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Modelling and Simulation of Thermo-Physical Property of Composite Material

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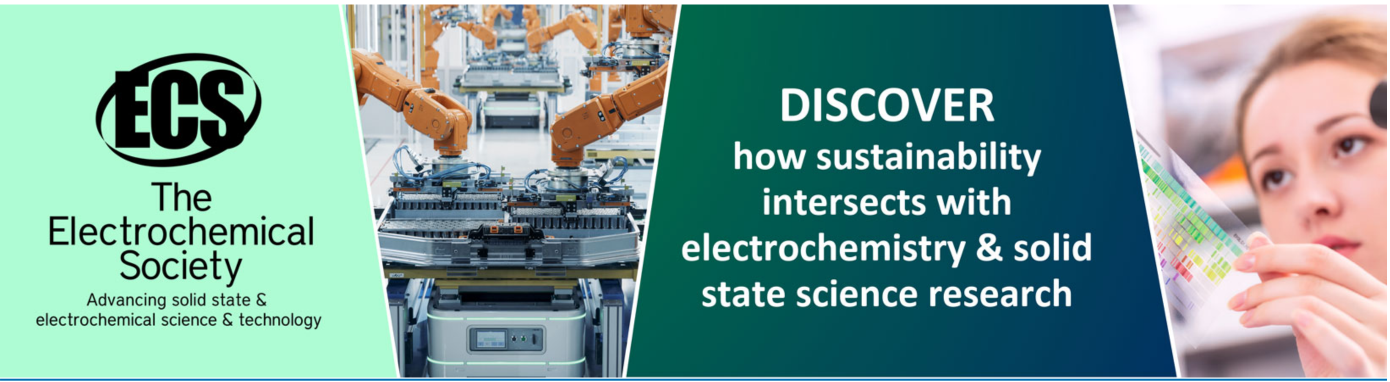

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Retraction

Retraction: Modelling and Simulation of Thermo-Physical Property of Composite Material (*IOP Conf. Ser.: Mater. Sci. Eng.* **1145** 012035)

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[1] Cabanac G, Labbé C and Magazinov A 2021 arXiv:2107.06751v1

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Retracted

Modelling and Simulation of Thermo-Physical Property of Composite Material

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Abstract. Thermo-physical property measurement is a significant methodology as these properties are the input for designing thermal systems. Properties of materials like thermal conductivity, thermal diffusivity and specific heat capacity has to be estimated in prior to estimate the thermal performance of any material. In the present work, numerical simulations were performed to estimate the thermo-physical properties of a polymer based composite material using porous medium modelling. The weight fraction of the composites and fibres are incorporated into the simulations through porosity. The transient heat diffusion equation are solved using ANSYS Fluent for a polymer based composite material using semi-infinite transient conduction approach. The thermal conductivity and thermal diffusivity are estimated simultaneously for various volume fractions of polyester and banana fibre. The temporal temperature distribution data predicted from ANSYS Fluent is curve fitted using MATLAB and the obtained values of thermal conductivity and thermal diffusivity are compared with the previously reported experimental results and are found to be within a deviation of 7 % for all cases.

1. Introduction and theoretical back ground

Transient thermal behaviour of materials are prevalent in applications involving periodic heating and cooling like IC engines, cold storage, cryogenics, metallurgy, catalytic reactors, air conditioning ducts, green buildings etc. The selection of materials to these applications is based upon the thermo-physical properties – thermal conductivity k, thermal diffusivity α and specific heat capacity C. By estimating two of the three thermo physical properties, the other can be estimated for any solid of known density ρ through Eq. (1).

$$\alpha = \frac{k}{\rho C} \tag{1}$$

The estimation procedure of any two properties in Eq. (1), differs considerably with the nature of the material and time instant from the initial condition. The thermal conductivity and thermal diffusivity of an insulator can be estimated simultaneously through semi-inifite transient heat transfer approach - the early regime with spatial effects of temperature variation with respect to time [1]. The sensitivity analysis can be performed to find the time window for experiments [2, 3]. However, owing to the greater thermal diffusivity of good conductors, these properties cannot be estimated simultaneously as heat diffuses faster in good conductors. So the thermal conductivity and the specific heat capacity are estimated separately using two different approaches [4, 5] in steady state and the thermal diffusivity is measured using Eq. (1).

