



Development of a predictive model for estimating the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids using support vector regression



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ARTICLE INFO

Keywords:

Materials science
Nanotechnology
Thermodynamics

ABSTRACT

The specific heat capacity of nanofluids ($C_{p_{nf}}$) is a fundamental thermophysical property that measures the heat storage capacity of the nanofluids. $C_{p_{nf}}$ is usually determined through experimental measurement. As it is known, experimental procedures are characterised with some complexities, which include, the challenge of preparing stable nanofluids and relatively long periods to conduct experiments. So far, two correlations have been developed to estimate the $C_{p_{nf}}$. The accuracies of these models are still subject to further improvement for many nanofluid compositions. This study presents a four-input support vector regression (SVR) model hybridized with a Bayesian algorithm to predict the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids. The bayesian algorithm was used to obtain the optimum SVR hyperparameters. 189 experimental data collected from published literature was used for the model development. The proposed model exhibits low average absolute relative deviation (AARD) and a high correlation coefficient (r) of 0.40 and 99.53 %, respectively. In addition, we analysed the accuracies of the existing analytical models on the considered nanofluid compositions. The model based on the thermal equilibrium between the nanoparticles and base fluid (model II) show good agreement with experimental results while the model based on simple mixing rule (model I) overestimated the specific heat capacity of the nanofluids. To further validate the superiority of the proposed technique over the existing analytical models, we compared various statistical errors for the three models. The AARD for the BSVR, model II, and model I are 0.40, 0.82 and 4.97, respectively. This clearly shows that the model developed has much better prediction accuracy than existing models in predicting the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids. We believe the presented model will be important in the design of nanofluid-based applications due to its improved accuracy.

1. Introduction

Recently, there has been an exponential growth in the number of studies conducted on nanofluids as a result of their enhanced heat transfer potential which makes them suitable for several energy-saving applications [1, 2]. Nanofluid based technologies can reduce the cost of energy to the tune of billions of dollars. In fact, it is estimated that the global market size of nanofluid heat transfer applications is above 2 billion dollars per year [3]. For instance, an improvement in chiller efficiency by 1% due to the usage of nanofluids is estimated to produce a

saving of about 320 billion kWh of electricity, corresponding to 5.5 million barrels of oil per year [3]. Due to the significance of nanofluid in effective energy management and ability to increase systems' efficiency, nanofluids have evolved as important materials that have profound potential in mitigating global challenges such as global warming and energy crisis [2].

Basically, nanofluids are suspensions of nanometer-sized particles in conventional cooling fluids such as ethylene glycol, engine oil, water, ethanol, and R11 refrigerant, etc [4]. Typically the nanoparticles are less than 100 nm in size and are made up of several classes of metallic,

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<https://doi.org/10.1016/j.heliyon.2019.e01882>

Received 16 November 2018; Received in revised form 23 February 2019; Accepted 30 May 2019

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non-metallic, oxides and other compounds [5]. The presence of nanoparticles in conventional fluids affects the thermophysical properties of the conventional coolants. Examples of areas where nanofluids are used include solar, biomedical applications, microelectronics, microfluidics applications [6, 7]. It is expected that the modern technological need for nanofluids will continue to rise in the future [8].

The most important nanofluids properties that are investigated for heat transfer applications include thermal conductivity, viscosity, thermal diffusivity, and specific heat capacity. Majority of the studies have been devoted to nanofluids' thermal conductivity enhancement. Moreover, around 5 percent of the literature is centered on other thermophysical properties (viscosity, thermal diffusivity, and specific heat capacity) [9]. No doubt, this amount of attention is clearly inadequate because other thermophysical properties equally play significant roles in many engineering applications. In particular, for the specific heat capacity of nanofluids, the literature survey suggests that limited efforts have been devoted to estimating the specific heat capacity of nanofluids.

