IPPI
Polyolefins Journal, Vol. 11, No. 3 (2024)
DOI: 10.22063/POJ.2024.3604.1302
ORIGINAL PAPER

A study of polypropylene and graphene and their nanocomposites using ANSYS

Aamir M. Shaikh[1] and Pravin R. Kubade[2*]

[1]Shivaji University, Kolhapur, Maharashtra, India
[2]Shri Guru Gobind Singhji Institute of Engineering and Technology (SGGSIE&T), Nanded, Maharashtra, India

Received: 10 April 2024, Accepted: 6 June 2024

ABSTRACT

Polymers can be natural or synthetic and are largely used in several applications due to their versatile properties. Polymers can vary widely in their properties and applications, and they are a fundamental part of our everyday life. Polypropylene (PP) is a thermoplastic polymer from the polyolefin family. It is among the most widely used plastics in various automotive and packaging industries. Although PP is widely used in commodity range, still its applications are restricted in niche areas due to lack of toughness which can be improved by incorporation of rubbery materials or fillers. Graphene (G) is one of the nanomaterials used to strengthen polypropylene. Graphene is recognized for its outstanding thermo-mechanical properties, making it a highly desirable material in various fields of science and technology. Benefits gained by incorporation of graphene nanoparticles into polypropylene are studied by researchers. In this study, a finite element analysis is performed which shows the mechanical behaviour of PP and G using ANSYS, which is one of the most powerful finite element analysis (FEA) softwares that can help to perform such simulations to understand stress, strain, deformation of components before actual experimentation. The bending load of 100 N and 1400 N in vertical z-direction are applied for 100% PP model, 100% G model and 50% PP+50% G model and the linear part of stress-strain curve is captured in this analysis. **Polyolefins J (2024) 11: 155-166**

Keywords: Polypropylene, graphene nanoparticles, von-Mises stress, finite element analysis.

INTRODUCTION

Polymer refers to a type of material that consists of large molecules made up of repeating sub-units called monomers. Polypropylene is produced through the polymerization of propylene monomers. These monomers bond together to form a long chain-like structure. Polymers are a vital class of materials that have revolutionized many industries and technologies due to their versatility, durability, and ease of processing. Polymer nanocomposites are advanced materials formed by combining polymers with nanoscale filler materials, known as nanoparticles. These nanoparticles typically have at least one dimension is of 1 to 100 nanometres. The merger of nanoparticles into polymer matrix leads to improved material properties, making nanocomposites an exciting area of research and development [1].

Mechanical testing of polymer nanocomposites is crucial to assess their mechanical characteristics and performance. These materials combine polymers with nanoscale fillers (such as nanoparticles, nanotubes,

*Corresponding Author - E-mail: pravinrkubade@gmail.com

CC BY NC SA

or nanoclays) to enhance thermo-mechanical and electrical characteristics. Mechanical testing methods like hardness, tensile, flexural (bending), impact, compression, fatigue test, etc., are used for polymer nanocomposites [2].

Tensile test measures a material's response to stretching forces. It provides information about tensile strength, elongation-at-break, Young's modulus, and other mechanical properties. For nanocomposites, it helps determine how the inclusion of nanoparticles affects the material strength and stiffness. Flexural testing (also known as bending testing) evaluates a material response to bending forces. It is particularly useful for assessing the flexural modulus and strength of polymer nanocomposites [3]. Impact testing assesses a material ability to withstand sudden loads or impacts. This is important for applications where the material needs to absorb energy in impact events. Hardness measures a material's resistance to permanent deformation under localized loading. Nanoindentation, a technique that uses an indenter to create a small indentation on the material surface, is used to check the hardness of nanocomposites at very small scales [4].

Compression testing involves applying compressive forces to a material to check its behaviour under such loading conditions. It is relevant for applications where the nanocomposite may experience compression forces. In wear and abrasion testing it evaluates a material resistance to wear and abrasion, which is important in applications where the material is subject to friction and sliding contact. Tribological properties of polymer nanocomposites can be significantly influenced by the inclusion of nanoparticles [5]. Creep tests measure the material response to a constant load over time, while stress relaxation tests measure the reduction in stress under constant strain. These tests are important for understanding the material long-term behaviour under constant loads [6]. Dynamic mechanical analysis (DMA) involves subjecting the material to a range of mechanical forces, including oscillatory forces, at various temperatures. It provides insights into the material viscoelastic behaviour, glass transition temperature, and damping properties [7]. Choice of testing methods based on the specific properties of interest and the intended application of the polymer-nanocomposite (PNC) material. Additionally, these tests may need to be adapted or modified to account for the unique characteristics introduced by the nanoscale fillers [8]. In past decades, many melt mixing/fabrication techniques are used to prepare the polymer nanocomposites with different concentration of fillers to make it ready for specific application [9]. However, it is observed that no work is reported on characterization of PP/G nanocomposites by using finite element analysis technique at various loads and static condition.

This study uses FEA software ANSYS to learn the deflection/deformation and stress of polypropylene (PP), graphene (G) and their nanocomposites (PP/G) preparing its 3-D model, which will eliminate the cost of characterization as well as time.

Polypropylene (PP)

Polypropylene has high chemical resistance. It resists different types of chemicals, making it suitable for various applications involving exposure to acids, bases, and other corrosive substances. Polypropylene (PP) is a lightweight material, making it model for claims where mass is a concern, such as in automobile and aerospace industries [10]. PP shows good mechanical strength and toughness, making it durable and able to withstand moderate impacts and loads. Polypropylene has limited water absorption rate, which is beneficial for applications requiring minimal water absorption. PP is an excellent electrical insulator, making it useful in electrical and electronic applications [11]. A melting point is slightly high for PP as compared to other, making it fit for applications involving high temperature environments. PP is recyclable, contributing to its popularity as a sustainable material in the plastics industry [12, 13].

Applications of polypropylene:

- PP is normally used in packaging industry like food packaging, bottles, containers, and bags, moisture resistance, and capacity to maintain the freshness of food products [14, 15].
- PP fibres are used textile applications like carpets, rugs, geotextiles, and various industrial fabrics [16].
- PP is utilized in the automobile sector for interior components, such as dashboards, door panels, and trims, because of its lightweight [17,18].
- In the production of toys, furniture, household appliances, and various consumer products [19].
- Due to chemical resistance and strength, PP is also utilized in various industrial applications like pipes, different fittings, containers, etc. [20, 21].

In general, polypropylene is a versatile and widely used material with numerous applications across various industries, owing to its favourable properties and cost-effectiveness [32].

