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Bayesian regularization optimization algorithm for the experimental thermophysical property for 80:20% water and ethylene glycol based ZrO_2 nanofluids

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Abstract. In the current study, water and ethylene glycol (W/EG 80:20%) are used as the base fluid, and sodium dodecyl benzene sulfonate is used as a surfactant to create nanofluids using ZrO_2 nanoparticles prepared using the sol-gel technique. For temperatures ranging from 20 ºC to 60 ºC and various volume loadings of nanoparticles, 0.2, 0.4, 0.6, 0.8, and 1.0%, respectively, the thermal conductivity, dynamic viscosity, density, and viscosity of these ZrO_2 nanofluids are experimentally evaluated. Artificial neural network based Bayesian regularization algorithm was used to find the correlation coefficient R^2 and root-mean square error. New correlations were also suggested for each of the thermophysical properties. Experiments show that temperatures and concentrations of nanoparticles have a significant impact on the thermophysical properties of nanofluids. In fact, it is shown that, at 20 ºC and 60 ºC, respectively, increasing the thermal conductivity of nanofluids by 1.0 vol% leads to increases of almost 10.16% and 24.53%. Additionally, at 1.0 vol and 20 ºC to 60 ºC, the dynamic viscosity is reduced from 61.94% to 50.79%. The correlations and outcomes of the developed artificial neural network are in perfect agreement with the experimental data.

Introduction

The majority of engineering fields have combined their heat transfer methods, and in recent years, research has focused heavily on creating smaller and more effective heat exchangers. Many research activities are now concentrated on increasing the low heat transfer capacities of conventional liquids like water (W), ethylene glycol (EG), or engine oils after extensive use of various approaches, such as modifying materials, using extended surfaces, or improving process standards. In this regard dispersing high conductivity nanoparticles, also referred to as nanofluids [1] has improved the thermal transport properties of heat transfer fluids, making them important research tools [2].

A wide range of nano-additives were used to create the nanofluids including metallic oxides, organic materials, and inorganic materials. Numerous studies have demonstrated that using single phase nanofluids may enhance the heat transfer capabilities of the thermal devices [3-4]. Sundar and Sharma [5] have observed an enhanced thermal conductivity (k_{nf}) with the use of water based Al_2O_3 nanofluids. Wang et al. [6] obtained an enhanced thermal conductivity by using Al_2O_3 and CuO nanoparticles into water, vacuum pump fluid, engine oil, and ethylene glycol. Murshed et al. [7] also found an increased thermal conductivity for TiO_2/water nanofluid. Liu et al. [8] have seen 24% augment in thermal conductivity of 0.1% water mixed Cu nanofluids. Mintsa et al. [9] revealed an augmented thermal conductivity with Al_2O_3/water, and CuO/water nanofluids.

Apart from the water, the mixture of water and ethylene glycol is used as a base fluid for the preparation of nanofluids. The freezing temperature of water can be enhanced by adding small quantity of ethylene glycol [10]. The water and ethylene glycol mixture fluids can be used as engine coolant in automobile radiators in the cold region countries. Vajjha and Das [11] found an increased thermal conductivity of CuO and Al_2O_3 nanofluids, but they used 60:40% of ethylene glycol and water (EG/W) mixture as a base fluid instead of water, because this water and ethylene glycol is used as engine coolant. Sundar et al. [12] have seen an augmented k_{nf} of 50:50% W/EG Al_2O_3 and CuO nanofluids. They determined thermal conductivity in the temperature range from 15 ºC to 50 ºC and in the volume loadings from 0% to 0.8%. Banisharif et al. [13] observed thermal conductivity enhancement of 9.5% and 14.3% at 0.1% vol. of 50:50% W/EG Fe_3O_4 nanofluid at temperatures of 263.15K and 293.15K respectively. Usri et al. [14] noticed an augmented thermal conductivity for 40:60%, 50:50% and 60:40% W/EG Al_2O_3 nanofluid in the temperatures of 30 to 70 ºC and over ϕ of 0.5% to 2.0 %. Alawi et al. [15] found raised k_{nf} for 70:30% and 50:50% W/EG CuO nanofluids. Sundar et al. [16] observed higher thermal conductivity enhancement for 20:80% EG/W Al_2O_3 nanofluid among 20:80%, 40:60% and 60:40% EG/W nanofluids. Sundar et al. [17] also observed an increased thermal conductivity by using 20:80%, 40:60% and 60:40% W/EG Fe_3O_4 nanofluids in the temperature range from 20 °C to 60 °C and in the volume concentration range from 0.2% to 2.0%.