Here, we briefly examine the relevance of the specific heat capacity of nanofluids. First, the specific heat capacity of nanofluid is a measure of the heat retention capacity of the nanofluid, and also one of the fundamental thermophysical properties that are used to characterize thermal fluids [9]. The evaluation of the heat equation and thermal diffusivity depends on the accurate determination of specific heat capacity values according to the Eqs. (1) and (2) shown below [9].

$$\frac{dT}{dt} = \alpha \nabla^2 T \quad (1)$$

Where T , t and α refer to the temperature, time and thermal diffusivity, respectively. The thermal diffusivity is related to the specific heat capacity through Eq. (2)

$$\alpha = \frac{k}{\rho \cdot C_p} \quad (2)$$

Where k stands for thermal conductivity, ρ and C_p refers to density and specific heat capacity, respectively [9]. In other words, accurate values of the specific heat capacity is required to evaluate fluid properties such as thermal diffusivity, dimensionless Prandtl number, and the pumping power [5, 10, 11].

So far, two main analytical models have been used in the literature to estimate the specific heat capacity of nanofluids. The first model, often referred to as model I is based on the idea of mixing theory for ideal gas mixtures, which is described by Eq. (3);

$$C_{p_{nf}} = \phi C_{p_n} + (1 - \phi) C_{p_{bf}} \quad (3)$$

Where $C_{p_{nf}}$, C_{p_n} and $C_{p_{bf}}$ refers to the specific heat capacities of the nanofluid, nanoparticles and basefluid, respectively [9]. The subscripts nf , bf and n , represent the nanofluid, base fluid and nanoparticles, respectively.

The second model (model II) is based on the assumption that both the nanoparticles and base fluids are in thermal equilibrium. It is expressed as shown in Eq. (4);

$$C_{p_{nf}} = \frac{\phi \rho_n C_{p_n} + (1 - \phi) \rho_{bf} C_{p_{bf}}}{\phi \rho_n + (1 - \phi) \rho_{bf}} \quad (4)$$

Eq. (4) has been applied in several studies in predicting the specific heat capacity of nanofluids [9]. Earlier studies have demonstrated that model II has a much closer agreement with experimental results compared to model I. In fact, most of the studies concluded that model I is inadequate in predicting the specific heat capacity of nanofluids [10, 12]. For instance, Le-Ping et al [13], measured the specific heat capacity of CuO/ethylene glycol nanofluid and their experiments revealed that Model II has good agreement with the experimental data while model I fails to predict the experimental data. Using molecular dynamics (MD) simulations approach, Ali Rajabpour [14] et al investigated the specific

heat capacity of CuO/Water nanofluids. Their results also revealed that model I is not sufficient for predicting specific heat capacity of nanofluids, however, there is an agreement between molecular dynamics (MD) simulations approach and Model II. Also, Sheng-Qi et al [15] measured the specific heat capacity of aluminum oxide/water nanofluid, then compared the experimental results with existing models. Their experimental results agreed with model II while model I fails to predict the specific heat capacity of the aluminum oxide/water nanofluid. Harry O'Hanley et al [16] measured the specific heat capacity of various water based-nanofluids. Their study revealed that model II has good agreement with experiments while model I shows a significant deviation from it. As indicated above, previous studies established that model II has good agreement with experimental data while model I is incapable of accurate estimation of specific heat capacity of nanofluid for most compositions. Critical examination of model II revealed that there is still room for improvement as far as its accuracy is concerned. This fact serves as the main motivation for our present study.

Quite recently, there has been growing interest in using machine learning approach for solving problems across diverse disciplines [17, 18, 19, 20]. In this respect, various machine learning techniques have been successfully applied in the study of thermophysical properties of nanofluids [4, 21, 22]. It is worthy to note that only a few studies have considered these techniques in predicting the specific heat capacity of nanofluids [23]. In this work, we developed a support vector regression model hybridized with Bayesian optimization for estimating the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids. Due to the limited experimental data on the specific heat capacity of metallic oxides, the model was built using experimental data of Al_2O_3 and CuO nanoparticles only. It is remarkable to state that the developed model exhibits a better accuracy compared to the other existing analytical models.

