# Simulation Analysis of Graphene Addition on Polymeric Composite

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#### ABSTRACT

Natural fibres in composite materials, such as kenaf fibres, are used to reinforce polypropylene (PP) due to their light weight and high mechanical performance required in various applications, such as automotive. Although natural fibres seem to be the most promising material, manufacturing parameters and material composition are crucial to determining balanced output performance. Therefore, this study provides essential knowledge on defining the parameters and the effect of addition of graphene content to kenaf fibres composites using computer simulation via Abaqus CAE software. Detailed analyses were compared with the experimental data of Young's modulus and tensile strength. General static and dynamic explicit analyses were conducted using Abaqus CAE simulations, and set at 40 wt. % kenaf fibres, 0, 1, 3, and 5 wt. % graphene. Short kenaf fibres were utilised together with graphene nanoplatelets and prepared using a hot-pressing technique with the temperature set at 190 °C and pressure of 5 MPa for 5 min. The findings indicated that the simulation and experimental data from previous studies data congruent which is Young's modulus and tensile strength increased with addition of graphene content. Thus, the simulated data could predict the experimental mechanical performance, in which 24 MPa of tensile strength was recorded for 3 wt. % of graphene additions.

Keywords: Kenaf; graphene; young's modulus; tensile strength

# INTRODUCTION

In the year 2021, industries are more concerned with the quality of product manufacturing with effective time and costs. In addition, some industries have emphasised the use of sustainable materials based on environmental technologies, which include social, economic, and environmental aspects (Chakraborty and Biswas 2020). Numerous studies have reported that the incorporation of natural fibres into composite materials could achieve equivalent mechanical performance, or in some cases, better than using synthetic fibres. Furthermore, the use of natural fibres as reinforcement materials in composites has provided an alternative way for producing eco-friendly materials compared to synthetic fibres (Hadiji et al. 2020). The impact of using synthetic fibres in composites on environmental degradation includes the generation of hazardous air pollutants and solid wastes. Hazardous air pollutants are caused by the curing of composites (Sands et al. 2001). Natural fibres, such as jute, sisal, flax, hemp, ramie, coir, pineapple, and kenaf have gained much attention as alternatives to synthetic fibres (Das et al. 2020; Bambach 2017). These natural fibres can be classified into bast, stalk, wood, fruit, seed, and grass according to their origin (Ridzuan et al. 2020).

Besides, these natural fibres are preferred over synthetic fibre because natural fibres, which originated

from plant fibres, are renewable and readily available most of the time (Guo, Sun, and Satyavolu 2020). These environmentally-friendly fibres can reduce carbon dioxide emission to the environment (Chopparapu et al. 2020; Fa 2013). Kenaf fibre, which has low density and high strength, is highly demanded in lightweight composites, particularly in the automotive industry or sometimes as interior parts of buildings (Gu, Kim, and Kim 2017; Sapiai et al. 2020). Furthermore, natural fibres have excellent tensile modulus and specific modulus, resulting in enhanced mechanical properties (Tholibon et al. 2019). In 1996, Ford Mondeo highlighted the use of kenaf-based composites for the inside car boards (Sreenivas, Krishnamurthy, and Arpitha 2020). Specifically, kenaf fibre has a high potential as polymer composites with excellent mechanical performance (tensile strength of 930 MPa, density of 1.45 g/cm<sup>2</sup>, and elastic modulus of 53 GPa) (Mahjoub et al. 2014). In order to enhance the mechanical properties of composite, the additional material of filler was an alternative way to be conducted. According to prior research, adding graphene to the natural fibre reinforced polymer was the greatest way to improve its strength and stiffness (Mustapha et al. 2019). Graphene material has enhanced several unique qualities for a variety of applications, including its extraordinarily high mechanical strength with a Young's modulus of 1 TPa and tensile strength of 20 GPa (Idumah and Hassan 2016).

However, there have a limited on detailed research on the influence of graphene addition on the mechanical characteristics of PP/kenaf composites yet. Also, there is none computer simulation that could help with estimating the material properties. Based on this knowledge, this study aims to define the parameters and compositions of fabricated kenaf composites using computer simulation for predicting the actual mechanical performance of kenaf composite materials. In order to determine the actual mechanical properties of kenaf composites, several experiments were performed at different graphene nanoplatelet (GNP) loadings.