This paper deals with the experimental determination of thermophysical properties of 20:80% EG/W mixture based ZrO_2 nanofluids and validated with Bayesian regularization algorithm approach. The experiments were performed in the volume concentration ranging from 0.2–1.0% and temperature ranging from 20–60ºC. From the sol-gel technique, the ZrO_2 nanoparticles were synthesized. The measured thermophysical properties were validated through the literature data. New equations were developed for the thermophysical properties. The regression coefficients were developed through the Bayesian Regularization algorithm approach.

Experimental study

Development of ZrO_2 nanoparticles

ZrO_2 nanoparticles were made through the sol-gel technique. The purified chemicals such as zirconium (IV) propoxide, propanol, NH_3, ethanol and ethylene glycol were procured through the Sigma-Aldrich Chemicals, USA. In a large beaker, the propanol, water and ammonium were taken and then agitated for 10 minute. The zirconium propoxide was added to the above solution and the whole mixture was stirred for 1 hour and observe the formation of while sol. The mole ratio of zirconium propoxide, water and propanol is fixed at 1:8:20. The formed sol is heated around 80 °C to remove the impurities and it is dried in a vacuum. Further the powder is dried in a furnace at a heating rate of 1°C per/min and kept at a temperature of 500 °C for 2.

Preparation of 80:20% W/EG ZrO_2/EG nanofluids

The base liquid is considered as 80:20% W/EG mixture. The stable 80:20% W/EG ZrO_2 nanofluids were prepared by adding SDBS surfactant. The ZrO_2 nanoparticles required for known particle loadings of 20 g of base liquid was calculated from Eq. (1).

$$W_{ZrO_2} = \left(\frac{\phi}{(1-\phi)}\right) \times \left(\frac{W}{\rho}\right)_{bf} \times \rho_{ZrO_2} \tag{1}$$

Where, the ρ_{ZrO_2} and ρ_w is 5680, and 1029.72 kg/m^3, the W_{bf} is 20 g, and W_{ZrO_2} weight of nanoparticles (g). The dry ZrO_2 nanoparticles of 0.22, 0.44, 0.66, 0.88, and 1.11g were used for 0.2, 0.4, 0.6, 0.8 and 1.0% vol. loadings of nanofluids.

Estimation of thermophysical properties

Thermal conductivity of nanofluids

The k_{nf} was evaluated through KD2 Pro (Decagon Devices Inc., USA) instrument. The KD2 Pro works under the principle of transient hot-wire technique. The instrument contains microcontroller and KS-1 sensor and its length and diameters of 60 and 1.3 mm was used. Accuracy of KS-1 sensor was ±2.5% and it measures the thermal conductivity in the ranging from 0.2 to 2 W/mK. The temperature of the nanofluids sample was controlled by Julabo temperature controller, Germany with an accuracy of ±0.1 ºC.

Dynamic viscosity of nanofluids

The A&D vibro viscometer, Japan considered for determine the dynamic viscosity of ZrO_2/water nanofluids, equipment consists of electric driven two gold coated vibrating plate sensors and it also consists of a temperature sensor for checking the temperature of the nanofluid sample. The accuracy of the instrument is ±1% and it measures the viscosity over the range from 0.3 to 10,000 mPa.s. Initially the equipment was calibrated with the know viscosity of the fluid (i.e. water) and then used for base fluid (80:20% W/EG) and nanofluids. The viscosity measuring fluid was poured in a cup and it is located on the table. Slowly adjust the table so that, the gold plates are partially immersed into the fluid. There is a mark on the gold plates, up the mark the gold plates should immerse into the fluid.