2. Methodology

2.1. Support vector machine (SVM)

SVM is a robust supervised machine learning technique originally developed for classification problems then later extended to regression tasks. Support Vector Regression (SVR) is an offshoot of SVM that is specifically used for regression tasks [21]. It is founded on the statistical learning theory proposed by Vapnik [24, 25, 26]. The main concept in SVR is mapping input data into higher dimensional feature space, then constructing a kernel function that permits the problem to be solved by linear regression function. SVR has a unique advantage over an artificial neural network (ANN) because it is less prone to overfitting problems due to the fact that its objective function is convex, hence global optimum is often reached [27]. Consequently, SVR results are consistent and reproducible, unlike ANN that may suffer from prediction uncertainties [28]. The solution to the non-linear regression problem consists of obtaining an appropriate function $f(x)$ that describes the output response to a d -dimensional input vector [18]. To keep this work concise, we have not detailed the underlying mathematical formulation for SVR. This has been presented in the literature which interested readers can refer to [4, 23, 29, 30, 31].

The main objective in SVR is to obtain a regression function $f(x)$ defined as in Eq. (5):

$$f(x) = \sum_{i=1}^l (\alpha_i^* - \alpha_i) \cdot \varphi(x_i), \varphi(x_j) + b \quad (5)$$

Where $\varphi(x_i), \varphi(x_j)$ is the inner product of vectors in the feature space which can be represented with a kernel function as shown in Eq. (6).

$$f(x) = \sum_{i=1}^l (\alpha_i^* - \alpha_i) \cdot K(x_i, x_j) + b, \text{ where } K(x_i, x_j) = \varphi(x_i) \cdot \varphi(x_j) \quad (6)$$

where l refers to the number of support vectors, $(\alpha_i^* \& \alpha_i)$ are the Lagrange multipliers, b is the bias term and $K(x_i, x_j)$ is the kernel parameter.

2.2. Parameters search: bayesian optimization (BO) strategy

Generally, the prediction performance of machine learning techniques relies on the accurate determination of its turning hyperparameters [32]. In the case of SVR, these parameters are; regularization factor (C), kernel parameter (γ) and epsilon (ϵ). As a result of the high computational cost or limitation of naïve techniques such as grid search or manual search, there has recently been strong interest in more sophisticated hyperparameter optimization techniques [21].

BO framework is an efficient parameter-searching tool used in a wide range of applications [33, 34]. BO seeks to find the global minimum of an unknown function $f(x)$ described mathematically as in Eq. (7):

$$x^* = \arg \min_{x \in X} f(x) \quad (7)$$

where X is defined as a compact subset of R_d and $f(x)$ is an unknown function whose gradients are undefined [35].

For the implementation of Bayesian optimization, two essential factors are to be determined. The first is a selection of a prior function that will capture our belief in the function to be optimized. For this purpose, the Gaussian function was selected due to its accuracy, analytic tractability, and robustness [36]. Second is the selection of an acquisition function used to create a utility function from the model posterior. The acquisition function provides insight as to where next to evaluate [33, 37]. The acquisition function is cheaper to evaluate compared with the unknown function which makes the optimization process easier and less computationally demanding.

In summary, a BO algorithm is shown in Table 1.

Steps 2–5 are repeated for 100 iterations in this study. Further information on details of the Bayesian optimization process can be obtained in the references [32, 37, 38].

3. Analysis

Generally, several factors influence the thermophysical properties of nanofluids. To develop an accurate predictive model, it is essential that only relevant factors that describe the thermophysical property to be investigated should be used in the development of the model. Such descriptors should uniquely characterize the material under investigation. In this study, the descriptors contained in the existing analytic models for specific heat capacity were selected as input variables for training the model [39]. The experimental data used in this study were gathered from published literature [39, 40]. The BSVR model proposed was developed using the following inputs as the descriptors;

- (i) The specific heat capacity of Al_2O_3 and CuO nanoparticles.

Table 1
Bayesian optimization of an unknown objective function [32].

Input: Input space D_0 ; GP prior μ_0, σ_0^2
1: for $t = 1, 2, 3, \dots$ do;
2: Select next point to evaluate x_{t+1} through the optimization of the acquisition function α
$X_{t+1} = \arg \max_{x \in D_t} \alpha(x; D_t)$
3: Evaluate the objective function to obtain y_{t+1}
4: Augment the data observed $D_{t+1} = \{D_t, (x_{t+1}, y_{t+1})\}$
5: update the Gaussian process model using μ_{t+1}
6: end
Result: Optimize the Gaussian process mean to find an optimized solution.

- (ii) The specific heat capacity of ethylene glycol.
- (iii) Volume fractions of Al_2O_3 and CuO nanoparticles
- (iv) The temperature.