The general heat diffusion equation in Cartesian coordinates for a material with internal heat

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generation q is given in Eq. (2).

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{q}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{2}$$

For a one dimensional heat diffusion with no heat generation, Eq. (2) reduces to Eq. (3)

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3}$$

Solving Eq. (3) using a similarity variable and applying constant heat flux boundary condition with a uniform wall heat flux of q over the surface, the temperature distribution at any x at a time instant t is obtained as

$$T(x,t) - T_i = \frac{2q}{k}\,\frac{\alpha T}{\pi}\,exp\,\frac{-x^2}{4\alpha t} \tag{4}$$

The temperature distribution, Eq. (4) is valid in the early regime of transient conduction in solids in which the temperature inside the solid is uninfluenced by the change in the surface heat flux [6]. Such a characteristic is exhibited by an insulator having poor thermal diffusivity during the early heat transfer regime. So the limiting condition for a material to be assumed as a semi-infinite solid is expressed in terms of non-dimensional time – Fourier number, given in Eq. (5)

$$Fo = (a/t)/2 \leq 0.2 \tag{5}$$

The time t obtained from Eq. 5 is taken as the limiting time for the conduct of experiments, beyond which the region away from the surface will be influenced by the change in the surface heat flux making the semi-infinite assumption invalid. From Eq. (5), it is inferred that a material with lesser α gives more t, the time duration of conduct of experiments. This justifies considering a polymer based composites as a semi-infinite solid.

The temperature distribution, Eq. (4) obtained by solving Eq. (2) is for a homogeneous material. The thermal conductivity and the thermal diffusivity involved in Eq. (4) are isotropic. The estimation of these properties for a composite material is challenging due to the non-homogeneous nature of the materials and anisotropic thermo-physical properties. The thermo-physical properties of a composite material is modelled as effective properties based on the thermo-physical property of a constituent material and volume fraction of these constituents [7].

Modelling composite materials as a non-homogeneous media and proposing models to predict the thermo-physical properties renders the model material specific within a narrow range of volume fractions and temperature limits. In the present work, the composite material – polyester with banana fibre is modelled as a porous medium - a homogeneous medium and the temporal temperature distribution results were compared with the previously reported experimental results.

2. Computational methodology

The computational domain used in heat transfer simulation is shown Fig. 1. The dimensions of the domain are estimated by the limiting Fourier number, Eq. (5). The computational domain is modelled as a porous medium in ANSYS Fluent with thermo-physical properties of material constituents shown in Table 1. The volume fraction, φ of materials are obtained by knowing the density ρ and weight percentage W of the resin and fibre using Eq. (6).

$$\varphi = \frac{(W\rho)_{Resin}}{(W\rho)_{Fibre}} \tag{6}$$

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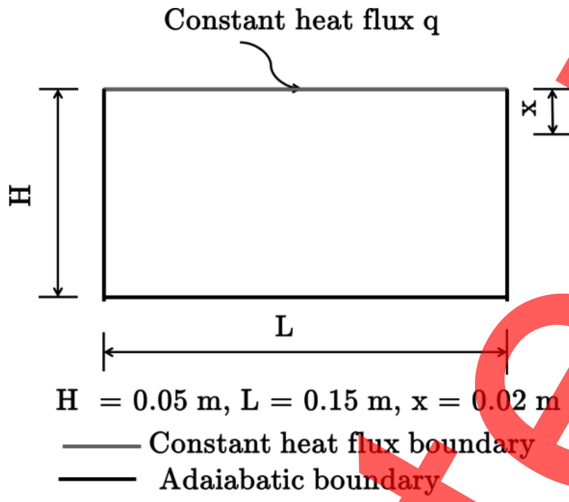