Graphene (G)

In graphene, carbon atoms are organized in single layer 2-D honey-comb lattice structure which imparts better thermo-mechanical and electrical properties. Graphene has sparked a widespread choice of research efforts and has led to the growth of various applications. However, despite its incredible potential, there are challenges in producing high-quality graphene at large scales and integrating it into practical applications. Researchers are endlessly discovering ways to overcome these challenges and unlock graphene's full potential for various industries [22].

Graphene is the basic structural element of other carbon allotropes, such as graphite, carbon nanotubes. Graphene is an excellent conductor of electricity, due to its unique structure. It is suitable for applications in electronics and conductive materials. Graphene is incredibly strong and has a high strength in tensile [23]. Graphene exhibits exceptional thermal conductivity, making it suitable for claims where effective heat transfer is crucial, such as in thermal management systems. [24, 25].

Graphene's potential applications are vast and include:

- Graphene-based material used in energy storage in batteries, supercapacitors. Also used in storage of energy due to their high surface area and conductivity [26, 27].
- Graphene is used in for various sensor applications, including chemical and biological sensing [28, 29].
- Graphene can be incorporated into composite materials to enhance their mechanical and thermo-mechanical properties [30].
- Graphene-based materials could be used in drug delivery due to their unique properties [32].

In spite of its huge potential, there are some challenges to overcome making graphene suitable for large scale production, cost effectiveness, and integration into practical devices. Researchers continue to work on these issues to unlock graphene's full range of applications.

Researcher used polypropylene (as a base material) and graphene nanoparticles to enhance mechanical properties of pristine polypropylene. This study aims to perform liner analysis using ANSYS Workbench wherein two sets of loads 100 N and 1400 N are applied to study the deformation/stress within the component with 100% PP, 100% G and 50% PP+50% G. The nanocomposites are prepared by different processes like melt mixing, ultra-sonication, extrusion, injection moulding, etc.

BOUNDARY CONDITIONS

To perform the finite element analysis (FEA), the important steps are pre-processing, solution and post-processing. First and most important step in FEA is pre-processing for that material selection, 3-D modeling, conditions at boundary like fixed surface/s, force applied with its direction/s are the parameters. By referring the ASTM standard, the 3D model is constructed having dimension 90 mm length along x-axis, 10 mm width along y-axis and 2.5 mm thick along z-axis (90 × 10 × 2.5 mm) used for flexural (bending) test. The two side surfaces (in the YZ plane) are fixed, and force is applied in vertical downward direction on top surface as shown in Figure 1.

In the first trial, pure polypropylene material is applied, in the second trial, pure graphene material is applied and in the third trial, composite material is applied.

The properties of polypropylene (PP) and graphene (G) are shown in Table 1. For this analysis, the important properties are density of material, Young's modulus and Poisson's ratio, etc.

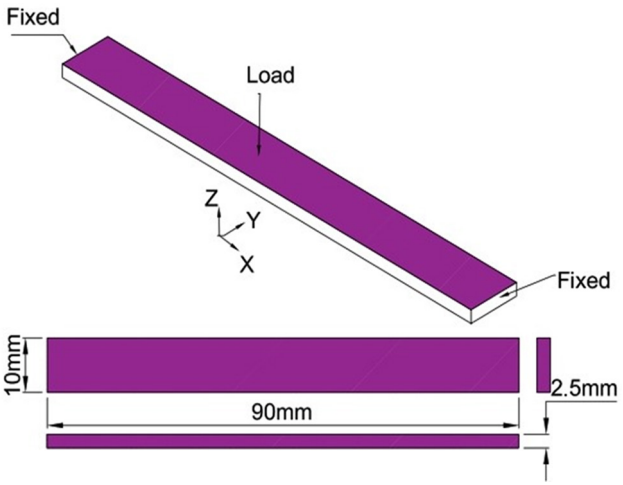


Figure 1. Three-dimensional object with boundary conditions.

Table 1. Nanocomposite materials properties [15, 27].

Properties	Polypropylene (PP)	Graphene (G)
Density (kg/m^3)	910	2267
Young's modulus (Pa)	1.1E+09	1E+12
Poisson's ratio	0.42	0.19

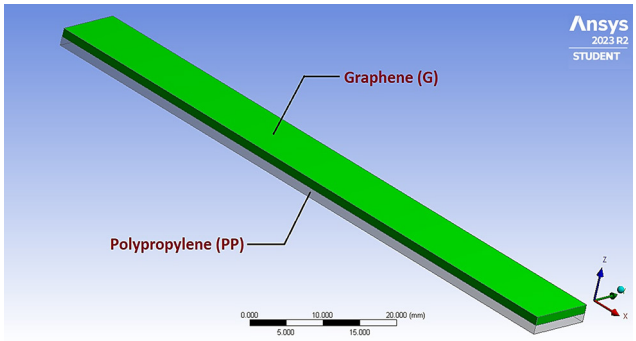


Figure 2. Composite of polypropylene (PP) and graphene (G).

In case of third trial (composite), the Design Modular of ANSYS is used to construct 3D model. The upper 3D model is constructed for graphene (G) while the lower 3D model is constructed for polypropylene (PP) as shown in Figure 2. The dispersion of nanoparticles adjusts its capacity to contribute to its properties in the composite. The strengthening of the composites depends on volume/weight percentage of nanoparticles added into the matrix. Incorporating nanomaterials at low weight percentage enhances the mechanical properties. In some cases, it is also found that the mechanical properties enhance with increase in the weight percentage of nanoparticles. In this perspective two-layer three-dimensional samples are prepared to obtain strengthening effect on the composite model. Initially the two-layer model is selected as a benchmark to study the behavior of the composite. However, different strengthening mechanisms can be obtained by increasing the layers with optimal weight

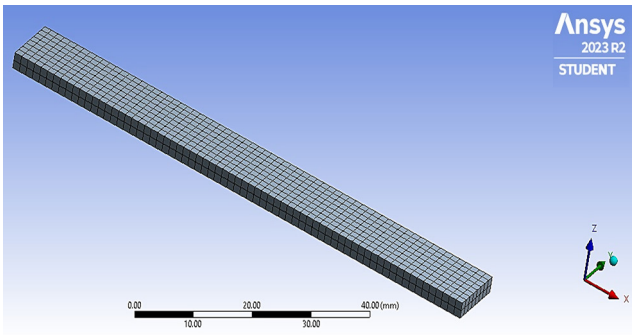


Figure 3. Meshing.

percentage of nanoparticles.

Discretization: In discretization step, the whole component is divided into number of parts [31]. Auto mesh generation with fine mesh control option in ANSYS workbench takes place with number of 1104 elements and 6693 nodes as shown in Figure 3.

