Thermomechanical properties prediction of wood-flour reinforced polymer composites using representative volume element (RVE)

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Abstract. The accurate prediction of the thermomechanical properties of newly developed polymer composites is important in the determination of their possible areas of application. In this study, a 3D model of representative volume element (RVE) with different wood flour weight ratios (5, 10, 15, 20, 25 and 30 %) was used to develop wood flour polymer composites. Micromechanical material modelling software (Digimat) was used in conjunction with finite element analysis software (Abaqus) to develop the polymer composites and to determine their thermomechanical properties (modulus of elasticity, Poisson's ratio, thermal conductivity, density, and hardness). The hardness, tensile strength and modulus of elasticity increase with an increase in the wt.% of wood flour, while the Poisson ratio, thermal conductivity and density decrease with an increase in the wt.% of wood flour. Also, the predicted thermomechanical properties using the micromechanical material modelling software (RVE) follow the same trend as those found in the literature.

Keywords: Wood flour, Representative volume element (RVE), Polymer, Digimat, Abaqus

1 Introduction

In a bid to create a pollution-free environment, materials such as wood flour (natural fibre like wood), cotton, sisal coir, jute, banana etc., known as environmentally friendly materials, are gaining tremendous patronage as a replacement for synthetic fibre composites. This is because these natural fibre composites have better electrical resistance, improved acoustic insulation and thermal properties, and high fracture resistance as compared to their synthetic counterpart [1, 2]. In addition to the already listed advantages, other benefits of natural fibres in composite development include low weight, low density, and cost-effectiveness. They are also renewable, possess acceptable specific properties, have relatively high stiffness and strength, and are known not to cause skin irritations when it comes in contact with the human body. The versatility of polymer composites and the constant rise of their usage has changed

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the course of research toward the development of alternative materials capable of addressing the environmental concern associated with them [3].
Adequate knowledge of the physical and thermo-mechanical behaviour of these natural fibres reinforced polymer composites will enable engineers to come up with the best designs for different engineering structures, and at a considerable cost. For example, the matrix properties, and thermal conductive nature of the used fibre, in addition to their shape orientation, thickness, volume fraction and the bond formed between the constituents, determine the thermal conductivity of a composite. The improved strength achieved when natural fibres are used as reinforcement in polymer composite has made them suitable for some structural applications, and their good thermal properties have made them a good candidate for use as ceiling boards in buildings [4].

Over the years, materials made from natural fibre composites are used as part of building components, because they help in the drastic reduction of energy consumption, via the reduction of heat transfer in air-conditioned buildings [5]. In automotive, wood-reinforced polymer composites are now used as part of the components for the fabrication of car roofs, car door panels, covers etc [6]. Natural fibre polymer composites are also popularly used for interior applications such as electrical appliance packages and furniture.

The determination of the mechanical properties of composites through computational modelling methods has shown to be effective, based on the parametric study conducted to expedite the process of design and development of composites [7, 8], as the predicted mechanical properties compared favourably well with those obtained experimentally. Representative volume element (RVE) is a popular technique used for evaluating the effective or bulk material properties of composites with randomly distributed short fibres [9, 10]. Finite element analysis (FEA) on the other hand computes the bulk material properties with respect to the volume fracture, the properties and the geometry of the constituent phases present in the composites [11]. Some of the RVE software frequently used are Digimat, FET2I, and CAE Fidesys; and some of the FEA software often used are Abaqus, Comsol and Ansys. In addition, finite element modelling of RVE of composite materials has played a crucial role in the field of material engineering, particularly in the understanding of micromechanics of composites debonding and cracking, which often develop at the interfaces of the fabricated material [12-14].

Polyethylene (PE) is an extensively used polymer due to its low cost and versatility. However, it is known to cause serious environmental problems since it takes a prolonged time to decompose [15]. Thus, the shift in attention in the research world toward turning this environmental waste into novel composites that is suitable for different applications [16, 17]. In a bid to expand the potential and usage of wood flour polymer composites, several types of research on wood flour polymer composites have focused on the comparison of the different ways of processing the composites, understanding the viscoelastic behaviour and better ways of improving their interfacial adhesion. Over the years, maleic anhydride (MA) grafted PE have been discovered as a very effective compatibilizer, and thus used to enhance interfacial compatibility between natural fibre and polymer matrix [15, 18].