#### METHODOLOGY

The main materials used in fabricating kenaf composites are polypropylene (PP), kenaf fibre, and GNPs as secondary filler. PP was supplied by Lotte Chemical Titan (M) Sdn. Bhd., PX 617 grade with the size of 90  $\mu$ m. This type of PP is suitable for hot process purposes with a melt flow rate of 1.7 g/10 min at 230 °C and a density of 0.9 g/cm³. Meanwhile, kenaf fibre was supplied by Lembaga Kenaf dan Tembakau Malaysia, Kelantan, Malaysia with an average kenaf length of 2–3 m. GNPs (C-500 grade) were used as the secondary filler and acquired from Sigma-Aldrich (Malaysia) Sdn. Bhd. with a surface area of 500 m²/g (Mohd Radzuan et al. 2020).

Kenaf composite fabrication processes started with kenaf preparation. Micron sized of kenaf fibre with 20 mesh of size was firstly soaked in 6% mol of sodium hydroxide solution for 3 h. Later, the soaked kenaf fibre was rinsed with distilled water and tested with litmus papers to ensure that the fibre is free of alkaline substances. Next, the fibre was dried in an oven for 24 h at 80 °C. In the meantime, the polymeric-based materials were prepared by mechanically mixing PP powder with GNPs for 5 min at 1,000 rpm. Later, the compound materials were mixed using ball milling (model Fritsch Pulverisette 6) at a rotational speed of 200 rpm for 1 h to obtain a homogeneous mixture. The compound materials were then mixed with kenaf fibre using a sigma-blade mixer at 190 °C and 45 rpm.

The compositions of composite samples were set at 40 wt. % kenaf content; 0 wt. %, 1 wt. %, 3 wt. %, and 5 wt. % of GNP content; and 55 wt. %, 57 wt. %, and 59 wt. % of PP content. The PP/GNPs compounds were allowed to melt in the compartment machine for 5 min, followed by the addition of kenaf fibre and the mixing process for another 10 min. Using a crushing machine, the hardened PP/kenaf/GNPs compounds were crushed into coarse powder before being fabricated in the size of 175 mm × 175 mm × 2 mm using a 50-ton hot press machine at the temperature of 190 °C and pressure of 5 MPa. The holding time was set to 5 min. The samples were cooled for 3 h in order to maintain their shape and minimise defects (e.g., delamination, warpage, and thinning). Later, the samples were cut in accordance with ASTM D 3039 for a tensile

test. The test was conducted using Instron 3365 universal testing machine with a load of 5 kN and speed of 0.1 mm/min

Computer simulation was conducted using Abaqus CAE software. Two types of simulation were carried out: static and dynamic explicit analysis. The analysis was carried out to determine the Young's modulus and tensile strength of kenaf composites and the effect of adding GNPs. For the simulation, related parameters and respective boundary conditions were applied based on previous research, which was assigned as the input for this study. After conducting the analyses, the values obtained from the simulation were compared with the experimental data from the previous research to determine the effect of GNPs on PP/kenaf composites (Idumah and Hassan 2016). The composite compositions that yielded the highest values of Young's modulus and tensile strength were identified.

#### GENERAL STATIC ANALYSIS

Appropriate values for the mechanical properties, including the Young's modulus, tensile strength, Poisson's ratio, and density, were set as the input based on the experiments performed. As the programme is based on the values rather than the units applied, the values entered must be consistent throughout the simulation. The time period was reduced to 1.0 s to minimise simulation time. Next, in the Constrain module, a new 'coupling' type barrier was set at the top of the sample. Meanwhile, in the Load module, the boundary conditions were set at the top and bottom of the sample to resemble the clamped parts on a tensile testing machine. After that, a meshed sample was produced for the Mesh module. A small sized mesh of 2 mm was used to produce the results from the simulation more accurately (Dutt 2015). However, a size that is too small will require much time to complete the analysis (More and Bindu 2015). The type of mesh chosen is the tetrahedral type, as other types of mesh are unsuitable for such components and many steps have to be taken to use them, as performed by other researchers (Tadepalli, Erdemir, and Cavanagh 2011). The number of elements was 1,240 and the number of nodes was 2,079. Finally, in the Job module, a new assignment (Job) needs to be generated and 'submitted' (Submit Job). This instruction would start the simulation analysis, and once completed, the data and results could be viewed in the Visualization module. Descriptions of the stress distribution, diagrams, and others could be extracted through this module (Q. Liu, Li, and Liu 2017).