Table 2 describes the relationships that exist between the descriptors and the specific heat capacity of nanofluids (target) in terms of Pearson's correlation coefficients (r). The results indicate that there is a significant relationship between the descriptors and target at 95% confidence level with the exception of the specific heat capacity of nanoparticles. It is important to note that the presence of a significant relationship between descriptors and target may suggest that the descriptors could be used to build an effective machine learning model. Since the specific heat capacity of the nanoparticles influences that of the nanofluids, it is expected that the specific heat capacity of the nanoparticles has some weight in predicting the specific heat capacity of nanofluids. Hence, it was included as fourth inputs even though correlation coefficients (r) and its p-value indicate that it is statistically insignificant as a predictor based on experimental data used in this study. Table 3 shows the basic statistical descriptions of the experimental data used in this study. As shown, the data used for the model development comprises of 189 datasets with the volume fractions ranging from 0.4 to 8.1 %.

4. Model

The computational work in this study was carried out in Matlab 2018b environment. The support vector regression algorithm randomizes and segments the experimental data into training and testing dataset in ratio 8:2, respectively. The training dataset was used for learning the connections between the various inputs and the corresponding outputs. Prior to the training process, the experimental data were normalized to enhance the computational efficiency of the algorithm. This learning process was achieved by automatic searching of the SVR hyperparameters space with the aid of the Bayesian optimization algorithm described in section 2.2. The optimal values of these parameters were achieved through the minimization of cross-validation error on the training dataset. The flowchart for the proposed model is shown in Fig. 1. After the training of the dataset, the new data set (test dataset) which has not been seen by the model during the training phase was used to validate the model predictive accuracy. The optimized SVR hyperparameters obtained are presented in Table 4. In achieving the optimal parameters, the model tried all possible kernel types. The kernel that returns the best result in this experiment is the Gaussian kernel. This result can be used for prediction of future dataset similar to the one investigated in this study.

5. Results and discussion

The effectiveness of the proposed model in predicting the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids was evaluated using various statistical measures such as root mean square error (RMSE), mean average error (MAE), mean relative average error (MRAE), average absolute relative deviation (AARD) and correlation

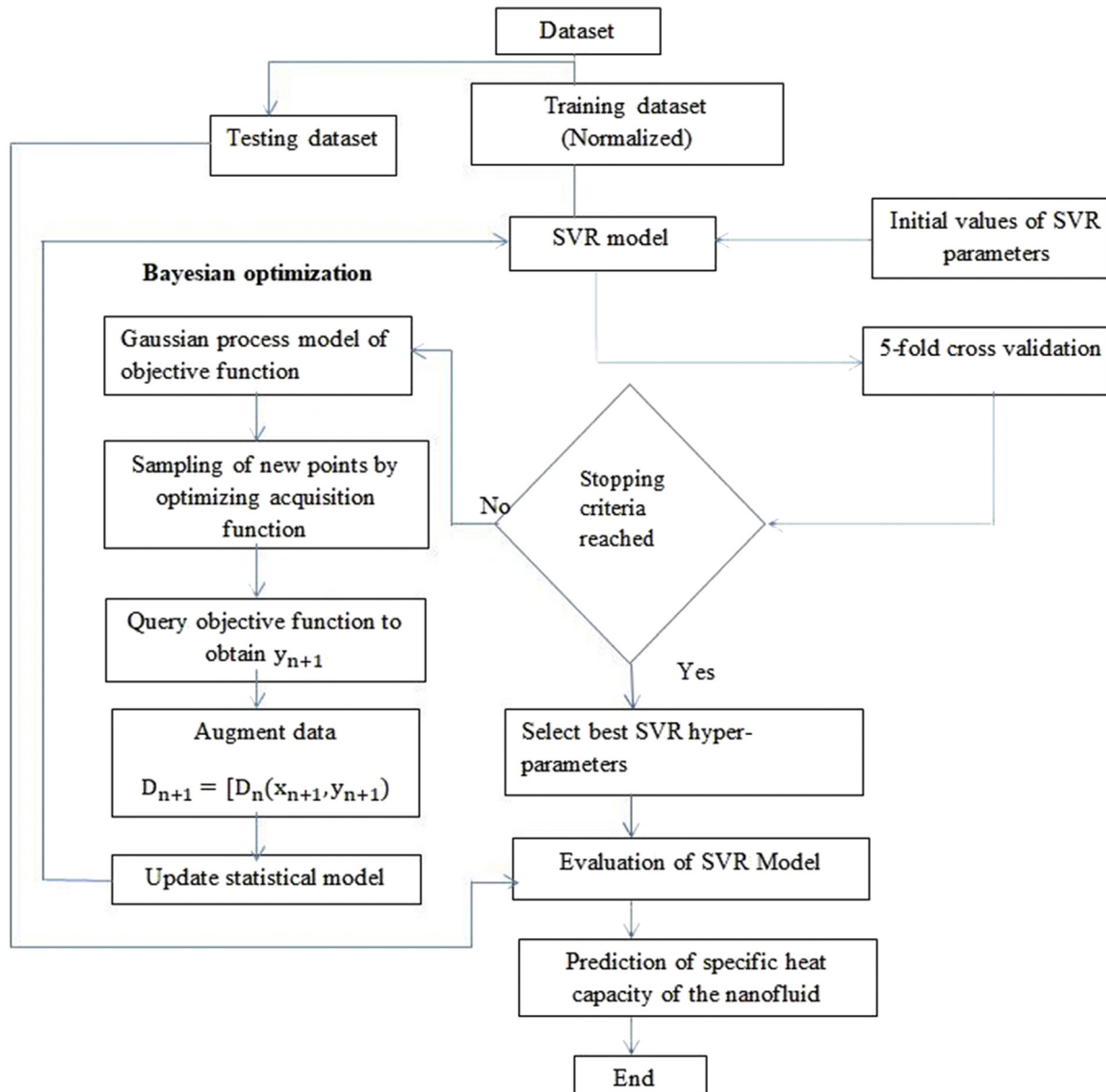
Table 2
Pearson Correlation between the input features and specific heat capacity nanofluids.