In the manufacturing of wood polymer composites (WPCs), the wood species that are commonly used are maple, pine, and oak, nevertheless, other species can be used. Since the physical, chemical, and microstructural properties of wood have a significant effect on the microstructure and the bulk properties of the developed WPCs, an appropriate selection of wood species is paramount in WPCs development [19]. For example, the use of wood flour from hardwood as reinforcement polymer composites tend to improve tensile strength more than when wood flour from softwood is used.

In this present study, representative volume element (RVE) software, Digimat in conjunction with finite element analysis software, Abaqus were used to develop and predict the thermomechanical properties of wood flour-reinforced polymer composites. Teak wood flour and low-density polyethylene (LDPE) were used in the fabrication of the composites. Teak wood flour (Tectona grandis Linn.) was used in this study because of its high patronage in furniture, decorative veneers, construction, cabinets, and the building of boats and ships.

2 Methodology

In studying the effect of the shape and size of the wood flour on the properties of the developed composites, the RVE software, Digimat makes the following assumptions: (i) the matrix (LDPE) and the inclusions (wood flour) are isotropic, homogeneous and are bonded to each other perfectly; (ii) the orientation and the distribution of the wood flour (inclusions) with small aspect ratio are homogeneous statistically; (iii) only elastic deformation is induced by the applied loading [20]. Based on these assumptions, it is hypothesized that for a given inclusion with a fixed volume or weight fraction, with an adequately small length to RVE size, the developed composites' properties such as the shear modulus, Young's modulus and Poisson's ratio are independent of the orientation of the loading [12].

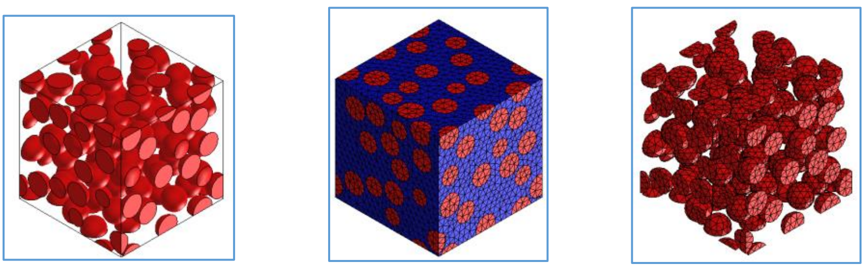
Digimat-FE was used to develop the composites with varying wood flour/polymer ratios as depicted in **Table 2**, and the material properties of the teak wood flour and LDPE used in the study are shown in **Table 1**. In the software, the LDPE was defined as the matrix while the wood flour was defined as an inclusion, after which the wt.% of the LDPE and wood flour are specified as shown in **Table 2**. Since the fabrication of wood flour polyethylene composites is a thermomechanical process (it requires the application of heat and pressure), thermomechanical analysis was selected in the software, where a pressure load of 50MPa and temperature of 180 ℃ was applied. The wood flour inclusion was assigned an ellipsoid shape with an aspect ratio of 2.0, and a perfectly bonded interface was assigned to the matrix-filler interface. Thereafter, the model of the composite was developed and the appropriate mesh size (0.05 mm) was assigned as depicted in **Fig. 1**. To ensure homogeneity in the properties of the developed composites, a periodic boundary condition was applied to the developed model. Upon the completion of the analysis in Digimat, the bulk material properties obtained from the software are used in finite element analysis software, Abaqus to determine and hardness of the developed composites.