After applying two side surfaces fixed and force value, software solves the elemental stiffness equation. Solution is converged at 36 iterations for displacement and force as shown in Figures 4 and 5, respectively.

The von-Mises rule is used to eliminate the failure of fragile materials for which the von-Mises stress is considered very low in comparison with the yield stress as per the standard for which following is the mathematical equation:

$$\sigma_{VM} \leq \sigma_y$$

Where, σ_{VM} = von-Mises stress.
σ_y = Yield stress.

$$\sigma_{VM} = \frac{1}{\sqrt{2}}\sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}$$

σ_1, σ_2 and σ_3 are principal stresses along x, y and z axis, respectively. In the cases of plane stress, $\sigma_3 = 0$. Also, the following governing equation and elemental

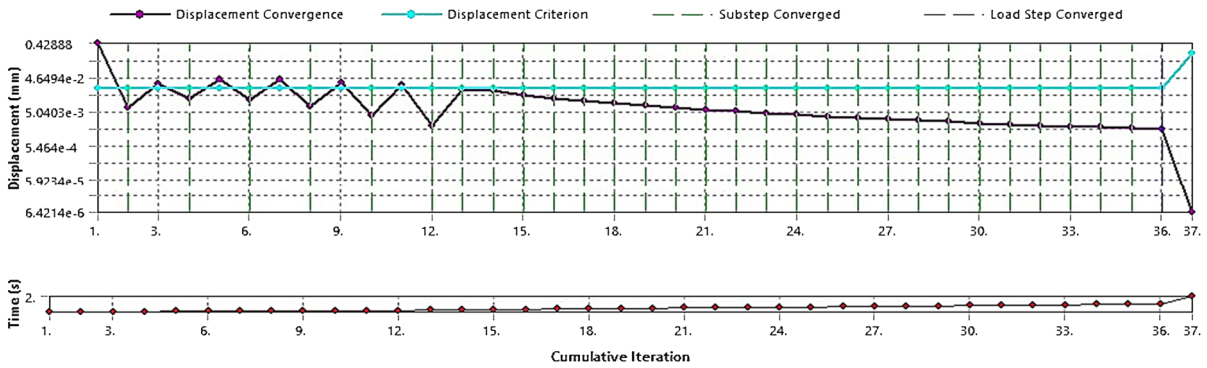


Figure 4. Displacement convergence of PP.

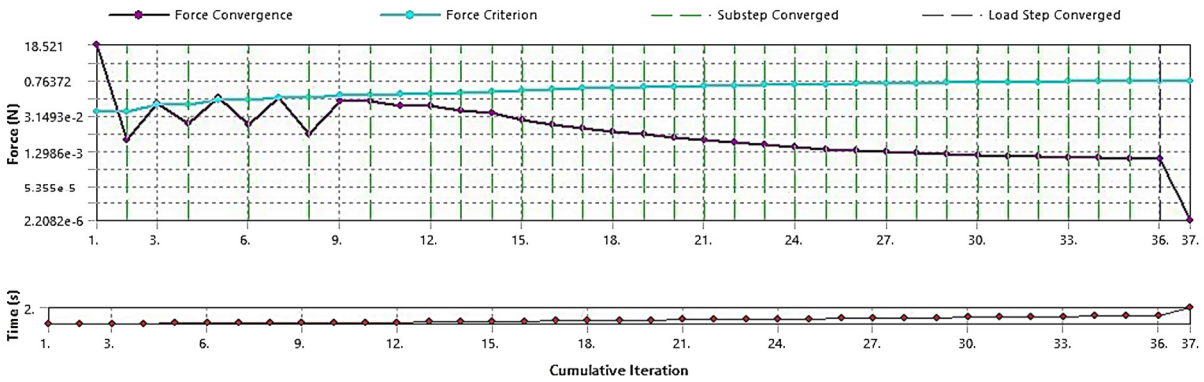
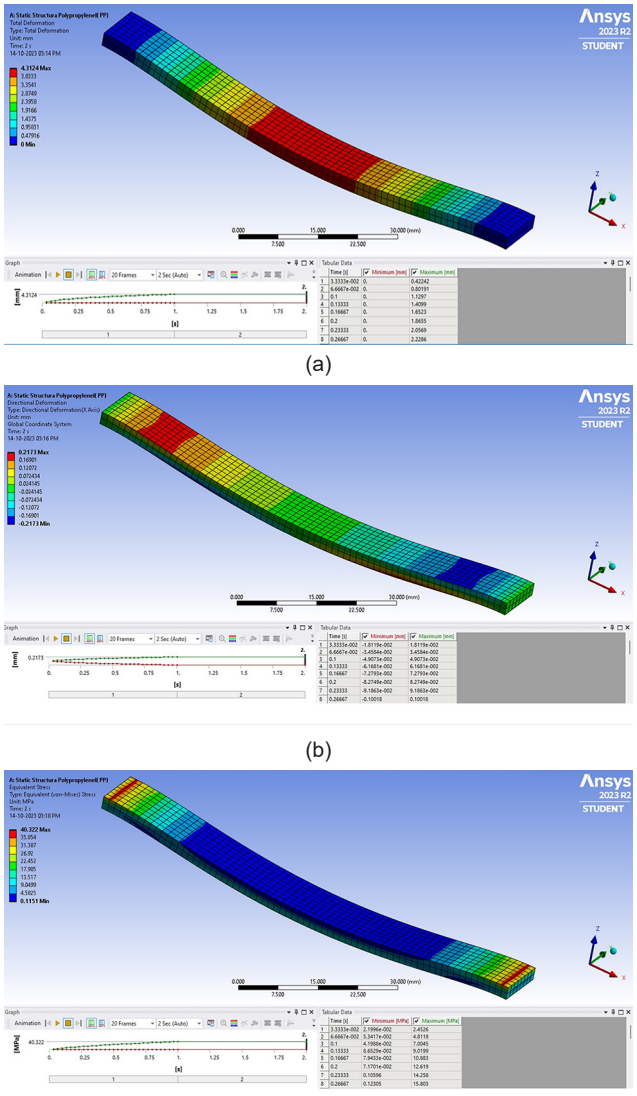


Figure 5. Force convergence of PP.

