cost factors, such as manufacturing overhead, labor, and long-term maintenance, to maintain clarity and enable a direct comparison based on readily quantifiable parameters. This simplification acknowledges the inherent variability and data acquisition challenges associated with those factors, particularly in early-stage research. Future research can build upon this foundation. It should incorporate a wider range of economic considerations to provide a more comprehensive assessment. This expansion will enhance the model's applicability to real-world scenarios and aid in informed decision-making for practical implementation.

An optimized nanocomposite of polypropylene (PP) and polyvinyl chloride (PVC), reinforced with carbon black and graphene, holds significant potential as a robust and efficient alternative to conventional PVC, opening doors to transformative applications across diverse industries. This innovative material presents possibilities for enhancing automotive interiors by potentially eliminating heat-induced odors and improving durability, while in the construction sector, it offers the prospect of replacing traditional PVC pipes and window frames to mitigate leaching and bolster long-term structural integrity. Within healthcare, there's potential for this composite to improve biocompatibility and sterilization efficiency in medical tubing and device casings. Furthermore, consumer goods like packaging, furniture, and sports equipment could benefit from this material's potential to deliver more durable and environmentally sustainable products. These applications illustrate the broad range of possibilities, positioning this nanocomposite as a high-performance, cost-effective, and sustainable solution poised to address critical industrial needs.

CONCLUSIONS

This research explored the potential of PP/PVC nanocomposites with graphene and carbon black reinforcements as alternatives to PVC, focusing on their mechanical properties and costeffectiveness. The key findings are:

- The PP/PVC blends, particularly the P4V6 series, showed promising inherent mechanical properties even before reinforcement. This suggests that the blending of PP and PVC in specific ratios can lead to materials with enhanced stiffness and potential for further improvement through reinforcement.
- Both graphene and carbon black nanofillers contributed to improved mechanical properties of the PP/PVC blends. However, graphene reinforcement generally led to enhancements in stiffness compared to carbon black.
- Increasing the concentration of both graphene and carbon black generally resulted in a reduction in deflection, indicating improved stiffness. However, the effect of graphene was more pronounced compared to carbon black.
- The economic analysis revealed that the P4V6 series composites with carbon black reinforcement (P4V6 C25, P4V6 C50, P4V6 C75) offer the best balance of costeffectiveness and performance. These materials exhibited a lower economic factor, making them economically attractive alternatives for various applications. Specifically, P4V6 C75, with its higher carbon black content, demonstrated the lowest economic factor while maintaining competitive mechanical properties.

Virtual experiments using Digimat and CATIA efficiently optimize PP/PVC nanocomposites with graphene and carbon black by predicting nanofiller effects on mechanical behavior. These simulations reduce experimental efforts, but ASTM D638 tensile tests remain essential for precise validation. To enhance accuracy, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) assess nanofiller dispersion and validate virtual models by revealing real material structures. Additionally, artificial intelligence (AI) and machine learning (ML) can be trained using past experimental data to refine predictions, optimize input parameters, and improve simulation reliability. By integrating AI, SEM/TEM validation, and standardized testing, the development of PP/PVC nanocomposites becomes more efficient that allows the creation of advanced materials with enhanced mechanical performance.

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REFERENCES:

1. Patil UA, Kubade PR (2024) The importance of alternative materials to PVC and effective plastic waste management strategies for a better future. In: Advancements in materials processing technology, R. Sahu, R. Krishna, R. Prasad (Eds.), Vol 2, 127-136 [CrossRef]
2. Patil UA, Kubade PR (2024) Exploring health risks of PVC and investigating potential alternatives through mechanical analysis and simulation. J Inst Eng (India) - C 105: 1571-1580 [CrossRef]
3. Patil UA, Kubade PR (2023) Recent advances in ternary blends of nanocomposite and their impact on the mechanical and thermal properties: A review. In: Proceedings of the International Conference on Applications of Machine Intelligence and Data Analytics. [CrossRef]
4. Painkal SK, Balachandran M, Jayanarayanan K, Sridhar N, Kumar S (2025) Synergistic enhancement in mechanical properties of graphene/MWCNT reinforced polyaryletherketone – carbon fiber multi-scale composites: Experimental studies and finite element analysis. Adv Ind Eng Polym Res 8: 20-36 [CrossRef]
5. Chaudhary N, Dikshit M (2021) A state of art review on the graphene and carbon nanotube reinforced nanocomposites: A molecular dynamics approach. Mater Today 47: 3235-3241[CrossRef]
6. Patra SC, Swain S, Senapati P, Sahu H, Murmu R, Sutar H (2022) Polypropylene and graphene nanocomposites: Effects of selected 2D-nanofiller's plate sizes on fundamental physicochemical properties. Inventions 8: 8 [CrossRef]
7. Innes JR, Young RJ, Papageorgiou DG (2022) Graphene nanoplatelets as a replacement for carbon black in rubber compounds. Polymers 14: 1204 [CrossRef]