Figure (1) Computational domain for simulations

Table (1) Properties of composites

Literature	Material	φ	$\alpha \times 10^{-7}$ m^2/s	K W/mK	C kJ/kgK	ρ kg/m^3
Idicula *et al.* [8]	Polyester	0	1.08 ± 0.09	0.181 ± 0.003	1408 ± 123	1190 ± 123
Idicula *et al.* [8]	Polyester	0.2	1.25 ± 0.09	0.153 ± 0.002	1199 ± 88	1021 ± 88
Idicula *et al.* [8]	Polyester	0.4	1.14 ± 0.09	0.140 ± 0.002	1246 ± 103	986 ± 123
Assis *et al.* [9]	Banana Fibre	1	8.20	0.55	1350	496

The computational methodology used in ANSYS FLUENT are discussed further. The heat transfer is assumed to be one dimensional, with no heat loss from the the lateral sides. The governing momentum equations, Eq. (2) is solved in the PM domain. The uniform heat flux boundary condition is used at the surface. The thickness of the channel is assumed such that the time t for heat diffusion is small enough for the material to be considered semi-infinite. The finite volume method is used to discretize the partial differential equations. Implicit, second order upwind solver is used with the velocity and pressure coupling achieved by the SIMPLE algorithm. The convergence criterion for the energy equation is set as 10^{-6}. Grid independence study is conducted for temperature for four successive grid levels at $q = 5000$ W/m^2. When the error between two successive levels of grid refinement is less than 1% for temperature profile, that grid size is chosen for all the subsequent computations. Quadrilateral uniform grids in both x and y directions with 76392 nodes is used in the computational study. The grid independence plots for $q = 5000$ W/m^2 is shown in Fig. 2.

The temporal temperature distribution at a spatial location is obtained with one of the surface subjected to constant heat flux of 5000 W/m^2. The percentage weight fraction is incorporated into the numerical simulations through volumetric porosity.

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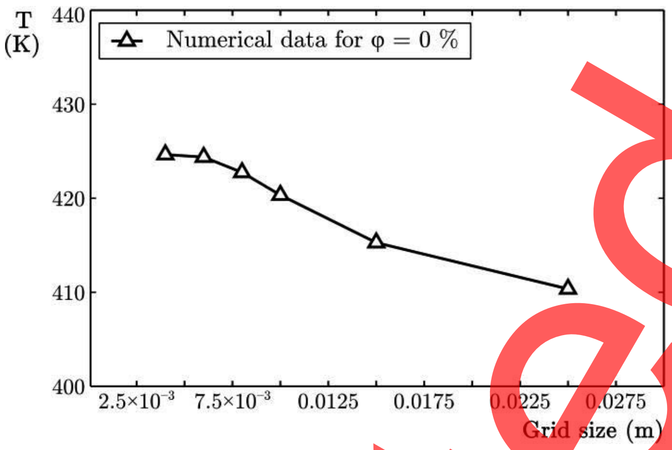

Figure (2) Grind independence temperature results for φ = 0%

3. Results and Discussions

(a) (b)

(c) (d)