The relationship between each descriptor and the target	The coefficient of correlation (r)	p-value
The specific heat capacity of ethylene glycol vs the specific heat capacity of the nanofluids	0.488	0.000
The volume fractions of the nanoparticles vs the specific heat capacity of the nanofluids	-0.807	0.000
The temperature of the Ethylene glycol base fluid vs the specific heat capacity of the nanofluids	0.498	0.000
The specific heat capacity of the nanoparticles vs the specific heat capacity of the nanofluids	0.139	0.056

Table 3

Basic Statistical description of the experimental dataset used for the development of the BSVR model proposed for metallic/ethylene glycol-based nanofluids.

Items	Variable	Count	Mean	Standard Deviation	Minimum	Maximum	Range
Input features	Temperature (K)	189	316.79	13.39	296.31	337.43	41.12
	Specific heat capacity of nanoparticles (J/K.g)	189	13.02	83.89	0.53	0.58	0.08
	Specific heat capacity of ethylene glycol (J/K.g)	189	2.51	0.06	2.41	2.60	0.20
	Volume fraction of the nanoparticles (%)	189	3.02	2.47	0.40	8.10	7.70
Target	Specific heat capacity of the nanofluids system (J/K.g)	189	2.33	0.13	2.05	2.58	0.53

**Fig. 1.** Flowchart for proposed Bayesian-support vector algorithm [38].**Table 4**

Optimised parameters for the proposed SVR model.

Optimized SVR parameters	Values
C	369.0036
Epsilon	0.0013
Kernel function	Gaussian
Kernel scale	15.9637

coefficient (r). The mathematical representations for these error estimates are given below as in Eqs. (8), (9), (10), (11), and (12):

$$RMSE = \sqrt{\frac{1}{n} \left\{ \sum_i^n (C_{p(pr)} - C_{p(ex)})^2 \right\}} \quad (8)$$

Table 5

Comparing the accuracies of the proposed and existing analytic models for estimating the specific heat capacity of metallic oxide/ethylene glycol nanofluids.