Density of nanofluids

The density of ZrO_2 nanofluids were measured by utilizing the Archimedes principle. The definition of density says, it is ratio between mass to volume. If we know the volume, then we measure the weight of the fluid by using the precision weighing machine. Initially 50 ml weight was measured after that 20 ml nanofluids and then measure the weight of the beaker. Then calculate the density values. The accuracy of the weighing machine is ±0.001 mg. The same procedure is adopted for measuring the density of other nanofluids concentrations. The law of mixtures can be used to determine the density of nanofluid, and which is given below:

$$\rho_{nf} = \rho_p \phi_p + \rho_{bf}\left(1 - \phi_p\right) \tag{15}$$

Specific heat of nanofluids

The nanofluids C_p have been measured by using DSC 2920 model of TA instruments. The cell is first validated with indium, water and then it is used for nanofluids. A nanofluid sample of 10 mg was placed in the instrument. The specific heat of nanofluids was measured over 20 to 60 ºC.

Bayesian regularization algorithm

As opposed to traditional backpropagation networks, Bayesian regularization neural networks are thought to be more dependable, robust, and efficient and may reduce or even do away with the need for cross-validation during the learning process. The Bayesian regularization technique makes use of a mathematical technique called ridge regression, which converted a nonlinear regression problem into a statistical task that was equally well-posed provide a more thorough explanation of Bayesian regularization. As part of the Levenberg-Marquardt approach, the backpropagation is typically used to compute the Jacobian $'jX'$ of the performance taking into account the weight and bias variables X. Following the Levenberg-Marquardt algorithm's basic tenets, each variable is adjusted as follows:

$$\left.\begin{array}{r} jj = jX \times jX \\ je = jX \times E \\ dX = \frac{-(jj + I \times mu)}{je} \end{array}\right\} \tag{18}$$

Where, E indicates all errors, while I reflects identity matrix. The adaptive controlling parameter mu is raised by the factor of mu_inc until the change lowered the performance.

A volumetric concentration (ϕ) and temperature (T) are the input in the proposed NN. The proposed NN is trained individually for each property, i.e., thermal conductivity (k), viscosity (μ), density (ρ), and specific heat (Cp). The schematic diagram is shown in **Fig. 1.**

Getting an optimum NN network is one of the critical tasks. Appropriate selection of hidden layers and the number of neurons in hidden layer determines the accuracy of the prediction. Therefore, experimental data is prepared with six volumetric concentrations ranging from 20 ºC to 60 ºC. Then, the training of the network is analyzed with minimum mean square error (MSE) over 1000 epochs and R-Value as expressed in the following equations.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(y_{\exp(i)} - y_{\mathrm{ANN}(i)}\right)^2 \tag{19}$$

$$R = \sqrt{1 - \frac{\sum_{i=1}^{N}\left(y_{\exp(i)} - y_{\mathrm{ANN}(i)}\right)^2}{\sum_{i=1}^{N}\left(y_{\exp(i)}\right)^2}} \tag{20}$$

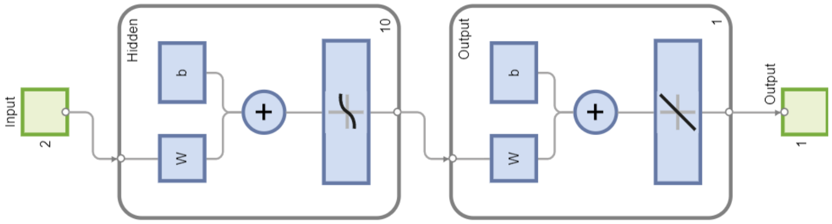

***Fig. 1:** The proposed NN network structure with ten neurons in the hidden layer*

Results and discussion

Thermophysical properties

Fig. 2(a) is plotted for the k_{nf} of ZrO_2 nanofluids at dissimilar particle volume loadings and temperatures. As it is observed that the thermal conductivity of increased with an increase of particle volume loadings and temperatures. At particle loadings of 0.2%, 0.4%, 0.6%, 0.8%, and 1.0% vol. of nanofluids at 20 ºC, the k_{nf} is raised by 3.86%, 5.69%, 7.72%, 8.13% and 10.16%, respectively, whereas at 60 ºC, the k_{nf} is augmented by 7.17%, 12.45%, 15.28%, 19.06% and 24.53% against the base fluid. The base liquid considered in the current analysis is 80:20% W/EG mixture and the thermal conductivity ratio of ZrO_2/80:20% W/EG nanofluid data is compared with Sundar et al. [17] of Fe_3O_4/80:20% W/EG nanofluid and it is shown in **Fig. 2(b)**. The thermal conductivity ratio, $k_r = k_{nf}/k_{bf}$ of the present ZrO_2/80:20% W/EG nanofluid is 1.245, whereas, the thermal conductivity ratio of the Fe_3O_4/80:20% W/EG nanofluid is 1.34 at ϕ = 1.0% and 60ºC.