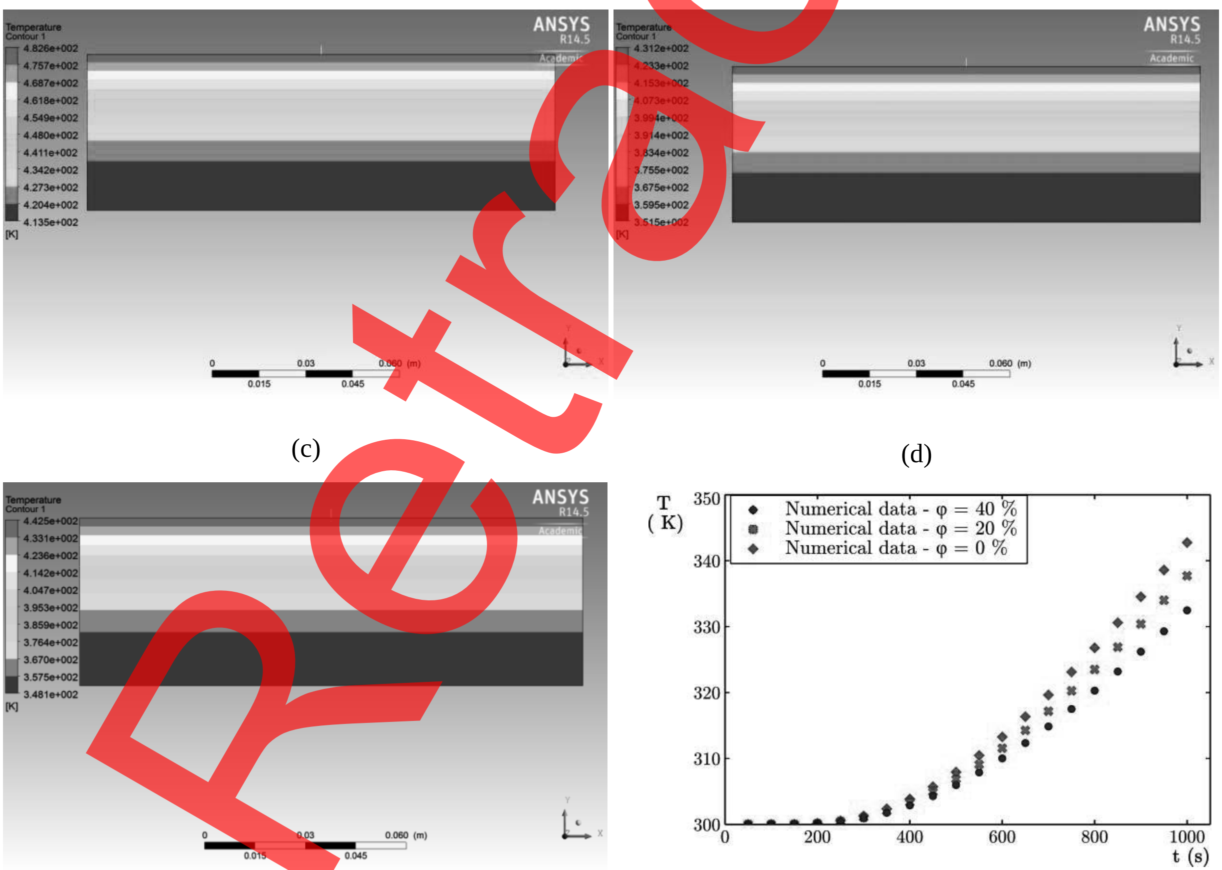

Figure (3) Temperaturure Vs time plots for (a) 100% polyester. (b) 80% polyester and 20% Banana fibre. (c) 60% polyester and 40% banana fibre. (d) Comparison plots for composite materials for different φ.

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The numerical results for temperature distribution for q = 5000 W/m^2 for polyester with 0%, 20% and 40% volume fractions are shown in Fig 3. From Fig. 3, it is inferred that the temperature far away from the top surface (at which the heat flux is applied) is uninfluenced the change in surface heat flux justifying the semi-infinite solid approximation. The temperature is maximum for composite material with 0% φ followed by 20 % and 40 % inferring the increase in the insulating nature of the material. The temporal temperature distribution plots of compsoite materials are compared in Fig. 3d.

The temperature distribution plots are imported as a discrete data into MATLAB and the corresponding temperature time plots are shown in Figs. 5 to 6. This also corresponds to the early regime of transient conduction. The time temperature data of the porous media computational domain is curve fitted with Eq. (4) in MATLAB using curve fit tool. The thermal diffusivity α and the thermal conductivity k are obtained. The obtained R^2 value for the curve fitting is 0.9985. The deviation between the predicted thermal diffusivity, conductivity and specific heat capacity with the experimentally reported values are compared through Figs. 4 to 6 and the % deviation are reported in Table 2.