### EXPLICIT DYNAMIC ANALYSIS

For the explicit dynamic analysis, the details on the mechanical properties (e.g., Young's modulus and Poisson's ratio) are similar to the general static analysis performed. The plastic deformation was based on the experiments performed for the mechanical properties of PP/kenaf composites (Rowell et al. 2016) and the values of ductile

damage were taken from previous studies (Nguyen et al. 2005). The same assembly steps were conducted, followed by the Step module. The explicit dynamic type was selected and the corresponding values were entered for mass scaling. The reference point was set at 2 cm from the top of the centre of the sample. A constraint type coupling was selected in the Interaction module. The reference point is presented in Figure 1. Only the boundary conditions were set for the Load module. Three types of boundary conditions are Symmetry, Antisymmetry, and Encastre. The same steps for the Mesh and Job modules as in the general static analysis were applied. The results could be generated afterwards in the visualization module (Främby and Fagerström 2021).



FIGURE 1. The coupling type constraint for the sample.

#### RESULTS AND DISCUSSION

## COMPUTER SIMULATION: GENERAL STATIC ANALYSIS

The tensile test results indicated the tensile strength of 22.8 MPa for 5 wt. % GNP addition. Meanwhile, the highest strain value recorded was 0.014279 with the Young's modulus value of 1,600 MPa. This corresponds to a 0.109 MPa (-0.47%) decrease in tensile strength compared to the pure kenaf/PP composite. However, a contradicting result was obtained, with an increment of 68% at 646 MPa for the Young's modulus. The findings from the simulation indicated that the stress-strain relationship for the pure PP/kenaf composites resulted in lower values of Young's modulus and tensile strength (954 MPa and 22.95 MPa, respectively) compared to PP/kenaf/GNPs at various loadings of 1 wt. %, 3 wt. %, and 5 wt. % (J. Z. Liang et al. 2016). In addition, the experiments performed recorded the Young's modulus of 1,090 MPa for 1 wt. % PP/kenaf/GNPs with the tensile strength of 23.07 MPa. This result shows that the Young's modulus and tensile strength increased by 14% and 0.5%, respectively, with the addition of graphene content of 1 wt. %. Meanwhile, the addition of 3 wt. % GNP content increased the Young's modulus to 1,200 MPa, whereas the tensile strength reduced to 22.88 MPa. The tensile strength started to deteriorate when the elasticity started to drop after adding more GNP content (Papageorgiou, Kinloch, and Young 2017). Furthermore, the decrease of tensile strength might be attributed to the void existence, which decreased the performance (Shen et al. 2013). Previous studies

observed a similar trend when 5 wt. % epoxy resin was introduced to carbon nanofibers, where voids were produced during fabrication and continued to grow with the addition of epoxy resin until 5 wt. % (Choi et al. 2005). The highest Young's modulus recorded was 1,600 MPa for 5 wt. % PP/ kenaf/GNPs. It can be shown that with the increase of GNP content, the Young's modulus gives a trend that attributes to high stiffness and uniform and homogeneous dispersion of GNPs in the polymer matrix (Idumah and Hassan 2016). Homogeneous dispersion of GNPs can be achieved using the melt-blending method, which offers a simple way of dispersing nanoparticles in a polymer matrix (A. Liang et al. 2018). A study using graphene-based nanocomposites fabricated via Raman spectroscopy demonstrated a similar trend as the filler content distributed evenly among the polymeric matrix (Papageorgiou, Kinloch, and Young 2017). Thus, 5 wt. % PP/kenaf/GNPs provides a significant toughening effect due to its high interface strength.

#### COMPUTER SIMULATION: EXPLICIT DYNAMIC ANALYSIS

An explicit dynamic analysis was also conducted to simulate the tensile testing of the PP/kenaf/GNPs composite samples. The values of stress and strain were only extracted from the elastic deformation region of the stress-strain graphs generated by the software, resulting in straight-line graphs. This is because the Young's moduli are calculated based on the gradients at the elastic deformation region only. The mechanical properties were evaluated either directly from the stress-strain curves by employing the gradient method for Young's modulus determination or using a newly developed phenomenological model for compressive deformation (Krupa et al. 2010). Meanwhile, lower tensile strength was recorded or varied from the experimental data collected because the step size set for the simulation is not sufficiently small or fine enough (target time increment: 5 × 10<sup>-7</sup>, factor: 1,000). Therefore, to prove that, the simulation conducted by other researchers was considered when there is a difference in the finest and coarse mesh model. 140 step sizes (i.e., 66 s of computing time) resulted in the finest mesh model, whereas the coarse mesh model only required 2 step sizes (i.e., 3 s of computing time) (Y. Liu and Glass 2013). Based on the finding, a smaller step size would yield more accurate simulation but caused a longer simulation process. Therefore, the values obtained from this dynamic explicit analysis were estimated to study the trends of the effect of GNP addition on the Young's modulus and tensile strength of the composites.