stiffness equation is to be used to calculate the unknowns:

$$[K]\{U\}=\{F\}$$

Result of polypropylene (PP) at 100 N load



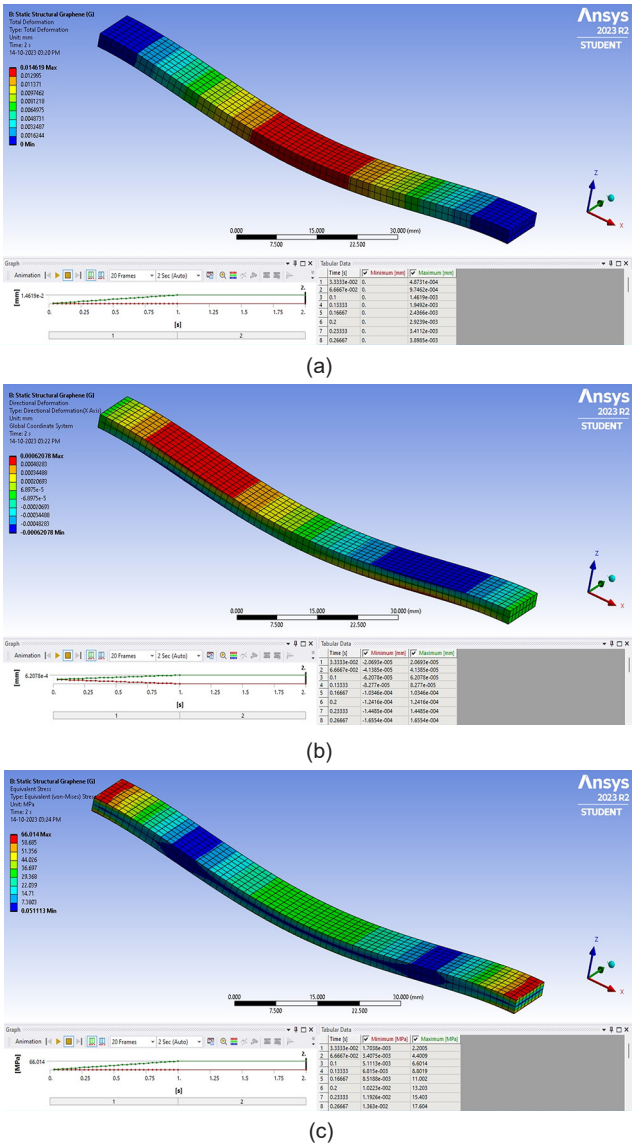
(a)

(b)

(c)

Figure 6. Total deformation (a), directional deformation (b) and von-Mises stress (c) for neat polypropylene (PP).

Result of graphene (G) at 100 N load



(a)

(b)

(c)

Figure 7. Total deformation (a), directional deformation (b) and von-Mises stress (c) for neat graphene (G).

where, [K] = Global stiffness matrix.
{U} = Unknown displacement vector.
{F}= Load or force vector.

RESULTS AND DISCUSSION

From ANSYS Workbench, following results are obtained. The first trial started at 100 N load in downward direction. The 3D models of neat polypropylene (PP), neat graphene (G) and their composites PP+G are analyzed.

Graphene is an extremely durable material, even on the microscopic level. After it is dispersed inside the polymer matrix like polypropylene, the issue turns as a strengthening agent, successfully decreases the deflection in the PP+G composites as compared to neat PP. The strong bonding within graphene provides boosted stiffness and compressive strength to the composite material.

From the above contour plots, the physics behind these improvements lie down in the unique structural characteristics of graphene nanomaterial, while the meshing comprises the contact of surface between 3-D model of graphene and the polypropylene matrix, which may result in improved dispersion. Accordingly, the mesh is deformed with the surface connectivity between two solid models.

From Figures 6 to 8 it has been noted that the total deformation and directional deformation for the polymer PP is higher than that for graphene. For polypropylene, the von-Mises stress value generated is 40.322 MPa (Max.) whereas for graphene, it is 66.014 MPa (Max.). In the case of PP+G nanocomposite, it is seen that the von-Mises stress value generated is 265.9 MPa (Max.). The total deformation of PP+G nanocomposite is in between deformation of PP and G. Moreover, the surface modification of graphene nanoparticles can further improve their dispersion in polypropylene matrix. Similarly, stronger interfacial interactions are observed due to overlapping of the PP+G meshing model, less deformation and stress, especially at 100 N load.

The normalized values are used to standardize and compare the data in the entire domain (PP+G composite). To study the behavior of PP+G composite, a simply supported beam (i.e. two side surfaces of the model are fixed, and load is applied at center) is selected. The mesh deformation increases with increase in distance from the fixed sides up to the midpoint of the model wherein the deformation is maximum (at center point).

Result of PP+G at 100 N load

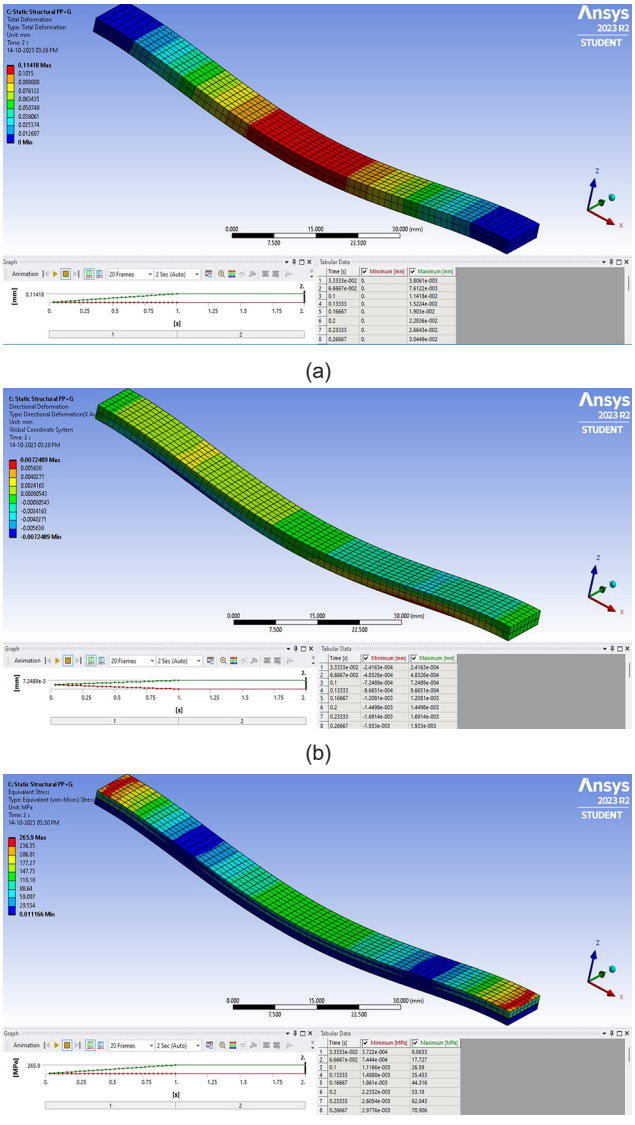


Figure 8. Total deformation (a), directional deformation (b) and von-Mises stress (c) for polypropylene + graphene (PP+G).

