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Research Paper

From lignocellulose to biocomposite: Multi-level modelling and experimental investigation of the thermal properties of kenaf fiber reinforced composites based on constituent materials

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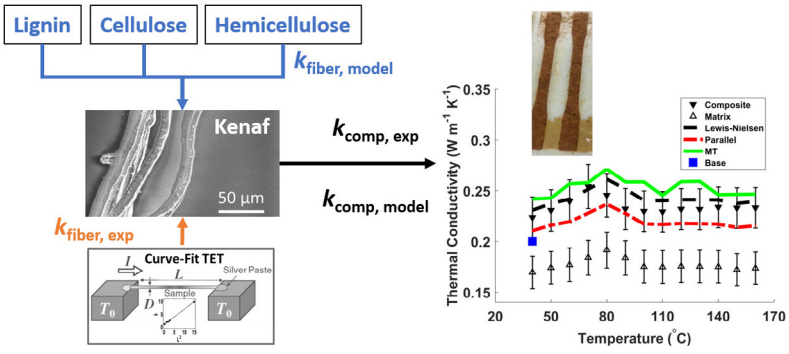
HIGHLIGHTS

- The thermal conductivity of Individual kenaf fibers was measured.
- A multi-level constituent-based composite thermal conductivity model was developed.
- Effective thermal conductivity of a kenaf fiber reinforced composite was measured.

GRAPHICAL ABSTRACT



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ABSTRACT

Natural fibers (such as kenaf) have garnered interest recently for use in composites because of their relatively high specific properties, low cost, and low environmental impact. Their thermal property information is limited, lacking experimental data on key properties such as thermal conductivity, specific heat, and CTE of the component fiber. This paper presents, for the first time, the thermal property data on kenaf fiber reinforced composites, and an approach to obtain the composite thermal properties based on constituent properties. Individual, plant-based fibers were measured independently and were then used to inform successful predictions of the effective thermal conductivity of the fiber reinforced composites. A unit cell model has been developed to predict the thermal properties of a planar, randomly oriented kenaf fiber-reinforced composite (near 22% volume fraction loading), which includes the effect of void content on the predicted thermal conductivity. A lower-level model is also developed for individual fiber thermal properties based on its constituents (lignin, cellulose, and hemicellulose). To validate this multi-level model, experimental measurements of the thermal diffusivity, coefficient of thermal expansion, and specific heat for the composite, the matrix, and the fibers were performed in the range from 30 °C to 160 °C, based on TMA, DSC, LFA, and transient electro-thermal (TET) techniques. Model results compare favorably with the experimental data, and are consistent with FEM modelling results based on fiber properties and fiber constituent materials (lignin, cellulose, and hemicellulose). This approach provides the

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basis for understanding component contribution to the fiber properties, as well as a technique to obtain fiber composite thermal property based on component properties. The composite thermal property data also fills an information gap and can be directly used in component design.

1. Introduction

Fiber-reinforced composite materials have shown their capacity to be useful and more effective in many fields because of their potential low density and high specific properties, as well as their tunable properties based on variation and orientation of the fiber content. Due to the awareness of the environmental issues and costs, recent studies have been focused on more eco-friendly features by developing composites using bio-fibers or silks such as banana [1], bamboo [2], kenaf [3], hemp [4], and spider silk [5]. Plant-based bio-fibers are valuable because of their high specific strength due to low density (kenaf = 1.45 g/cm^3 [6], spider silk = 1.36 [7], Kevlar = 1.44 [8], carbon fiber = 1.8 [9], jute = 1.3–1.4 [10]), bio-degradability [11], low cost ($0.40–$0.55/kg) compared to $2/kg for glass fibers [6]), and their low energy consumption during production [6,12].

Kenaf (*Hibiscus cannabinus* L.) is a crop, originated from Africa and widely cultivated around the world for use as fiber, paper pulp, or biofuel [13]. It has been investigated as a binderless thermal insulator [14], as well as for use in a hybrid fiber composite with other fibers [15,16]. However, traditional thermal characterization of natural fiber reinforced composites are focused on the thermal stability of the composite via DMA [12,17,18], TGA [10,17,19–22] and DSC [10,21,23–25]. Thermal expansion of the composites are sometimes measured as well by TMA [10,11,17,26]. However, thermophysical properties (such as thermal conductivity) are not as often reported, although they are essential for thermal applications of the composite and for modelling thermal behavior. When performed, these investigations use a laser flash method (typically an LFA machine [25,27,28]) for thermal diffusivity (α), DSC for specific heat, and density often from literature values.