Statistics	BSVR model proposed		Model I	Model II
	Training	Testing		
RMSE	0.0087	0.0127	0.1267	0.0228
MAE	0.0054	0.0093	0.1120	0.0184
MRAE	0.0024	0.004	0.0497	0.0082
AARD	0.2350	0.4043	4.9673	0.8157
r	0.9975	0.9953	0.9200	0.9964

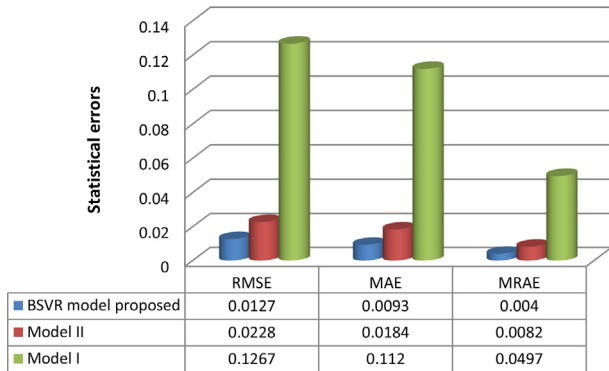


Fig. 2. Graphical representation of various errors obtained from our model and the existing analytic model.

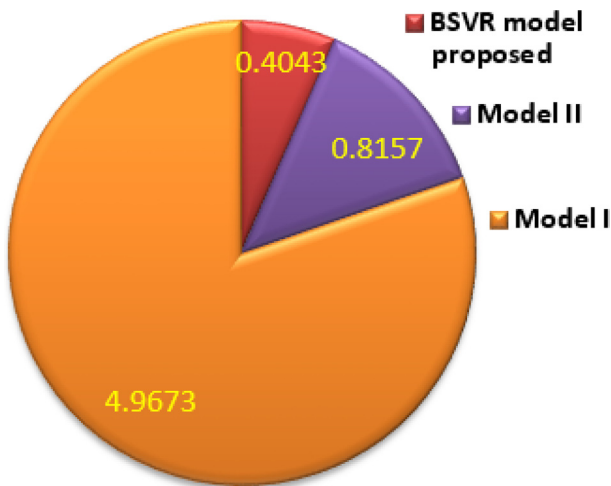


Fig. 3. Comparison of the average absolute relative deviation (AARD) obtained from our model and existing analytic models.

$$MAE = \frac{\sum_{i=1}^n |C_{p(pr)} - C_{p(ex)}|}{n} \quad (9)$$

$$MRAE = \frac{\sum_{i=1}^n \left| \frac{C_{p(pr)} - C_{p(ex)}}{C_{p(pr)}^* - C_{p(ex)}} \right|}{n} \times 100\% \quad (10)$$

$$AARD \% = \frac{\sum_{i=1}^n \left| \frac{C_{p(pr)} - C_{p(ex)}}{C_{p(pr)}} \right|}{n} \times 100\% \quad (11)$$

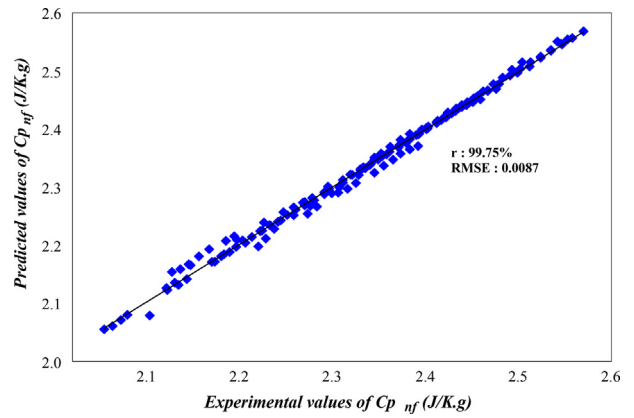


Fig. 4. Relationship between the predicted and experimental values of the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids for training data.

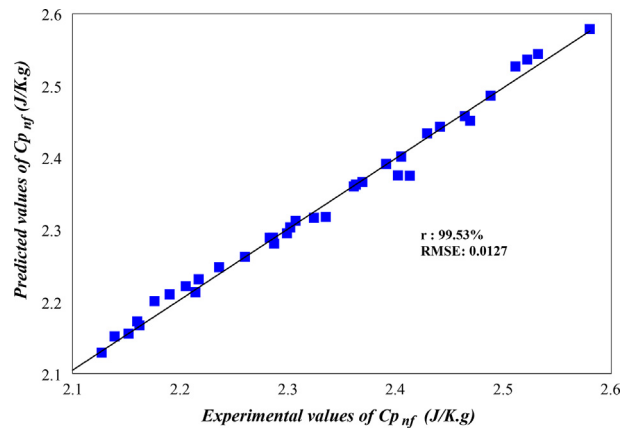


Fig. 5. Relationship between the predicted and experimental values of the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids for testing data.