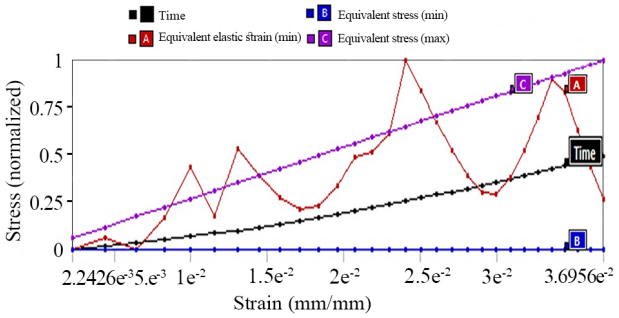


Figure 9. Normalized values for stress and strain (Min. and Max.).

Table 2. Maximum stress and strain at 100 N.

Polypropylene (PP)		Graphene (G)		PP+G	
Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Stress (Max.) [MPa]	Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Stress (Max.) [MPa]	Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Stress (Max.) [MPa]
2.24E-03	2.4526	2.20E-06	2.2005	3.02E-05	8.8633
4.40E-03	4.8118	4.41E-06	4.4009	6.04E-05	17.727
6.41E-03	7.0045	6.61E-06	6.6014	9.06E-05	26.590
8.25E-03	9.0199	8.81E-06	8.8019	1.21E-04	35.453
9.96E-03	10.883	1.10E-05	11.002	1.51E-04	44.316
1.15E-02	12.619	1.32E-05	13.203	1.81E-04	53.180
1.30E-02	14.258	1.54E-05	15.403	2.11E-04	62.043
1.45E-02	15.803	1.76E-05	17.604	2.42E-04	70.906
1.58E-02	17.275	1.98E-05	19.804	2.72E-04	79.769
1.71E-02	18.685	2.20E-05	22.005	3.02E-04	88.633
1.83E-02	20.042	2.42E-05	24.205	3.32E-04	97.496
1.95E-02	21.352	2.64E-05	26.406	3.63E-04	106.36
2.07E-02	22.620	2.86E-05	28.606	3.93E-04	115.22
2.18E-02	23.850	3.08E-05	30.807	4.23E-04	124.09
2.29E-02	25.047	3.30E-05	33.007	4.53E-04	132.95
2.40E-02	26.213	3.53E-05	35.208	4.83E-04	141.81
2.50E-02	27.350	3.75E-05	37.408	5.14E-04	150.68
2.61E-02	28.462	3.97E-05	39.608	5.44E-04	159.54
2.71E-02	29.550	4.19E-05	41.809	5.74E-04	168.40
2.80E-02	30.616	4.41E-05	44.009	6.04E-04	177.27
2.90E-02	31.661	4.63E-05	46.210	6.34E-04	186.13
2.99E-02	32.687	4.85E-05	48.410	6.65E-04	194.99
3.09E-02	33.694	5.07E-05	50.611	6.95E-04	203.86
3.18E-02	34.685	5.29E-05	52.811	7.25E-04	212.72
3.27E-02	35.660	5.51E-05	55.012	7.55E-04	221.58
3.36E-02	36.620	5.73E-05	57.212	7.86E-04	230.44
3.44E-02	37.565	5.95E-05	59.413	8.16E-04	239.31
3.53E-02	38.497	6.17E-05	61.613	8.46E-04	248.17
3.61E-02	39.415	6.39E-05	63.814	8.76E-04	257.03
3.70E-02	40.322	6.61E-05	66.014	9.06E-04	265.90
3.70E-02	40.322	6.61E-05	66.014	9.06E-04	265.90

In the present study, the interval time for 31 sub steps is selected (in analysis setting) from which equivalent elastic strain (Min.) and equivalent stress (Min. and Max.) can be obtained, which are clearly depicted in Figure 9. The values of strain (i.e., the ratio of change in length to original length) are different from instant to instant, which is fluctuating in nature because of instantaneous loading conditions 100N and 1400N (A-curve). In the entire domain, the minimum value of stress is shown as zero due to a simply supported beam, which restricts the deformation of mesh at fixed side surfaces (B-curve). Maximum deformation is observed at the center point of the model due to lack of support at this location and possibly results in sagging. In equivalent stress (Max.), the stress is directly proportional to stain, and it is linear in nature because of combined effect of gradually applied load (C-curve). As time step increases, the corresponding values of stress and strain increase proportionally (Time-curve). With the help of all these curves, the behavior of PP+G is studied in terms of mechanical properties such as strength, elasticity, and elongation under different load conditions for safe design.

The trend or the nature of equivalent stress and

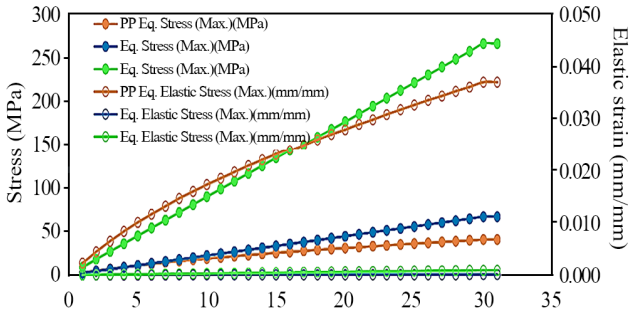
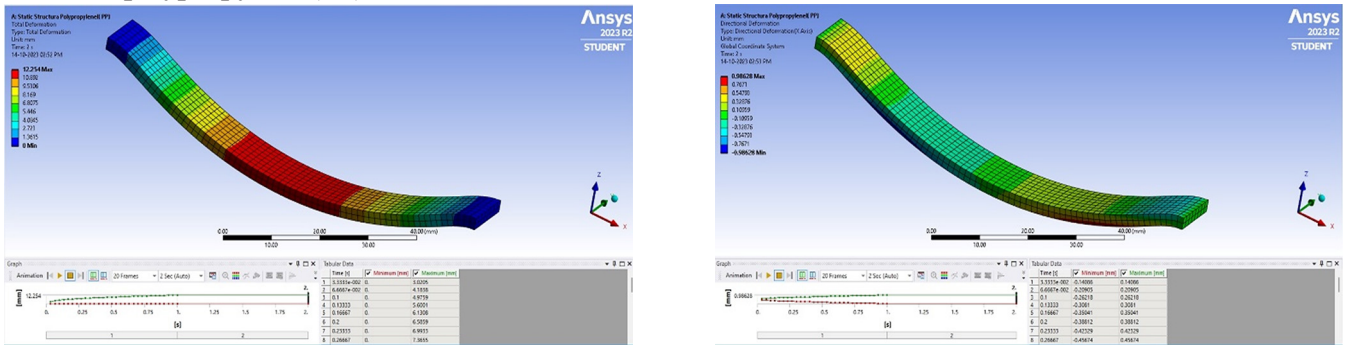


Figure 10. Stress-strain curve for PP, G and PP+G at 100 N load.