Table 1. Material properties of LDPE and teak wood flour used

Material properties	LDPE	Teak wood flour
Density (kg)	930	720
Thermal conductivity (W/mK)	0.34	0.12
Thermal expansion (K^{-1})	2.0×10^{-4}	7.0×10^{-6}
Modulus of elasticity (GPa)	1.08	9.32 [21]
Poisson's ratio	0.44	0.43
Specific heat (J/kgK)	2 600	1 760

Table 2. % composition of LDPE and teak wood flour

S/N	LDPE (wt.%)	Teak wood flour (wt.%)
1	95	5
2	90	10
3	85	15
4	80	20
5	75	25
6	70	30



(a) (b) (c)

Fig 1. (a) Assembly model, (b) mesh model of assembly and (c) mesh model of filler (teak wood flour)

In order to determine the hardness of the developed wood flour polymer composites developed, the bulk material properties obtained from the RVE software, Digimat was used in Abaqus to simulate Brinell hardness, after which the diameter of the indent obtained for the different wt.% of teak wood flour LDPE composite was substituted in the Brinell hardness expression to determine the individual Brinell hardness. **Fig. 2** shows the indent on one of the samples, stress and strain developed during the simulation of Brinell hardness of the wood flour polymer composites developed.

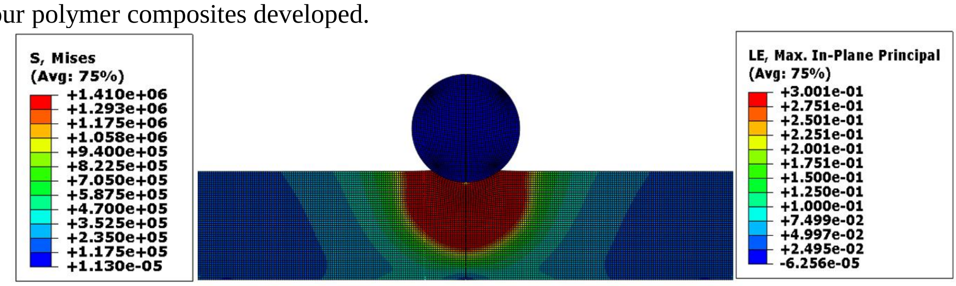


Fig 2. Simulation of Brinell hardness

With the value of the applied load known and the diameter of the indent and ball, also known, the Brinell of the developed wood flour polymer composites are computed.

3 Results and discussion

The distribution of the von Mises stress and principal strain in the developed teak wood flour LDPE composites with 5 wt.% and 30 wt.% respectively are shown in **Fig 3**. The portion of the composites where inclusions come closest to one another experiences the most strain.

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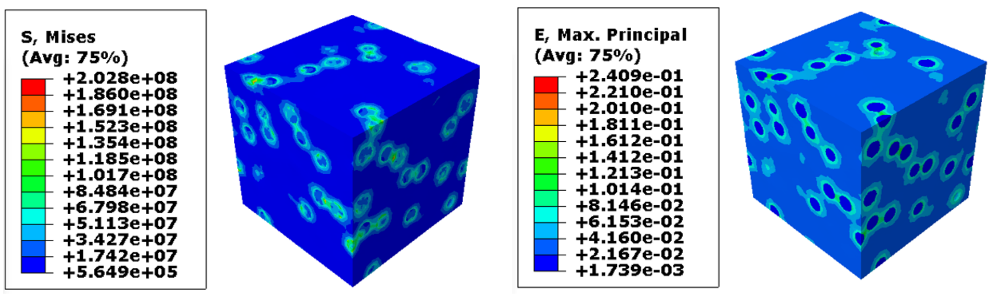
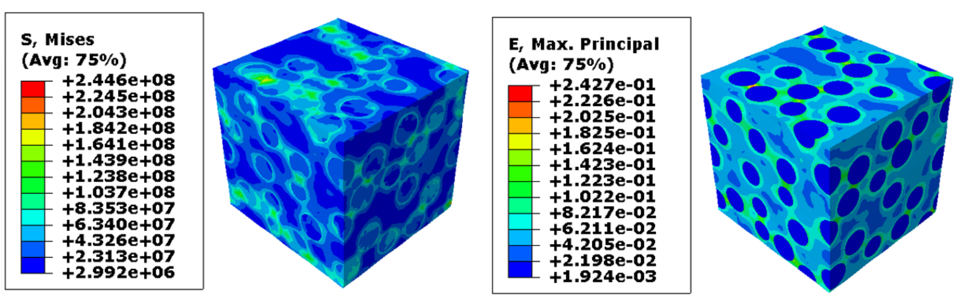
Hence, this results in the development of a higher stiffness in the region, while the region of the composite with embedded stiff inclusions in the soft matrix bears the highest stress. Similar stress and strain behaviour was reported in a study conducted on the reinforcement PEDOT:POS with graphene and borophene, using RVE [22].