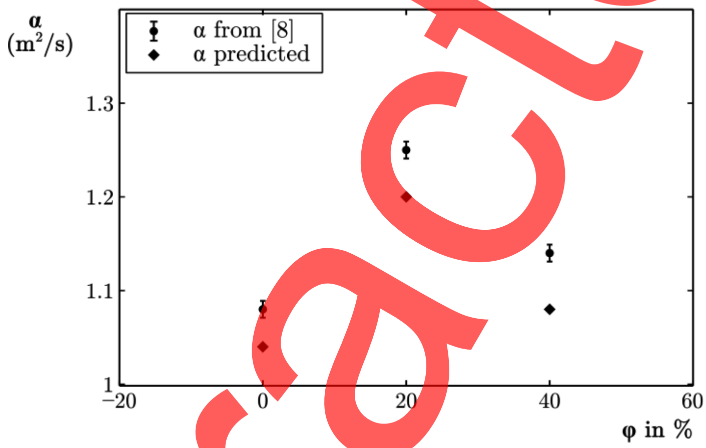

Figure (4) Comparison plots of thermal diffusivity

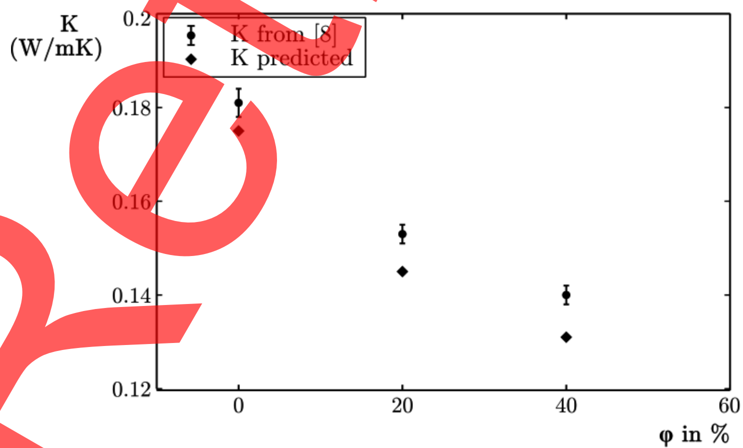

Figure (5) Comparison plots of thermal conductivity

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Table (2) Percentage deviation with results of Idicula *et al.* [8]

Material	α	K	C
Polyester with 0% fibre	3.42	3.84	3.7
Polyester with 20% fibre	5.17	4.16	3.15
Polyester with 40% fibre	6.87	5.55	4.26

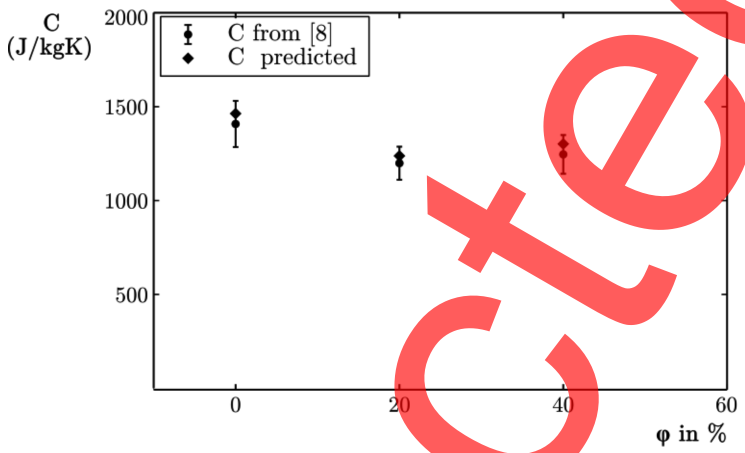

Figure (6) Comparison plots of specific heat capacity

The reported numerical results also conformed the dependence of the thermo-physical property on the volume fraction and thermo-physical property of the constituent materials as reported in [10-13].

4. Conclusion

The thermo-physical properties of a polymer based composite model were estimated using semi-infinite transient conduction approach. Numerical simulations were performed using ANSYS Fluent with the thermo-physical properties of constituent materials using porous medium modelling to estimate the temperature distribution of the composite material within the material with respect to time and space. The obtained temperature distribution was curve fitted with Eq. (3), using MATLAB to estimate the thermal conductivity and thermal diffusivity simultaneously. The obtained curve-fit thermo physical properties are in better agreement with the previously reported experimental heat transfer results within a deviation of 7 %.

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