The RSM approach to develop a new correlation for density of metal-oxide aqueous nanofluids

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Abstract
Density is one of the basic thermo-physical properties of a fluid that should be analysed before conducting performance analysis of the fluid. In the present study, the influence of design parameters on the density of nanofluids was investigated using response surface methodology (RSM). The quadratic model generated by RSM is used to predict the performance parameters, i.e. temperature and mass concentration with reasonably good accuracy. Improved empirical correlations were proposed based on the experimental data for density prediction of the metal oxide nanofluids. Experimentally measured densities of two different nanofluids at the nanoparticle mass fraction of up to 0.2% and the temperature range of 20°C-40°C were examined. The enhancement of densities compared to the density of base fluid at 20°C and 40°C, are about 0.217% for 0.2% fraction of ZnO nanoparticles. In addition, the densities of SiO$_2$ nanofluids are improved 0.117% compared to the density of distilled water. Finally the RSM outputs were compared with the results obtained from the experimental data. It was observed that the optimal RSM model is accurate and the absolute maximum deviations measured values from the predicted densities of ZnO and SiO$_2$ nanofluids are 0.008% and 0.014% respectively.

1. Introduction

Nanofluids were invented by Choi [1], after understanding mixing nanoparticles (1-100 nm) with a base fluid improves heat transfer. Materials generally used as nanoparticles include chemically stable metals (e.g. gold, copper), metal oxides (e.g., alumina, silica, zirconia, titania), dioxide ceramics (e.g. Al$_2$O$_3$, CuO), metal carbides (e.g. SiC), metal nitrides (e.g. SiN), carbon in various forms (e.g., diamond, graphite, carbon nanochannels, fullerene) and functionalized nanoparticles, Cheng [2].

In the previous decade, scientists had tested different kinds of nanomaterials for making nanofluids. Al$_2$O$_3$, SiO$_2$, ZnO, CuO, zirconia and silver are more common metal and metalloid oxides for preparing nanofluids compared to other metal oxide nanofluids [3-6].

Although nanofluids have high potential to improve heat transfer compared to water, more pumping power is required in order to achieve a desired flow rate. This is due to the fact that
nanoparticles, which are used to make nanofluids are weighty. It is important to understand certain fluid properties that are essential for thermal performance. Such properties are primarily density, viscosity, and thermal conductivity.

Amongst the different thermo-physical properties of nanofluids, viscosity and thermal conductivity were more interested for the researchers [7-10]. A few number of researchers worked on other properties such as specific heat and density. Viscosity and thermal conductivity are not enough to evaluate heat transfer coefficient theoretically. Specific heat and density are also essential for heat transfer information. Since these properties have significant influence on nanofluid flow and heat transfer characteristics, so they should be determined accurately [11]. Therefore, some density measurements have been presented for different nanofluids at various conditions [12], while suggesting the reported theoretical correlation for the estimation of nanofluids density is based on simple model [13]. Nanoparticle concentration increment displays the role of the interaction on the fluid density since the effect of particle size and size distribution on density is almost negligible [11]. Attempt to obtain models based on accurate experimental data in a proper manner would be a powerful technique for understanding and predicting a process. In these cases, novel approaches such as a response surface methodology (RSM) and an artificial neural network (ANN) are efficient in predicting the density of nanofluids based on the available data [14].

Recently, Sha and Edwards [15] comprehensively investigated the applications of ANNs in material science. Hassan et al. [16] predicted the density, porosity, and hardness of an aluminium-copper based composite material using ANNs. Singh et al. [17] applied ANNs to predict the effective thermal conductivity of moist porous materials. A review paper [18] showed that the implementation of ANN technique has greatly promoted research in materials science and technology. Karimi and Yousefi [14] applied the hybrid model, including back-propagation network (BPN) and genetic algorithm (GA) to estimate the nanofluids density. Sadollah et al. [19] investigated the effect of different process factors on the stability of nanofluid by using optimization methods. They had compared the results predicted by utilizing RSM and ANNs. Thus the purpose of this paper is to minimize the total mean squared error between net output and desired output through optimization. The presented model determines the effective density of the nanofluids as a function of temperature, nanoparticle mass fraction, nanoparticle and the base fluid densities.

2. Methodology:

2.1. Materials

Silicon dioxide ($SiO_2$) nanopowder with assay 99.5% and particulate size ranges from 10 to 20 nm were purchased from Sigma-Aldrich Co., Selangor, Malaysia. $SiO_2$ nanofluid has been prepared by dispersing nanoparticles in base fluid. Distilled water was used as a base fluid for the preparation of $SiO_2$ nanofluids. An ultrasonic disruptor has used to produce nanofluids from the specific nanoparticles and the selected base fluids. No surfactant additives were added during the preparation process. In the present case after 30 minutes of intensive sonication, the stable suspensions were obtained according to the desired mass concentrations (wt.%) of $SiO_2$.

Zinc oxide ($ZnO$) spherical shaped nanopowder with assay 97% and particulate size was less than 50 nm were purchased from Sigma-Aldrich Co., Selangor, Malaysia. The $ZnO$ nanoparticles sedimented within several minutes as zinc oxide is insoluble in water and also, the particles remained within the clusters without being dispersed. Enhanced stability of the $ZnO$ nanofluids is observed with sodium hexametaphosphate (SHMP). SHMP with purity 96% was purchased from Sigma-Aldrich Co., Selangor, Malaysia. After 60 minutes of intensive sonication, the stable suspensions were obtained according to the desired mass concentrations (wt%) of $ZnO$. The most stable suspension as per our sedimentation studies contained surfactant and nanoparticles in wt% ratio 1:10 (SHMP: $ZnO$).
2.2. Experimental works

The density of a fluid is defined as a ratio of the mass to the volume, which it occupies (equation 1).

\[ \rho = \frac{m}{v} \]  

(1)

The density of the liquid is higher than the density of gas for the same quantity of the fluid, because gases are more elastic than liquid and therefore they tend to occupy the maximum space (volume).