The stress-strain graphs are plotted, as seen in Figure 2. It can be observed that the gradients of the graphs increased with the increasing amount of GNP content, denoting the increment in the Young's modulus. The values of the Young's modulus and tensile strength are listed in Table 1. The values of Young's modulus increased from 656.79 MPa for PP/kenaf to 875.06 MPa for the 5 wt. % PP/kenaf/GNPs sample, whereas the tensile strength increased from 17.64 MPa for PP/kenaf to 24.99 MPa for the 5 wt. % PP/kenaf/GNPs

sample. Other researchers determined that the addition of 5 wt. % GNP content into polymer composites enhanced the mechanical properties as the Young's modulus and tensile strength improved significantly without the reduction in elastic properties (Deepa Urs et al. 2020). In addition, GNPs as a filler are expected to exhibit better performance in polymer composites due to their higher surface constant area (Shen et al. 2013). Prior research found that the addition of GNP content in the epoxy matrix higher than 5 wt. % would deteriorate the Young's modulus and tensile strength due to the presence of agglomeration and fibre pull-outs (Idumah

and Hassan 2016). The increase of GNP content in the epoxy matrix reduced the Young's modulus from 3.0 GPa for 5 wt. % GNPs/epoxy composites to 2.72 GPa for 6 wt. % GNPs/epoxy composites. A similar trend was also observed for tensile strength, where the strength dropped from 27 MPa for 5 wt. % GNPs/epoxy composites to 23.5 MPa for 6 wt. % GNPs/epoxy composites (Papageorgiou, Kinloch, and Young 2017). Thus, this experiment shows a similar trend as 5 wt. % GNPs in PP/kenaf/GNPs composites have higher values of Young's modulus and tensile strength.

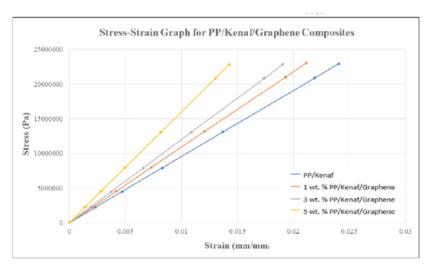


FIGURE 2. Stress-strain graphs of PP/kenaf/GNPs samples.

COMPARISON BETWEEN SIMULATION AND EXPERIMENTAL DATA

Upon completing the simulation, the results were compared with the experimental data obtained from previous research using the same materials of GNPs/kenaf/PP composites with 0–5 phr prepared by melt extrusion process (Idumah and Hassan 2016). The results for Young's modulus and tensile strength from the general static analysis simulation compared to previous research are shown in Table 1. The simulation is deemed successful as the results are similar to that of previous research for Young's modulus; however, the tensile strength for simulation demonstrated the percentage difference of 7%-32% compared to the previous research (Idumah and Hassan 2016). The values of Young's modulus obtained have a good correlation between the simulation and experimental data of prior research, especially with the maximum GNP addition of 5 wt. %. This phenomenon indicates an increasing stiffness of kenaf/PP/GNPs composites. According to previous research, the increase of Young's modulus for both data obtained from simulation and experiment is due to the addition of 0.5 wt. % GNPs, leading to a 75% increase in strength and reduction in elongation at break (Khabaz-Aghdam et al. 2020). The values obtained are within the same range (8%–25% difference) and the trends are similar, where the values of tensile strength for simulation increased initially with the addition of GNP fillers and then decreased gradually with further addition of GNP content. It is shown that the addition of GNPs in

composites for both previous research and simulation would improve the tensile strength. Prior research found that with further addition of GNP content, the tensile strength tends to decline due to defect or aggregation of GNPs generated during fabrication, and for the GNP content of 0.3 wt. %, the aggregation became more severe (Lee, Wang, and Tsai 2016; Mohd Radzuan et al. 2020). A similar trend was observed by previous researchers, where the tensile strength increased from 17.5 MPa (pure PP/kenaf) to 21.3 MPa (3 wt. % PP/kenaf/GNPs) before reducing to 17.3 MPa for the 5 wt. % PP/kenaf/GNPs sample. The simulation yielded an increment from 22.95 MPa (pure PP/kenaf) to 23.07 MPa (1 wt. % PP/kenaf/GNPs). However, with the increase of GNP content, the tensile strength reduced from 22.88 MPa (3 wt. % PP/kenaf/GNPs) to 22.85 MPa for the 5 wt. % PP/kenaf/ GNPs sample. The percentage difference in tensile strength for simulation and experimental values is possibly due to the inaccurate input during the setting-up (initial) stage of the analysis, leading to inaccurate results.