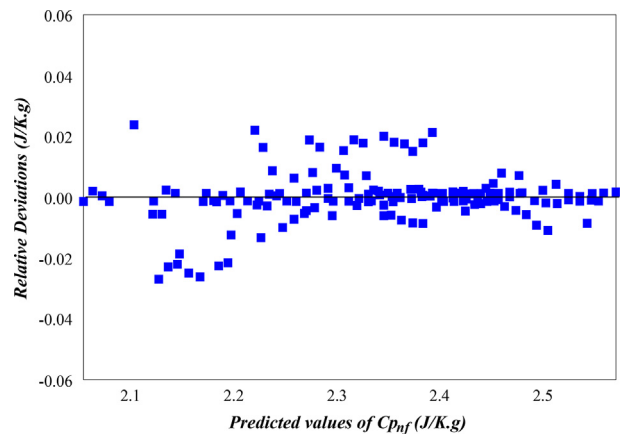


Fig. 6. Relative error distributions over the predicted values of specific heat capacity of metallic oxides/ethylene glycol-based nanofluids for the training dataset.

$$r = \frac{\sum_{i=1}^n (C_{p(ex)} - \overline{C_{p(ex)}})(C_{p(pr)} - \overline{C_{p(pr)}})}{\sqrt{\sum_{i=1}^n (C_{p(ex)} - \overline{C_{p(ex)}})^2 (C_{p(pr)} - \overline{C_{p(pr)}})^2}} \quad (12)$$

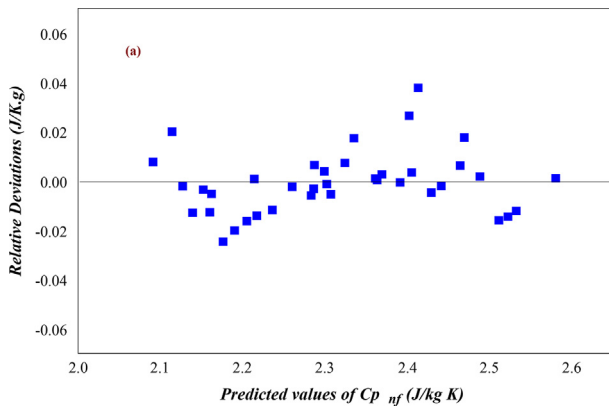


Fig. 7. Relative error distributions over the predicted values of specific heat capacity of metallic oxides/ethylene glycol-based nanofluids for the testing dataset.

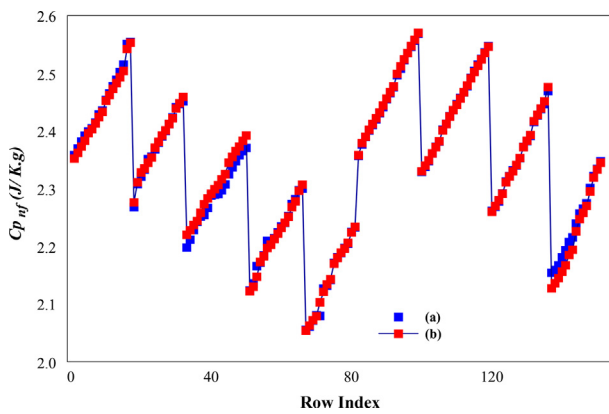


Fig. 8. Comparison of the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids using the training dataset: (a) BSVR model prediction (b) Experimental values.