The densities of distilled water and nanofluids were measured experimentally by KEM Density/Specific Gravity Meter DA-645. The accuracy of density measurement and temperature are 0.00005 g/cm\(^3\) and 0.3 °C respectively. The measurements were recorded 3 times for each temperature. The average results show in figure 1 and figure 2 which are display the density measurements of distilled water, SiO\(_2\) and ZnO nanofluids for different weight concentrations at the temperature range of 20 °C to 40 °C.

Nanofluids exhibit higher density compared to the conventional fluid such as water. The density of nanofluids depends on the concentration of the nanoparticles. Density of a fluid decreases with the increasing of its temperature and also increases with the increasing of its pressure. It is an important property of the fluid. Based on the density, the flow of the fluid can be classified as either incompressible or compressible. For incompressible flow, the density of the fluid is constant; whereas for compressible flow the density changes with respect to the temperature and pressure of the fluid.

2.3. RSM Optimization Process

RSM is an empirical statistical modeling technique employed for multiple regression analysis using quantitative data obtained from properly designed experiments to solve multivariate equations simultaneously [20, 21]. RSM is used to determine the optimum density, for the nanofluids. A central composite full of three independent variables was used. The independent variables selected for the optimization were temperature, mass concentration and density ratio of the base fluid to the nanoparticles. Regression analysis was performed on the data obtained from the experiments. Coding of the variables was done according to the following equation (equation 2):

\[ x_i = \frac{X_i - X_{CP}}{\Delta X_i} \quad i = 1, 2, ..., k \]  

(2)
Where \( x_i \) is the dimensionless value of an independent variable; \( X_i \) refers to the real value of an independent variable; \( X_{CIP} \) is the real value of an independent variable at the center point; and \( \Delta X_i \) is the step change of the real value of the variable \( i \) corresponding to a variation of a unit for the dimensionless value of the variable \( i \). The experiments were carried out in duplicate, which was necessary to estimate the variability of the measurements. Replicates at the center of the domain in three blocks permit the checking of the absence of bias between several sets of experiments. The relationship of the independent variables and the response was calculated by the second-order polynomial equation (3).

\[
Y_{PRE} = \alpha_0 + \sum_{i=1}^{k} \alpha_i X_i + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \alpha_{ij} X_i X_j + \sum_{i=1}^{k} \alpha_{ii} X_i^2
\]  

(3)

Where, \( Y_{PRE} \) is the predicted response; \( \alpha_0 \) a constant; \( \alpha_i \) the linear coefficient; \( \alpha_{ii} \) the squared coefficient; and \( \alpha_{ij} \) the cross-product coefficient, \( k \) is the number of factors.

The mean squared error (MSE) was used to quantify the difference between predicted and actual values. The MSE can be expressed as follows:

\[
MSE = \frac{1}{k} \sum_{i=1}^{k} (Y_{PRE} - Y_{EXP})^2
\]  

(4)

The response surface method is a sequential process and its procedure can be summarized as shown in Figure 3.

3. Result and Discussion

The response surface methodology is employed using Minitab Version 17.3.1 software for the optimization of a problem with 3 optimization variables. A quadratic response surface is the approximated density for \( SiO_2 \) and \( ZnO \) based on the Least Square method. Weight fraction (\( \Phi \)), Temperature (\( T \)), base fluid density (\( \rho_f \)) and density ratio of base fluid to nanoparticle (\( \rho_f/\rho_{np} \)) are input variables and nanofluid density (\( \rho_{nf} \)) is the output variable. The quadratic equation for finding the best-fitted curves to experimental data points for \( SiO_2 \) and \( ZnO \) are represented by equations 5 and 6, respectively.
\[
\rho_{\text{Prem}(SiO}_2) = 1000.02 + 5.182 \varnothing + 0.0055 T + 2.2 \varnothing^2 - 0.005 T^2 - 0.0008 \varnothing T
\] (5)

\[
\rho_{\text{Prem}(ZnO)} = 999.640 + 21.112 \varnothing - 0.001 T - 39.60 \varnothing^2 - 0.005 T^2 - 0.011 \varnothing T
\] (6)

Where, \( T \) is a temperature and \( \varnothing \) is the nanoparticle weight fraction.

Thus the trained of the net model has used to predict the nanofluid density and the comparison of the predicted and the experimental values are presented here (figure 4 & figure 5). As it can be seen that good agreements were achieved between the predicted and the experimental values of the densities with the mean squared error of MSE = 0.251\% for \( SiO_2 \) and MSE = 1.24\% for \( ZnO \) nanofluids and the high correlation coefficients of \( R = 0.9992 \) for \( SiO_2 \) and \( R = 0.9986 \) for \( ZnO \).

4. Conclusions

In this study the response surface methodology has successfully been applied for estimating the densities of \( SiO_2 \) and \( ZnO \) nanofluids. The proposed model could evaluate the densities as a function of temperature, nanoparticle mass fraction, base fluid densities and the density ratios of the base fluid to the nanoparticles. Based on the experimental data, the trained net has shown good agreement between the predicted and the experimental values of the densities with the mean squared error, (MSE) and the high correlation coefficients, (R) for \( SiO_2 \) nanofluids. Similarly, acceptable R and MSE were achieved for \( ZnO \) nanofluids. Furthermore, experimental data demonstrate the density increases with the increase of mass concentrations and decreases with the increase of temperatures following the conventional trend of nanofluids.

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