8. Farida E, Bukit N, Ginting EM, Bukit BF (2019) The effect of carbon black composition in natural rubber compound. Case Stud Therm Eng 16: 100566 [CrossRef]
9. Kim BJ, White JL (2004) Compatibilized blends of PVC/PA12 and PVC/PP containing poly(lauryl lactam-block-caprolactone). J Appl Polym Sci 91: 1983-1992 [CrossRef]
10. Toprakci O, Akcay AT, Toprakci HAK (2024) Enhancing calendering process conditions by blending poly(vinyl chloride) with polyethylene, polypropylene and poly(methyl methacrylate). Mater Sci Res India 21: 210203 [CrossRef]
11. Al-Arbash A, Al-Sagheer F, Ali A, Ahmad Z (2005) Thermal and mechanical properties of poly(hydroxy-imide)-silica nanocomposites. Int J Polym Mater 55: 103-120 [CrossRef]
12. Murthe SS, Sreekantan S, Mydin RBSMN (2022) Study on the physical, thermal and mechanical properties of SEBS/PP (styrene-ethylene-butylene-styrene/polypropylene) blend as a medical fluid bag. Polymers 14: 3267 [CrossRef]
13. Samira M, Ahmed M, Nadia N, Mohamed S, Rachida Z (2013) Thermal and mechanical properties of PVC and PVC-HDPE blends. Res Rev J Mater Sci 1: 6-11 [CrossRef]
14. Trzepieciński T, Ryzińska G, Biglar M, Gromada M (2017) Modelling of multilayer actuator layers by homogenisation technique using Digimat software. Ceramics Int 43: 3259-3266 [CrossRef]
15. Nayak B, Sahu RK (2019) Experimental and Digimat-FE based representative volume element analysis of exceptional graphene flakes/aluminium alloy nanocomposite characteristics. Mater Res Exp 6: 116593 [CrossRef]
16. Landervik M, Jergeus J (2015) Digimat material model for short fiber reinforced plastics at Volvo Car Corporation. In: 10th European LS-DYNA Conference.
17. Magidov I, Mikhaylovskiy K, Shalnova S, Topalov I, Gushchina M, Zherebtsov S, Klimova-Korsmik O (2023) Prediction and Experimental Evaluation of Mechanical Properties of SiC-Reinforced Ti-4.25Al-2V Matrix Composites Produced by Laser Direct Energy Deposition. Materials 16: 5233 [CrossRef]
18. Kumar SA, Narayan YS (2019) Tensile testing and evaluation of 3D-printed PLA specimens as per ASTM D638 type IV standard. Lecture Notes in: Innovative Design, Analysis and Development Practices in Aerospace and Automotive Engineering (I-DAD 2018), Chandrasekhar U, Yang LJ, Gowthaman S (eds), Springer, pp: 79-95 [CrossRef]
19. Chang KH, Choi KK (1992) An error analysis and mesh adaptation method for shape design of structural components. Comput Struct 44: 1275-1289 [CrossRef]
20. Jalammanavar K, Pujar N, Raj RV (2018) Finite element study on mesh discretization error estimation for Ansys workbench. In: 2018 International Conference on Computational Techniques, Electronics and Mechanical Systems (CTEMS): 344-350 [CrossRef]
21. Sanjaya Y, Prabowo AR, Imaduddin F, Binti Nordin NA (2021) Design and analysis of mesh size subjected to wheel rim convergence using finite element method. Procedia Structural Integrity 33: 51-58 [CrossRef] 10.1016/j.prostr.2021.10.008
22. Sahu SK, Sreekanth PR (2023) Evaluation of tensile properties of spherical shaped SiC inclusions inside recycled HDPE matrix using FEM based representative volume element approach. Heliyon 9: e14034 [CrossRef]
23. Sahu SK, Sreekanth PR, Devaraj S, Kumar VR, Phanden RK, Saxena KK, Ma Q (2024) Assessment of mechanical properties by RVE modeling and simulation of recycled HDPE reinforced with carbon nanotubes. Int J Int Des Manuf (IJIDeM) 19: 2143-2157 [CrossRef]

24. Badgayan ND, Sahu SK, Samanta S, Sreekanth PR (2018) Assessment of bulk mechanical properties of HDPE hybrid composite filled with 1D/2D nanofiller system. Mater Sci Forum 917: 12-16 [CrossRef]
25. Yesaswi CS, Sahu SK, Sreekanth PR (2022) Experimental investigation of electro-mechanical behavior of silver-coated teflon fabric-reinforced nafion ionic polymer metal composite with carbon nanotubes and graphene nanoparticles. Polymers 14: 5497 [CrossRef]
26. Pradhan S, Sahu SK, Pramanik J, Badgayan ND (2022) An insight into mechanical & thermal properties of shape memory polymer reinforced with nanofillers; a critical review. Mater Today 50: 1107-1112 [CrossRef]
27. Sanaka R, Sahu S, Sreekanth PR, Giri J, Mohammad F, Al-Lohedan HA, Saharudin MS, Ma Q (2025) Heat-responsive PLA/PU/MXene shape memory polymer blend nanocomposite: Mechanical, thermal, and shape memory properties. Polymers 17: 338 [CrossRef]
28. Zhao X, Huang D, Ewulonu C, Wu M, Wang C, Huang Y (2021) Polypropylene/graphene nanoplatelets nanocomposites with high conductivity via solid-state shear mixing. e-Polymers 21: 520-532 [CrossRef]