Result of polypropylene (PP) at 1400 N load



(a) (b)

Figure 11. Total deformation (a) and directional deformation (b) for neat polypropylene (PP).

equivalent strain (Max.) is captured or extracted from software whose values are shown in Table 2 at 100 N load for polypropylene, graphene and PP+G. These values help us design components on the safer side.

The horizontal axis carries a few instances i.e. sub-steps in analysis setting starting from 1 to 31 while the vertical axis carries the equivalent stress (Max.) in MPa for PP, G and PP+G. The graphs of stress-strain for the material polypropylene (PP), graphene (G) and PP+G are obtained from software facility in which initial trial of this static structural case was performed by applying a vertical download load of 100 N as shown in Figure 10. It is very clear from the figure that, firstly, the slope of all the curves is less. Whereas, for PP+G, the curve slope is high as compared to the curve slope of PP and G, which indicates the greater strength of the nanocomposites.

Second load at 1400 N

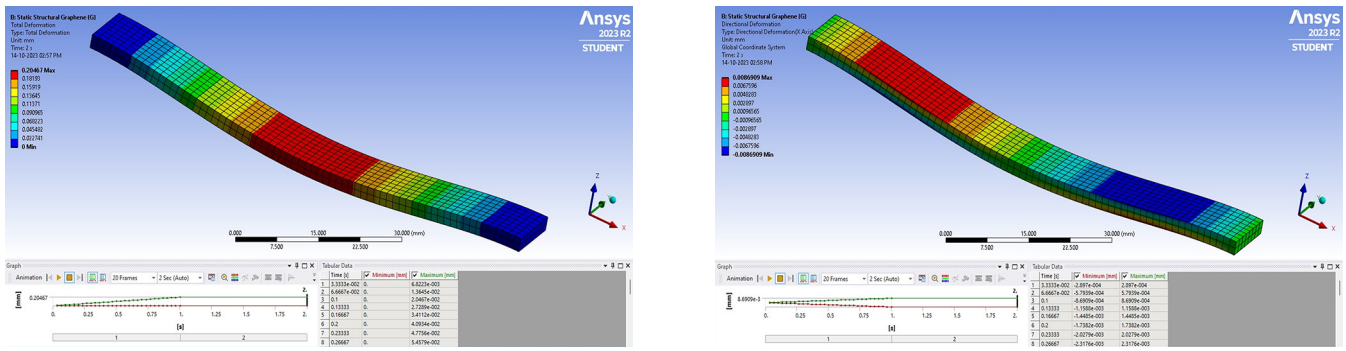
The second trial started at 1400 N load in downward direction whose results for neat polypropylene (PP), neat graphene (G) and their composite (PP+G) is obtained. For the safe side, it is necessary to check the deformation in component by increasing the load condition. From ANSYS Workbench, the following results are obtained.

Due to changing load conditions i.e. from 100 N to 1400 N, the deflection in neat PP meshing model increases because of its compact structure which acts as a barrier to the diffusion of gases and liquids. The increase in the mechanical properties of PP+G nanocomposites can be observed at 1400 N load due to the compactly packed structure of graphene.

Graphene is stronger, chemically inert, and resistant to degradation under several loading and environmental conditions. Adding graphene into polypropylene results in improving resistance to chemical degradation, toughness, and durability of PP+G nanocomposites. The ANSYS model of PP+G nanocomposites for deformed and undeformed meshing exhibits less stress and deflection as of neat PP.

The colour contour plot indicates the deformation values of PP+G at 1400 N load, wherein blue and red colours show lower and higher values, respectively. From Figures 11 to 13 it is observed that the total

Result of graphene (G) at 1400 N load



(a) (b)

Figure 12. Total deformation (a) and directional deformation (b) for neat graphene (G).

Result of PP+G at 1400N load

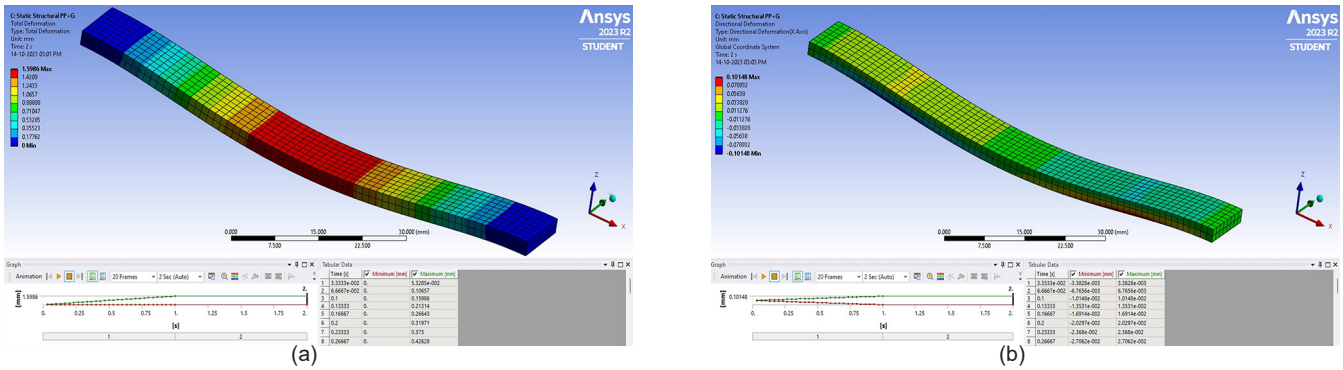


Figure 13. Total deformation (a) and directional deformation (b) for polypropylene + graphene (PP+G).

Table 3. von-Mises stress at 100 N and 1400 N load.

Stress (Max)	at load 100 N			at load 1400 N		
	Polypropylene (PP)	Graphene (G)	PP+G	Polypropylene (PP)	Graphene (G)	PP+G
von-Mises Stress (MPa)	40.322	66.014	265.9	237.83	924.2	3722.6

Table 4. Deformation at 100 N and 1400 N load.

