



Modeling thermal conductivity augmentation of nanofluids using diffusion neural networks

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ABSTRACT

In the present investigation, neural network method is employed to estimate thermal conductivity of nanofluids consisting of multi-walled carbon nanotubes (MWCNTs) suspended in oil (α -olefin), decene (DE), distilled water (DW), ethylene glycol (EG) and also single-walled carbon nanotubes (SWCNTs) in epoxy and poly methylmethacrylate (PMMA). The results obtained have been compared with other theoretical models as well as experimental values. The predicted thermal conductivities are in good agreement with the literature values.

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1. Introduction

Within the different classes of tubes made of organic or inorganic materials, carbon nanotubes (CNTs) are extremely promising for applications in materials and medicinal chemistry [1]. Since the discovery of CNTs by Iijima [2], CNTs have received much attention in theoretical and experimental studies on condensed matter physics and material sciences. CNTs are fascinating materials which combine the microscale (length) with the nanoscale (diameter) dimensions.

It should be mentioned that the investigations dealing with the thermal properties of nanotubes has not received as wide attention as the modeling of the mechanical properties, electronic properties, or even the modeling of flows through nanotubes. Because of existence of some impurities in synthesized nanotubes the measurements of the thermal conductivity of nanotubes or any other transport properties in different solvents are subject to some degree of uncertainty.

The thermal conductivity of a material is one of its thermodynamic response functions. The definition of thermal conductivity, k ,

is based on the macroscopic equation of heat flow known as the Fourier's law

$$J_q = -k\nabla T(x, t) \quad (1)$$

where J_q is the amount of heat flowing through a unit surface per unit time and T is the temperature of the material. Two contributions are made to the thermal conductivity, one is due to charge carriers (electrons) and the other is due to lattice vibrations (phonons).

The question of estimating the thermal properties of individual SWCNTs and MWCNTs as well as of their bundles has been addressed in a number of computational investigations. Therefore a couple of predictive computational modeling techniques of carbon nanotubes have become the focal point of research in computational nano-science area. In general, from a theoretical point of view, nanotubes can be modeled in terms of inter-atomic potentials describing the various forces experienced by the carbon atoms in the nanotubes and by those foreign atoms interacting with the tubes such as fluid particles. For example, by knowing the inter-atomic potentials, computational tools consisting of the molecular dynamic simulation (MD) [3–8] and the Monte Carlo (MC) [9] methods have been employed to model the transport properties of CNTs. MD simulation revealed that isolated SWCNTs had a very similar thermal conductivity as those of a hypothetical isolated graphene sheet with the same number of atoms at certain temperatures [10].

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