The measured dynamic viscosity of ZrO_2 nanofluid is plotted in **Fig. 2(c)** at different particle loadings and temperatures. Interestingly at higher particle loadings the viscosity is higher, but at the same time measured between 20 ºC to 60 ºC the μ_{nf} is gradually decreased. The increased μ_{nf} may directly impact on the friction factor. The μ_{nf} is raised by 25.16% to 17.46% (ϕ = 0.2%), 36.47% to 25.40% (ϕ = 0.4%), 44.52% to 31.75% (ϕ = 0.6%), 55.48% to 38.10% (ϕ = 0.8%), and 61.94% to 50.79% (ϕ = 1.0%) from 20 ºC to 60 ºC, in comparison with base fluid data. The larger resistance between the fluid layers leads to a larger μ_{nf} values. The similar nature of viscosity enhancement has noticed by Minakov et al. [30] for Al_2O_3, TiO_2, ZrO_2, CuO, Fe_2O_3, and Fe_3O_4, as well as nanodiamonds nanofluids. The present study 80:20% W/EG mixture ZrO_2 nanofluids are validated through the Sundar et al. [22] of Fe_3O_4/80:20% W/EG nanofluid and it is provided in **Fig. 2(d)**. The viscosity ratio, $\mu_r = \mu_{nf}/\mu_{bf}$ of the present ZrO_2/80:20% W/EG nanofluid is

1.619, whereas, the viscosity ratio of Fe_3O_4/80:20% W/EG nanofluid is 1.606 at ϕ = 1.0% and 20ºC.

The density of ZrO_2 nanofluids were plotted in **Fig. 3(a)**. The density is increased for nanofluid at higher particle volume loadings and those are lowered at higher temperatures. The density of base fluid is 1029.72 kg/m^3, whereas the density is increased to 1076.22 kg/m^3 at 1.0% vol. loadings at 20ºC. Moreover at 60ºC, the density of the base fluid is 1011.99 kg/m^3 and the density of the 1.0% vol. of nanofluid is increased to 1058.67 kg/m^3. Similar kind of an enhanced density with nanofluids have been presented by Sharifpur et al. [27] and Shoghl et al. [28] by using water -CuO, -MgO, -CNT, -TiO_2, -Al_2O_3 and -ZnO nanofluids.

Measured C_p values were presented in **Fig. 3(b).** As it is seen from the figure, with respect to increase of temperature, the C_p is increases, but the with respect to increase of particle volume loadings, the C_p is decreases. The C_p of base fluid (80:20% W/EG) is 3815 J/kg K, whereas the C_p of 1.0% nanofluid is 3781.05 J/kg K at 20 ºC. Similarly, the C_p of base fluid is 3907 J/kg K, but the C_p of 1.0% nanofluid is 3872.13 J/kg K at 60 ºC.