Fig. 4 shows the stress-strain curve within the elastic region of the developed polymer composites. Since the composited developed are still with the elastic region (0.03 strain), they exhibit linear behaviour. However, the strength of the composites was observed to increase with an increase in the wt.% of the teak flour. Similar behaviour was observed in a study conducted by Bledzki et al. [6], where PLA and polypropylene were reinforced with soft wood flour.



(a)



(b)

Fig 3. Stress and strain distribution plots for teak wood flour LDPE composite with (a) 5 wt.% and (b) 30 wt.% teak wood flour

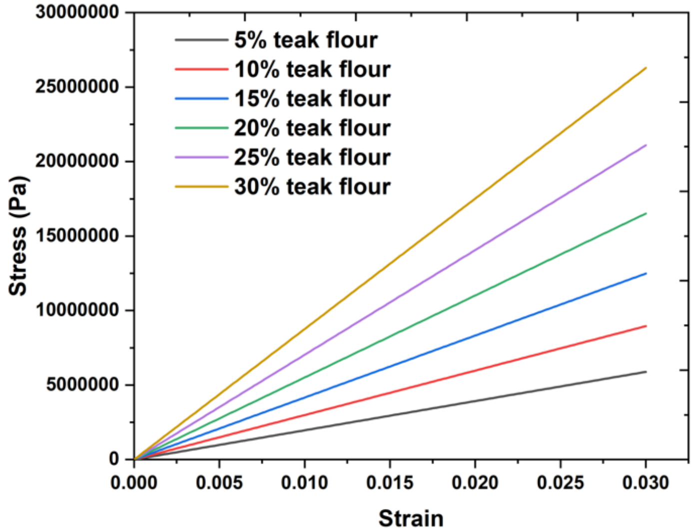


Fig 4. Stress versus strain plots of the teak flour LDPE composite at different wt.% of teak wood flour

Fig. 5 shows the thermal conductivity, modulus of elasticity, and Poisson's ratio of the developed teak wood flour LDPE as a function of the wt.% of the teak wood. From the plot, it was observed that the thermal conductivity of the developed composite decreases with the increasing wt.% of the teak flour. The decrease in thermal conductivity of the developed polymer composites with an increase in the wt.% of the wood flour is due to the increment in the porosity that emanates from the wood flour degradation and the subsequent formation of volatile organic compounds (VOCs) [23]. Similarly, the Poisson's ratio of the composite decreased with an increase in the wt.% of wood flour, but the modulus of elasticity increased with an increase in the wt.% of the wood flour. The reason for this behaviour can be attributed to the fact that the wood flour phase has a higher rigidity as compared to the polymer matrix [24]. The increase in the elastic modulus of the composites with an increase in the wt.% of the teak flour can be attributed to the higher elastic modulus of the teak flour as compared to that of the LDPE, and the fact that the polymer matrix has a lesser rigid phase as compared to teak wood flour filler [24].