The results from the dynamic explicit analysis are also consistent for both general static analysis and experimental data obtained from previous research (Deepa Urs et al. 2020; Idumah and Hassan 2016). The Young's modulus of the samples increased from 656.79 MPa for the pure PP/kenaf sample to 875.06 MPa for the 5 wt. % PP/kenaf/GNPs sample, while the tensile strength increased from 17.64 MPa for the PP/kenaf sample to 24.99 MPa for the 5 wt. % PP/kenaf/GNPs sample. Figure 3 presents the findings from

the explicit dynamic analysis for tensile testing of 0 wt. %, 1 wt. %, 3 wt. %, and 5 wt. % PP/kenaf/GNPs composite samples. From Fig. 3, it can be seen clearly the location where the crack was already happened at the bottom part of the sample. Due to the maximum numbers of stress resulted from the simulation in which it has shown by red region. With the addition of graphene by 1, 3 and 5 wt. % PP/kenaf/GNPs, a high strength and high specific area of graphene have resulted to strengthened on resistance to the crack extension of samples (J. Liu et al. 2019). Previous research has shown that adding filler loading such as graphene to polymer composites reduces ductility values, resulting in

enhanced post-cracking performance (Çuvalci, Erbay, and İpek 2014).

The datasets for Young's modulus and tensile strength from the explicit dynamic analysis are tabulated in Table 1. From the table, it can be determined that the Young's modulus and tensile strength from the explicit dynamic analysis increased with the increase of GNP content. Thus, a comparison between simulation and experimental data shows that the simulation data obtained are similar to the experimental data resulted from the addition of GNPs to PP/kenaf, which increased both Young's modulus and tensile strength.

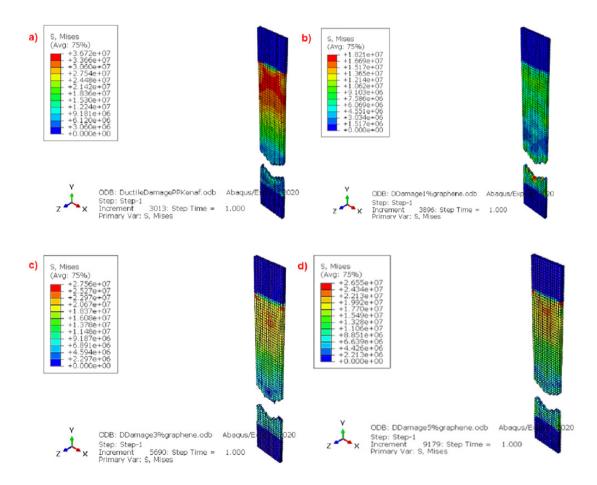


FIGURE 3(a). Tensile testing sample: PP/kenaf composite, 3(b). tensile testing sample: 1 wt. % PP/kenaf/GNPs composite, 3(c). tensile testing sample: 3 wt. % PP/kenaf/GNPs composite, and 3(d). tensile testing sample: 5 wt. % PP/kenaf/GNPs composit

TABLE 1. Values of Young's modulus and tensile strength from the dynamic explicit analysis and general static analysis.

Sample Composition	Dynamic Explicit Analysis		General Static Analysis			
	Young's Modulus (MPa)	Tensile Strength (MPa)	Young's Modulus (MPa)		Tensile Strength (MPa)	
			Simulation	Previous Research	Simulation	Previous Research
PP/Kenaf	656.787	17.637	954	954	22.95	17.50
PP/Kenaf/GNPs (1 wt. %)	715.125	18.922	1,090	1,090	23.07	17.70
PP/Kenaf/GNPs (3 wt. %)	756.048	20.001	1,200	1,200	22.88	21.30
PP/Kenaf/GNPs (5 wt. %)	875.057	24.993	1,600	1,600	22.85	17.30

#### CONCLUSION

It can be concluded that the addition of GNPs to PP/kenaf composites increases Young's modulus and tensile strength. The highest Young's modulus and tensile strength can be compared with the composition of PP/kenaf without GNP content. From the general static analysis for simulation, the highest Young's modulus was 1,600 MPa for the 5 wt. % PP/kenaf/GNPs sample, while the highest tensile strength was 23.07 MPa for the 1 wt. % PP/kenaf/GNPs sample. Meanwhile, the dynamic explicit analysis obtained the highest Young's modulus of 875.057 MPa and tensile strength of 24.993 MPa for the 5 wt. % PP/kenaf/GNPs sample. Hence, the addition of GNPs improves the suitability of materials to be used in the fabrication of interior components of vehicles.

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# DECLARATION OF COMPETING INTEREST

None

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