Multi-level thermal modelling techniques are often focused on using atomistic simulations (molecular dynamics [29] and density functional theory [30]) to inform mesoscale models (phase field [31]) and finally through homogenization to macroscale (Mori-Tanaka). Particularly in the nuclear energy field, where irradiation can cause microstructural evolutions of voids, grain boundaries, and phase separations in nuclear fuels, multi-level simulations are being developed to predict the thermal conductivity of UO_2 ceramics [32]. However, these models are very computationally expensive and require knowledge of the microstructure. The focus of the current study is to present models based on experimentally measured thermal property values of the constituent materials that require very little computation resources, to aid in the engineering design of biological fiber reinforced composites.

The current study seeks to develop a multi-level model to predict the thermal conductivity of the kenaf composite based on a simple base-level model for the properties of the fiber based on the constituent materials (lignin, hemicellulose, cellulose) and higher-level models based on fiber and resin properties to determine the effective composite values. Validation experiments were conducted to determine the thermal properties, including thermal diffusivity, thermal conductivity, specific heat capacity, and thermal expansion between 30 °C and 160 °C for a kenaf composite, its resin, and fibers. The temperature range was selected to provide data from room temperature to slightly above the glass transition temperature (T_g). These results will then be compared to a unit cell-based FEM model and other analytical models (including derivation of a micromechanics-based model). Measured property data is also compared to literature values of the constituent materials of the kenaf fiber(cellulose, hemicellulose, lignin). This quasi-multiscale (termed multi-level) modelling of natural fiber thermophysical properties from constituent materials to bulk behavior is lacking in the literature [33] and necessitates experimental validation with proper measurements of the bulk values. This work provides a preliminary study on traditional matrix composites in preparation for extending techniques to green/eco-composites.

2. Materials and experimental methods

2.1. Materials

To form the composite, kenaf bast fibers (averaging 70 mm in length) were obtained in bulk from Bast Fiber LLC. They were chopped to a length of 10–15 mm and soaked in a 3% NaOH solution for 12 h to remove impurities on the surface. The fibers were dried in an oven at 80 °C for 8 h. The dried fibers were then shredded using carding brushes, resulting in lengths from 1 to 5 mm. They were then mixed with an epoxy matrix (PT2050 B1 by PTM&W Industries) at a 22% fiber volume fraction, based on volume calculations of the fiber from mass and density data, and ignoring void that formed during curing. The mixture was then placed in the dog-bone shaped tensile specimen molds (Fig. 1a). Pressure was applied with tightening clamps and the composite was cured at 80 °C for 12 h. Vacuum bagging was not used because there was no way of ensuring a flat top surface in the end product.

The samples used for the current study came from standard dog-bone specimens after mechanical testing occurred. The samples were cut and polished to the necessary shape for use in the different measurement instruments. The fiber pattern is randomly oriented, with a slight bias in the x-y horizontal plane, similar to the in-plane randomly oriented fiber reinforced hemp composite in Ref. [4]. This bias is quantified during the measurement of the CTE of the composite (Section 3.2.3), with the result being that thermal expansion of the different axes agree, within experimental uncertainty, and the effect of the bias on thermal properties was taken to be minimal.

2.2. Experimental methods

2.2.1. Density

The density of the composite was 1134 kg/m^3 (±100 kg/m^3) based on the displaced liquid volume, the resin at 1110 kg/m^3 from manufacture specifications, and kenaf fiber at 1450 kg/m^3 [2].

2.2.2. DSC

The specific heat (c_p) measurements of a fiber bundle, the resin, and the kenaf composite were carried out with a NETZSCH 404 F3 Pegasus. The apparatus performed the test with a 30.1 mg sample for both the resin and the composite. The heating scan rate was set at 5 K/min, with a temperature range from 30 °C to 160 °C in a nitrogen environment. An Al_2O_3 holder was used and the reference sample employed was a sapphire disc.