Deformation (Max)	at load 100 N			at load 1400 N		
	Polypropylene (PP)	Graphene (G)	PP+G	Polypropylene (PP)	Graphene (G)	PP+G
Total deformation (mm)	4.3124	0.01461	0.1141	12.254	0.2046	1.5986
Directional deformation (mm)	0.2173	0.0006207	0.007248	0.9862	0.00869	0.1014

deformation and directional deformation for PP are higher than those for graphene. For polypropylene and graphene, von-Mises stress value generated is 237.83 MPa (Max.) and 924.2 MPa (Max.), respectively. Whereas for composites PP+G the von-Mises stress value generated is 3722.6 MPa (Max.) which is quite high. Total deformation of PP+G is in between deformation of neat PP and neat G.

The values of internal resistance against deformation (von-Mises stress) was obtained by ANSYS as shown in Table 3.

From the results, it is observed that both the total deformation and directional deformation increase with the increase in load for PP, G and PP+G. Additionally, the combination of PP+G shows a different deformation behaviour compared to individual materials, indicating a potential synergistic effect between them.

The comparative result for vertically downward load at 1400 N is shown in Figure 14, which clearly depicts the curves of PP, G and PP+G. The difference in the curves (Figures 10 and 14) is due to the change in the magnitude of load. In Figure 14, the slope of PP+G is greater than that of neat PP. Much less deformation is observed in PP+G compared with neat PP.

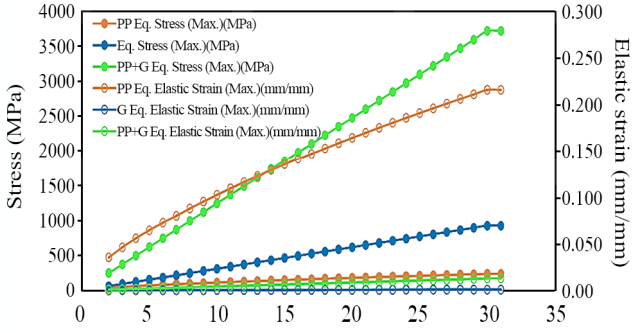


Figure 14. Stress-strain curve of PP, G and PP+G at 1400 N load.

CONCLUSION

The behavior of polypropylene, graphene and their composites was examined using ANSYS workbench under static structural analysis. Reinforcement of polypropylene was observed when graphene was incorporated under loads of 100 N and 1400 N. The deformation obtained at different load conditions are as follows:

(a) 4.3124 mm, 0.01461 mm and 0.1141 mm for PP, G

Table 5. Maximum stress and strain at 1400 N.

(PP)		Graphene (G)		PP+G	
Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Polypropylene Stress (Max.) [MPa]	Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Stress (Max.) [MPa]	Equivalent Elastic Strain (Max.) [mm/mm]	Equivalent Stress (Max.) [MPa]
2.18E-02	23.854	3.08E-05	30.807	4.23E-04	124.09
3.53E-02	38.503	6.17E-05	61.613	8.46E-04	248.17
4.62E-02	50.408	9.25E-05	92.420	1.27E-03	372.26
5.58E-02	60.806	1.23E-04	123.23	1.69E-03	496.34
6.45E-02	70.300	1.54E-04	154.03	2.11E-03	620.43
7.25E-02	78.958	1.85E-04	184.84	2.54E-03	744.51
7.99E-02	87.933	2.16E-04	215.65	2.96E-03	868.60
8.77E-02	96.51	2.47E-04	246.45	3.38E-03	992.69
9.52E-02	104.74	2.78E-04	277.26	3.81E-03	1116.8
0.10243	112.67	3.08E-04	308.07	4.23E-03	1240.9
0.10940	120.34	3.39E-04	338.87	4.65E-03	1364.9
0.11616	127.78	3.70E-04	369.68	5.08E-03	1489.0
0.12273	135.00	4.01E-04	400.49	5.50E-03	1613.1
0.12912	142.03	4.32E-04	431.29	5.92E-03	1737.2
0.13536	148.90	4.63E-04	462.10	6.34E-03	1861.3
0.14146	155.60	4.94E-04	492.91	6.77E-03	1985.4
0.14742	162.16	5.24E-04	523.71	7.19E-03	2109.5
0.15326	168.59	5.55E-04	554.52	7.61E-03	2233.5
0.15899	174.89	5.86E-04	585.33	8.04E-03	2357.6
0.16461	181.08	6.17E-04	616.13	8.46E-03	2481.7
0.17014	187.15	6.48E-04	646.94	8.88E-03	2605.8
0.17557	193.12	6.79E-04	677.75	9.31E-03	2729.9
0.18091	199.00	7.09E-04	708.55	9.73E-03	2854.0
0.18617	204.79	7.40E-04	739.36	1.02E-02	2978.1
0.19135	210.49	7.71E-04	770.16	1.06E-02	3102.1
0.19646	216.10	8.02E-04	800.97	1.10E-02	3226.2
0.20149	221.64	8.33E-04	831.78	1.14E-02	3350.3
0.20646	227.11	8.64E-04	862.58	1.18E-02	3474.4
0.21136	232.50	8.95E-04	893.39	1.23E-02	3598.5
0.21621	237.83	9.25E-04	924.20	1.27E-02	3722.6
0.21621	237.83	9.25E-04	924.20	1.27E-02	3722.6

and PP+G, respectively, at 100 N load.

(b) 12.254 mm, 0.2046 mm and 1.5986 mm for PP, G and PP+G, respectively, at 1400 N load.

Polypropylene showed a higher total deformation compared to graphene and PP+G at both 100 N and 1400 N loads. Whereas graphene showed the least total deformation compared to PP and PP+G at both 100 N and 1400 N loads due to the combined mesh effect.

Prior to fabrication and testing, simulation of PP+G composite was performed since it provided an important method of analysis which was easily validated and understood by applying von-Mises failure criteria. From ANSYS software, the equivalent strain, equivalent stress, total deformation, and directional deformation were extracted easily, indicating the behavior of PP, G and PP+G under different loads. For polypropylene at load 100 N, the total deformation was approximately 38 times more than that of PP+G. Similarly, it is approx. 8 times more than that of PP+G at 1400 N. However, much less deformation was observed in PP+G. Hence, it is concluded that PP+G gives better results in terms of resistance to deformation compared with neat PP. Explicit dynamics analysis can capture linear as well as nonlinear stress-stain curves. So, there is a scope to perform explicit dynamic analysis to understand nonlinear stress-stain behavior of polymer nanocomposites.

CONFLICTS OF INTEREST

The authors declare that they have no conflicts of interest.

ACKNOWLEDGEMENTS

Aamir M. Shaikh would like to thank Dr. Pravin R. Kubade for supervising the research activities.