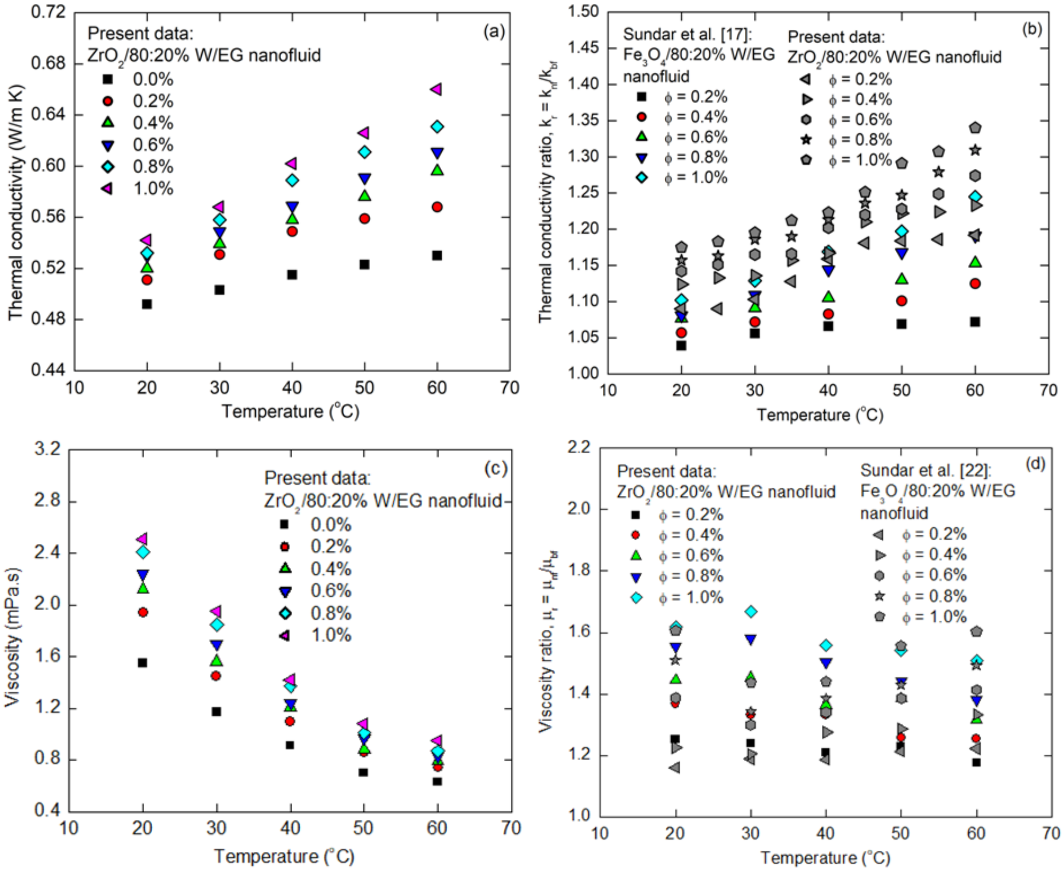

Fig. 2: *(a) Thermal conductivity with respect to temperature, (b) thermal conductivity ratio, (c) viscosity with respect to temperature, and (d) viscosity ratio*

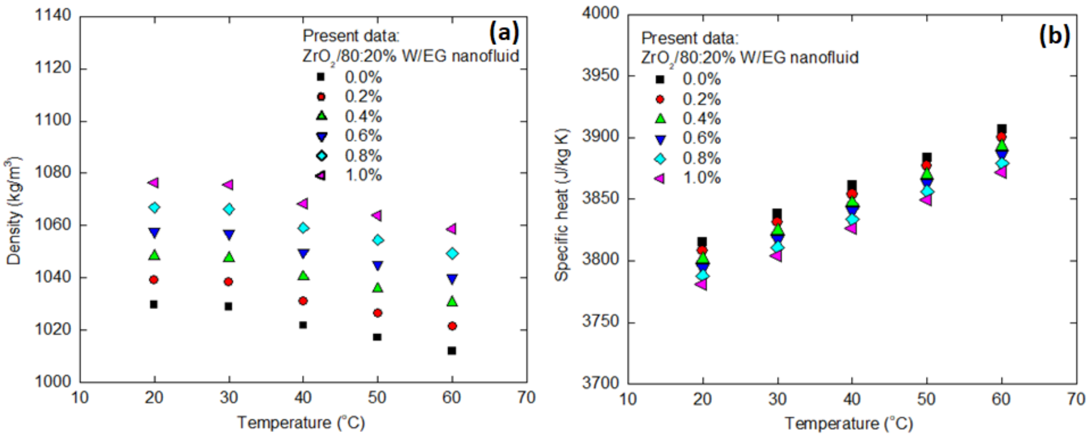

Fig. 3(a): *Density of ZrO*$_2$*/80:20% W/EG nanofluid,* ***(b)*** *Specific heat of ZrO*$_2$*/EG nanofluids*

Bayesian regularization algorithm approach

The proposed network is trained separately for four properties. To avoid the over fitting problem of artificial neural network (ANN), the data is divided into 86% training, 7% testing, and 7% validation dataset. During the training phase, 1000 epochs are used. The training stops if the target mean square error (MSE) is achieved or after completing a number of the epoch. **Figure 4** presents the proposed R^2 analysis for k_{nf}, (a) train values, (b) confirmation of train values, (c) test values, and (d) total values. It is observed from the figure, the training data, R^2 is equal to 0.99966, whereas, for all the data (both training and test data), the R^2 is equal to 0.99938. A good performance can be expressed with the closeness of sample data towards the equality line. The R^2 values obtained for all datasets are close to one, which shows that the developed model is well trained, giving the best performance for predicting the data.

