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Intelligent modeling of rheological and thermophysical properties of green covalently functionalized graphene nanofluids containing nanoplatelets

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ABSTRACT

Regarding the importance of accurate predictions in industrial applications, this research aims to investigate the ability of artificial neural networks (ANNs) to carry out modeling and multi-criteria optimization of the rheological and thermophysical properties of an environmentally-friendly covalently functionalized nanofluid containing graphene nanoplatelets (CGNPs). In this contribution, different ANN structures are assessed and the NNs with 2-7-1, 2-4-1, 2-7-1 and 2-5-1 structures having a linear transfer function (purelin) and a hyperbolic tangent sigmoid (tansig) transfer function in the output and hidden layer are found to give the least difference between the network outputs and the experimental data for the thermal conductivity, viscosity, specific heat capacity, and density, respectively. Moreover, new correlations for thermal conductivity and viscosity of the nanofluid are proposed and the LASSO (Least Absolute Shrinkage and Selection Operator) and SVM (Support Vector Machine) methods are also presented for comparative purposes. It is observed that all models performed in a very comparable fashion, giving an idea of the easy nature of the problem.

So it is recommended to train simple linear models like LASSO or SVM for such problems and perhaps the complex NNs are not necessary in some cases of practical prediction applications such as cooling or heating systems containing nanofluids. Furthermore, finding the optimal conditions is another crucial aspect of engineering problems. In this regard, a multi-criteria optimization of the hydrothermal characteristics of the nanofluid (i.e., to find the optimal cases with highest thermal conductivity and the relatively least viscosity) is conducted using the genetic algorithm coupled with a compromise programming approach.

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1. Introduction

Recently, the superb thermophysical properties of nanofluids have led to the implementation of these nanofluids as the nano-coolants for improvement of heat transportation in various applications [1–5]. Among different carbon-based nanomaterials, graphene nanoplatelets (GNPs) have gained significant attentions due to their mechanical, electrical and thermal properties [6–9]. Yu et al. [10] reported an improvement of about 86% in the thermal conductivity for 5.0 vol.% graphene dispersion in ethylene glycol media. Baby and Ramaprabhu [11] reported the thermal conductivity improvements of 14% and 64% for 0.056 vol.% highly stable exfoliated graphene-based nanofluids at 25 and 50 °C. Sarsam et al. [12] exhibited the maximum enhancement of 26% in the thermal conductivity of the nanofluid in the presence of 0.1 wt.% triethanolamine-treated GNPs at 40 °C.

However, the application of GNPs is limited since the homogeneous dispersion of these nanoplatelets is difficult to achieve due to their extreme hydrophobicity which leads to the aggregation of nanoplatelets [13]. In order to address this limit, covalent and non-covalent functionalization of graphene can be employed to modify the particle surfaces for the further stability of GNPs' dispersions in organic and aqueous media [13]. The functionalization process using a mixture of concentrated sulfuric and nitric acids is the most common technique for treating the carbon nanotubes [14]. However, from the environmentally-friendly perspective, this approach is not recommended due to its contribution to the environmental pollutions. In this regard, Sadri et al. [15] developed a new eco-friendly technique to covalently functionalize the GNPs

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using gallic acid (GA) in an aqueous solution. In fact, since the GA is a natural antioxidant and has a stabilizing nature and anti-oxidation, non-corrosive and non-toxic properties [16,17], they investigated the free radical graft of GA onto the surface of GNPs to improve its thermal performance.

On the other hand, the rigorous anticipation of nanofluid properties is of fundamental importance. Most of the times, development of practical and reliable correlations are very difficult [18,19]. This difficulty and the increasing need for accurate methods for predicting the experimental data have led to the introduction of intelligent systems such as artificial neural networks (ANNs) [20,21], which require much less time and cost to solve complex problems [22]. In this regard, many investigations have focused on the capability of ANNs for modeling the nanofluid thermal properties due to their superb features such as simplicity, extensive capacity and high-speed processing [23,24].

Hemmat Esfe et al. [25] developed a neural network to predict the thermal conductivity of MgO/ethylene glycol (EG) nanofluids at 25–55 °C. Afrand et al. [26] modeled the viscosity of the SiO_2–MWCNTs/SAE40 nanofluid using an ANN. Heidari et al. [27] used about 1500 experimental data points on the viscosity of various nanofluids and developed an ANN in terms of the base fluid viscosity and temperature, and nanoparticles size, density, and concentration. Afrand et al. [28–30] evaluated thermophysical properties of water-based Fe_3O_4, MgO, functionalized CNT nanofluids with different concentrations and temperatures and proposed the ANNs to precisely predict the experimental results. Bahiraei and Hangi [31] investigated the thermophysical properties of Fe_3O_4 nanofluids at 0–4 vol.% concentration and the temperature range of 25–60 °C. They developed a model for thermal conductivity and viscosity using neural network and revealed that the ANN is capable of accurate prediction of thermophysical properties of nanofluids.