REFERENCES

1. Okamoto M (2023) Polymer nanocomposites. Adv Polym Eng 4: 457-479
2. Hallad SA, Banapurmath NR, Khan TY, Umarfarooq MA, Soudagar ME, Hunashyal AM, Gujjar SV, Yaradoddi JS, Ganachari SV, Elfasakhany A, Siddiqui MI (2021) Statistical analysis of poly nanocomposites for mechanical Properties. Molecules 26: 4135
3. Buehler MJ, Misra A (2019) Mechanical behavior of nanocomposites. MRS Bulletin 44: 19–24
4. Stephen C, Thimmappa BHS, Selvam R, Shivamurthy B (2019) Polymer nanocomposites for high-velocity impact applications-A review. Compos Commun 17: 72-86
5. Tian Y, Zhang H, Zhao J, Li T, Bie B-X, Luo S-N, Zhang Z (2016) High strain rate compression of epoxy based nanocomposites. Compos- A: Appl Sci Manuf 90: 62–70
6. Chang Z, Wang Y, Zhang Z, Gao K, Hou G, Shen J, Zhang L, Liu J (2021) Creep behavior of polymer nanocomposites: Insights from molecular dynamics simulation. Polymer 228: 123895
7. Jayanarayanan K, Rasana N, Mishra RK (2017) Dynamic mechanical thermal analysis of polymer nanocomposites. In: Thermal and rheological measurement techniques for nanomaterials characterization, Elsevier, pp: 123-157
8. Chan JX, Wong JF, Petrů M, Hassan A, Nirmal, U, Othman N, Ilyas RA (2021) Effect of nanofillers on tribological properties of polymer nanocomposites: A review on recent development. Polymers 13: 2867
9. Rasana N, Jayanarayanan K, Ramachandran KI (2020) Experimental, analytical and finite element studies on nano (MWCNT) and hybrid (MWCNT/glass fiber) filler reinforced polypropylene composites. Iran Polym J 29:1071-1085
10. Gijsman P, Fiorio R (2023) Long term thermo-oxidative degradation and stabilization of polypropylene (PP) and the implications for its recyclability. Polym Degrad Stabil 208: 110260
11. Wang J, Dai Q, Si R, Guo S (2019) Mechanical, durability, and microstructural properties of macro synthetic Polypropylene (PP) fiber-reinforced rubber concrete. J Clean Prod 234:1351-1364
12. Calhoun A (2010) Polypropylene. In: Multilayer flexible packaging: Technology and applications for the food, personal care, and over-the-counter pharmaceutical industries, Ed. Wagner JR, William Andrew Publishing , 31-36
13. Massey LK (2007) Polypropylene In: Plastics design library, the effects of UV light and weather on plastics and elastomers (2nd Ed), Ed: Massey LK, William Andrew Publishing, 215-221
14. Alsabri A, Tahir F, Al-Ghamdi SG (2022) Environmental impacts of polypropylene (PP) production and prospects of its recycling in the GCC region. Materials Today: Proceedings 56: 2245-2251
15. Maddah HA (2016) Polypropylene as a promising plastic: A review. Am J Polym Sci 6: 1-11
16. Moritomi S, Watanabe T, Kanzaki S (2010) Polypropylene compounds for automotive applications. Sumitomo Kagaku 1: 1-16
17. Aamir M. Shaikh, Pravin R. Kubade (2023) Effect of nanofillers on rolled polymer nanocomposites: A review. Materials Today: Proceedings
18. Himma NF, Anisah S, Prasetya N, Wenten IG (2016) Advances in preparation, modification, and application of polypropylene membrane. J Polym Eng 36: 329-362
19. Kubade PR, Tambe P, Kulkarni HB (2017) Morphological, thermal and mechanical properties of 90/10 (WT %/WT %) PP/ABS blends and their polymer nanocomposites. Adv Compos Lett 26: 182-188
20. Kubade P, Tambe P (2016) Influence of surface modification of halloysite nanotubes and its localization in PP phase on mechanical and thermal properties of PP/ABS blends. Compos Interfaces 24: 469-487
21. Patil J, Patil H, Sankpal R, Rathod D, Patil K, Kubade PR, Kulkarni HB (2021) Studies on mechanical and thermal performance of carbon nanotubes/polypropylene nanocomposites. Materials Today: Proceedings 46: 7182-7186
22. Lee KS, Kim H, Shim BS (2013) Graphene: an emerging material for biological tissue engineering. Carbon lett 14: 63-75
23. Adak NC, Chhetri S, Sabarad S, Roy H, Murmu NC, Samanta P, Kuila T (2019). Direct

observation of micro delamination in graphene oxide incorporated carbon fiber/epoxy composite via in-situ tensile test. Compos Sci Technol 177: 57-65
24. Lee JH, Shim CM, Lee BS (2013) Graphene in edge-carboxylated graphite by ball milling and analyses using finite element method. Int J Mater Sci Appl 2: 209-220
25. Atif R, Inam F (2016) Modeling and simulation of graphene based polymer nanocomposites. Advances in the last decade. Graphene 5: 96-142
26. Ijaz H, Raza H, Gohar GA, Ullah S, Akhtar A, Imran M (2020) Effect of graphene oxide doped nano coolant on temperature drop across the tube length and effectiveness of car radiator -A CFD study. Therm Sci Eng Prog 20: 100689
27. Sanes J, Sánchez C, Pamies R, Avilés MD, Bermúdez MD (2020) Extrusion of polymer nanocomposites with graphene and graphene derivative nanofillers: An overview of recent developments. Materials 13: 549
28. Mishra BP, Mishra D, Panda P, Maharana A (2020) An experimental investigation of the effects of reinforcement of graphene fillers on mechanical properties of bi-directional glass/ epoxy composite. Materials Today: Proceedings 33: 5429-5441
29. Xu F, Gao M, Wang H, Liu H, Yan F, Zhao H, Yao Q (2023) Polymer-based graphene composite molding: A review. RSC Adv 13: 2538-2551
30. Yazdi HA, Parvaneh V, Shariati M (2019) Investigating mechanical properties of polyacetal/ graphene nanocomposites by a structural-mechanical model. IEEE 10th International Conference on Mechanical and Aerospace Engineering (ICMAE), Brussels, Belgium. 333-337
31. Shaikh AM, Ghatge DA (2023) CFD Simulation for fluid flow through a circular chamber by using ANSYS. In: Recent advances in material, manufacturing, and machine learning, CRC Press, pp. 1025-1034
32. Shaikh AM, Kubade PR (2024) A review on rolling process for polymer nanocomposites with different nanofillers to enhance properties. In: 2nd International Conference on Smart Sustainable Materials and Technologies (ICSSMT 2023). ICSSMT 2023, Springer, 39-48