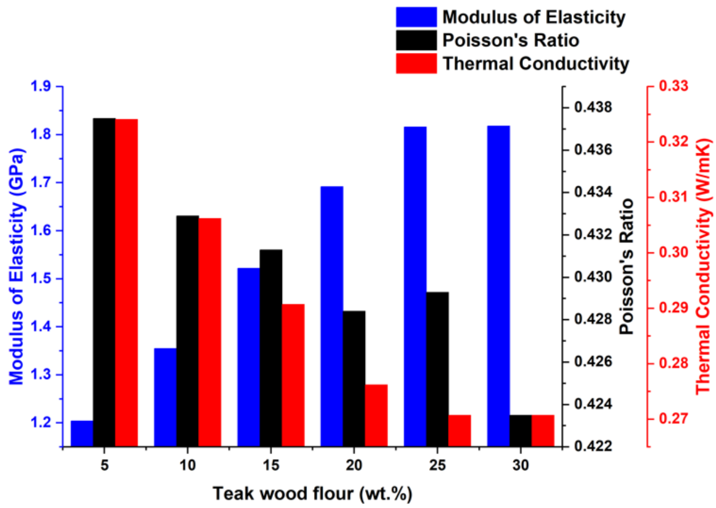


Fig 5. Elastic modulus, Poisson's ratio, and thermal conductivity of teak wood flour LDPE composite

Fig. 6 shows the Brinell hardness results and the density of the developed wood flour composites as a function of the wt.% of teak wood flour. Due to the viscoelastic behaviour of wood flour, the density of the composite was observed to decrease with an increase in the wt.% of the teak flour, and the formation of volatile organic compounds during fabrication is responsible for the appreciable decrease in the density of the composite as the wt.% of the wood flour is increased [23]. Similar behaviour was reported in a study conducted on the effects of wood flour on the properties of pressed wood plastic composites [25].

The hardness of the developed composites increased with an increase in the wt.% of teak flour such that the composite with 30 wt.% teak flour gave the highest hardness. This increment in the hardness of wood flour with an increase in the wt.% of wood flour could be attributed to the fact that an increase in the % composition of wood flour in the composite result in a restriction of plastic flow behaviour which is trapped by the teak flour, and this eventually leads to an increase in resistance of the composite to indentation. Similar behaviour in the hardness of the developed composites was reported when wood flour was used to reinforce polyester resin [26].

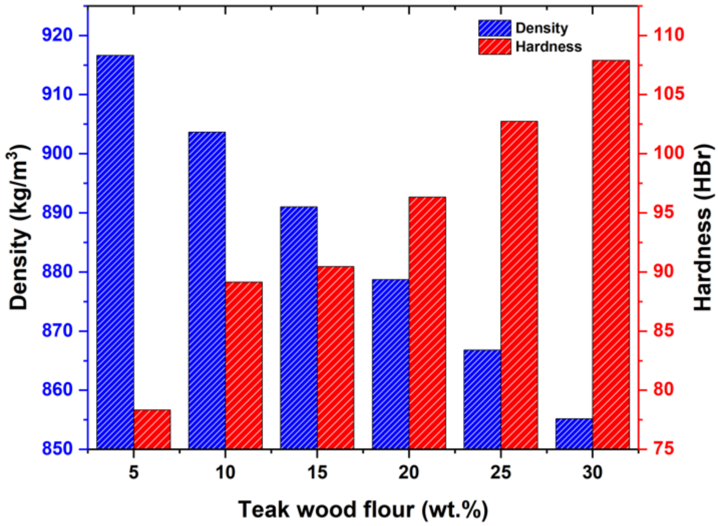


Fig 6. Density and hardness of teak wood flour LDPE composite

4 Conclusions

In this work, a computational technique was used to develop wood flour polymer composites using different weight ratios of teak wood flour and low-density polyethylene. Representative volume element (RVE) software (Digimat) in conjunction with FEA software (Abaqus) was used to design and determine the thermomechanical properties of the developed wood flour polymer composites. The strength, modulus of elasticity, and hardness of the developed composites were observed to increase with an increase in the wt.% of teak wood flour while the density, Poisson's ratio, and thermal conductivity decreased with an increase in the wt.% of the added wood flour. The thermomechanical results obtained using RVE and FEA software follow the same trend as those obtained experimentally in the literature, when wood/sawdust was used to reinforce polymer, and the hardness values predicted using this software are within the range for wood flour polymer composites.

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