In general, the comparison between the performance of the ANN model and the results obtained from experimental data discloses that the neural network can more accurately predict the thermophysical properties of studied nanofluids than conventional methods.

Based on what is discussed above, this study aims to employ the multilayer perceptron neural network to model the rheological and thermophysical characteristics of the covalently functionalized nanofluids containing graphene nanoplatelets synthesized from a green and bio-based technique at different temperatures. In this regard, the experimental data of thermal conductivity, viscosity, density, and specific heat capacity were taken from the work of Sadri et al. [15]. Different numbers of neurons and hidden layers are investigated for the achievement of the optimal network structure. Moreover, the significance and the normalized importance of input variables including temperature and the concentrations of GNPs on the rheological and thermo-physical characteristics of solutions are determined. For comparison purposes, the Least Absolute Shrinkage and Selection Operator (LASSO) [32,33] and support vector machine (SVM) [34] are also employed for the problem under study. In this regard, a multi-criteria optimization on the hydrothermal characteristics of the nanofluid is conducted to find the optimal cases with highest thermal conductivity and the relatively least viscosity using the genetic algorithm coupled with a compromise programming approach.

2. Preparation of nanofluid

The nanofluid considered in this study is synthesized though an environmentally friendly technique by Sadri et al. [15]. They covalently functionalize the GNPs to enhance its stability in polar solvents by employing dried clove buds. In this regard, the hydrogen peroxide and ascorbic acid were used to graft β-caryophyllene, eugenyl acetate, and eugenol onto the GNPs. The ascorbic acid and hydrogen peroxide served as the redox initiator and the free-radical oxidizer, respectively. This eco-friendly technique is comprised of two stages: (1) preparation of the clove extract (Fig. 1) and (2) the functionalization procedure. As can be seen, first, 15 g of ground cloves was added to 1000 ml of deionized water at the constant temperature of 80 °C. Then, an agitator was used to homogenize the solution for 30 min at 80 °C. Finally, a 45 μm polytetrafluoroethylene (PTFE) membrane was employed to filter the clove extract.

Regarding the functionalization, the solution of 1000 ml of clove extract and 5 g of pristine GNPs was stirred into a beaker for 15 min until a uniform black suspension was achieved. Then, after adding by degrees 25 ml of hydrogen peroxide into the suspension, 10 min sonication was conducted. Next, it was heated for 14 h at 80 °C. After that, the suspension was centrifuged at 14,000 rpm and repeatedly washed with deionized water to reach the pH of 7. Then, a vacuum oven was used to dry the resultant functionalized samples at 60 °C. Finally, in order to prepare the clove-treated GNPs (CGNPs) water-based nanofluid, different concentrations of CGNPs (0.025, 0.075 and 0.1 wt.%) were dispersed in the deionized water for 10 min [15].

For more information, the initiation reaction and the free radical grafting technique are illustrated in Fig. 2. As can be seen, the hydroxyl radicals form though the reaction of the hydrogen peroxide and vitamin C [35,36]. Then, the free radicals are formed on the structures of the eugenol and eugenyl acetate due to the attack of the hydroxyl radicals, resulting in the grafting of the activated

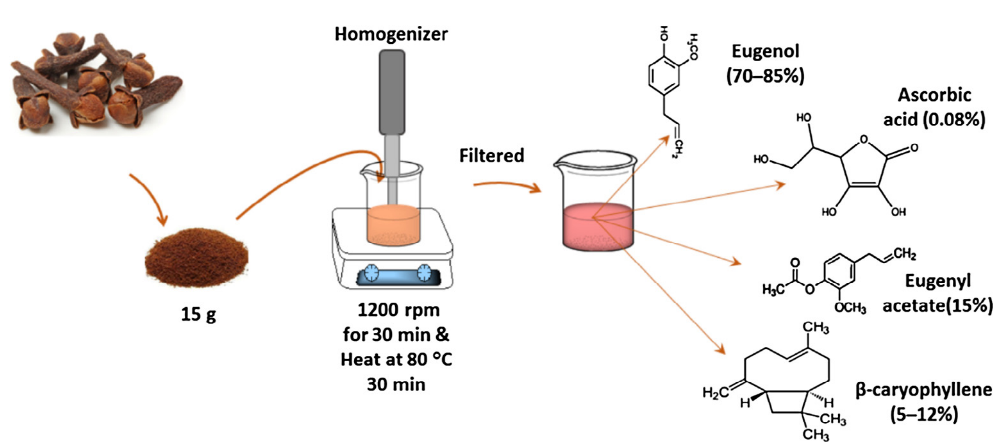

Fig. 1. Procedure of preparation of the clove extract [15].

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