Figure 5 presents the proposed R^2 examination for viscosity, (a) train values, (b) confirmation of train values, (c) test values, and (d) total values. As seen from the figure, the training data, R^2 is equal to 0.99772, but whereas, for all the data (both training and test data), the R^2 is equal to 0.99747. A good matching of the data can be expressed with the closeness of sample data towards the equality line. The R^2 values obtained for all the viscosity datasets are nearly equals to one, which indicates the proposed model is well trained and providing the best results. **Figure 6** presents the proposed correlation coefficient R^2 analysis for density, (a) train values, (b) confirmation of train values, (c) test values, and (d) total values. As it is seen that, the training data, R^2 is equal to 0.99999, but whereas, for all the data (both training and test data), the R^2 is equal to 0.99998. Perfect matching of the experimental and optimized data was observed. The R^2 values obtained for all the density data points are almost equals to one, which provides the proposed model data is well predicted the experimental data.

Figure 7 presents the proposed R^2 analysis for specific heat, (a) train values, (b) confirmation of train values, (c) test values, and (d) total values. As it is seen that, the training data, R^2 is equal to 1, and also all the data (both training and test data) R^2 equal to 1. The R^2 value of specific heat is 1 it means that the used model data is well predicted the experimental data.

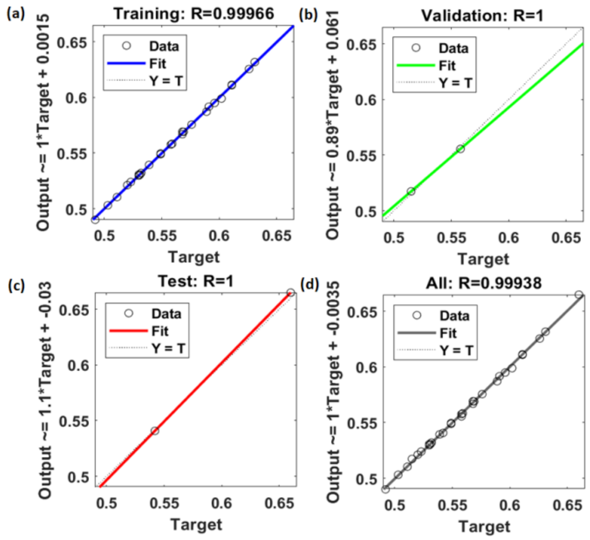

Fig. 4: *Proposed R^2 examination for thermal conductivity: (a) train values, (b) confirmation of train values, (c) test values, and (d) total values.*

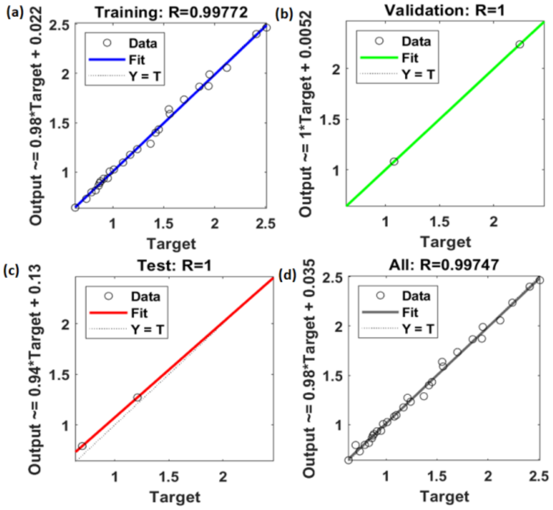

Fig. 5: *Proposed R^2 examination for viscosity: (a) train values, (b) confirmation of train values, (c) test values, and (d) total values*

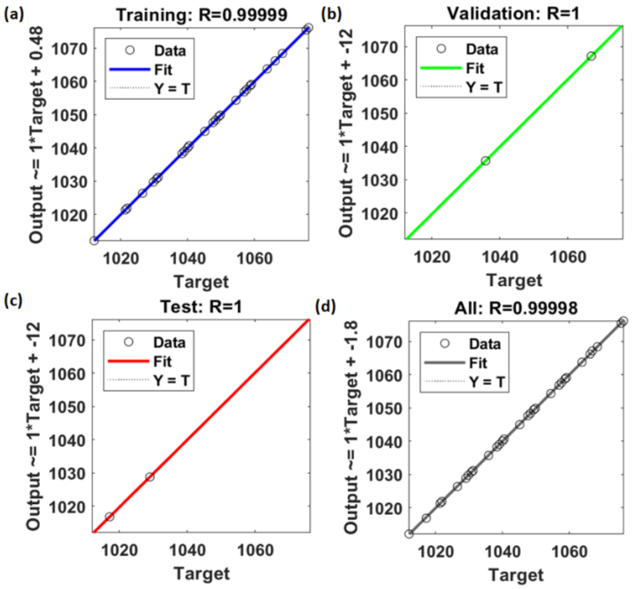

Fig. 6: *Proposed R^2 examination for density: (a) train values, (b) confirmation of train values, (c) test values, and (d) total values*

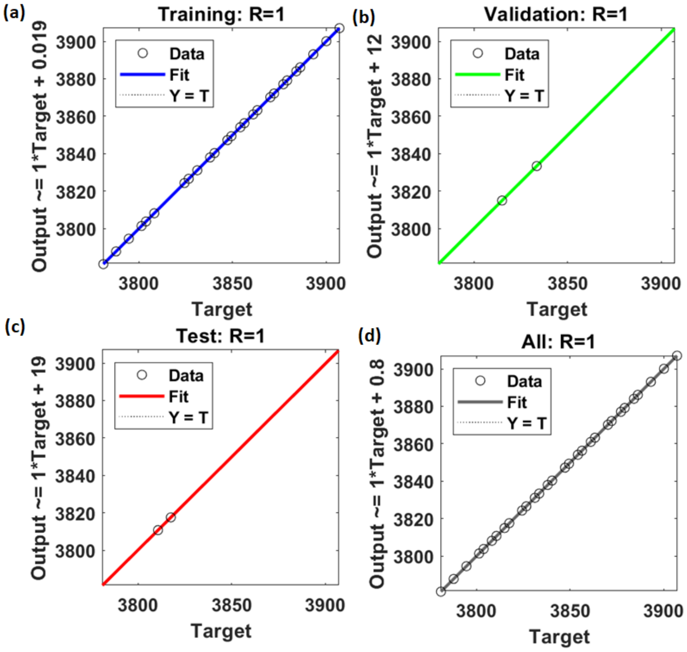

Fig. *7: Proposed R^2 examination for specific heat: (a) train values, (b) confirmation of train values, (c) test values, and (d) total values.*

Conclusions

Experiments were performed for the analysis of 80:20% W/EG ZrO_2 nanofluids at dissimilar loading concentrations and temperatures. The ZrO_2 were developed through sol gel procedure. The developed nanofluids were offered ±30 mV of zeta potential which states that the nanofluids are stable. With increased particle volume loadings and temperatures, the thermal conductivity of nanofluids is enhanced. At higher particle loading of 1.0%, the thermal conductivity enhanced is 24.53% at 60ºC. With the increased temperature, the dynamic viscosity of the nanofluid is decreased, but oppositely, with an increased particle loading, the viscosity is enhanced. Higher particle concentration of 1.0%, the viscosity increased is 61.94% at 20 ºC against base fluid. Other side density is larger and specific heat is lowered to an increase of particle volume loadings.

Correlation coefficient R^2 and mean square error was analyzed using the neural network of Bayesian regularization algorithm approach for all the properties. The correlation coefficient R^2 of specific heat is 1, whereas, correlation coefficient R^2 for thermal conductivity, dynamic viscosity, and density is 0.99966, 0.99772, and 0.9999, respectively. The measurements were appropriately augmented for all the data points used by the neural network approach. Bayesian regularization algorithm utilizes the more accurate tool for modeling the experimental data of nanofluids.

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