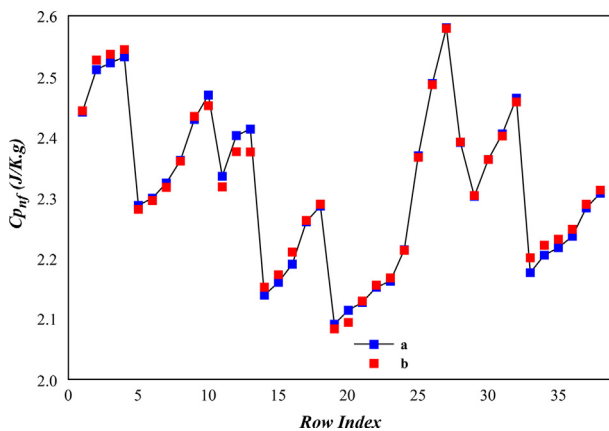


Fig. 9. Comparison of the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids using the testing dataset: (a) BSVR model prediction (b) Experimental values.

where n is the total number of the dataset. $C_{p(ex)}$ and $C_{p(pr)}$ refers to the experimental and the

predicted values of specific heat capacity the nanofluid, respectively. While $\bar{C}_{p(ex)}$ and $\bar{C}_{p(pr)}$ refer to their respective mean. $C_{p(pr)}^*$ is the estimated values of the reference model.

A reliable model should have a low value of errors (RMSE, MAE,

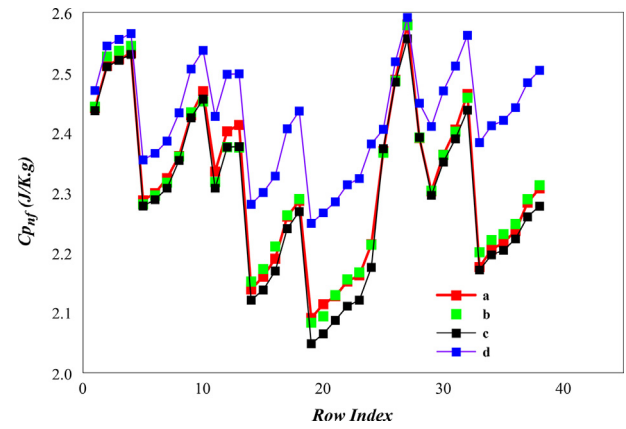


Fig. 10. Comparison of the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids using the testing dataset: (a) Experimental values (b) BSVR model prediction (c) Model II prediction (d) Model I prediction.

AARD) and a near unity value for the correlation coefficient. Table 5 reflects the training and testing results (actual performance) of the proposed machine learning model alongside the computed results of the existing analytic models. These results clearly show that the proposed model has better accuracy as the errors were much lower than those of the existing models. The improvement in the accuracy of the proposed model is seen more clearly in Figs. 2 and 3. Figs. 2 and 3 depict the comparison of the predictive ability of the proposed BSVR and existing models. It is obvious that Model I has the lowest accuracy while the accuracy of our proposed model is twice better than Model II.

Figs. 4 and 5 show the cross plot between the predicted and the experimental data of the specific heat capacity of the nanofluids for the training and testing data, respectively. Our model has near unity correlation coefficients (Pearson's) with the experimental data during the training and the testing phase. Figs. 6 and 7 reflect the residue analyses for the training and testing results, respectively. The relative errors were evenly distributed around the axis origin which thus further affirms the reliability of the proposed scheme. Furthermore, in order to show the degree of agreement between the proposed model and the experimental values, we superimposed the result of our model on the experimental data as shown in Figs. 8 and 9. The proposed model shows excellent agreement with measured results during the training and testing phases. It is important to states that given the accuracy obtained for the testing dataset, we believe the model proposed is better for predicting the specific heat capacity of the nanofluid compositions under consideration. Furthermore, Fig. 10 shows the comparison of our model in relation to the analytic models on a single plot. There is a significant discrepancy between model I and the experimental data while model II exhibits a good agreement with the experimental data. These observations are consistent with previous studies mentioned in the literature. Critical examination of Fig. 9 clearly shows that the proposed model yielded a much better accuracy than model II in a fashion consistent with other errors analysis discussed above. This performance is attributed to the wide generalization ability of the SVR algorithm, the efficiency of the Bayesian optimization technique and also the right selection of descriptors used in model development.

6. Conclusion

In this work, a four-input Bayesian support vector regression (BSVR) model has been successfully developed to estimate the specific heat capacity of metallic oxides/ethylene glycol-based nanofluids. The SVR parameters were optimized with Bayesian optimization technique and the model was built using as inputs; the volume fractions of metallic oxide nanoparticles (CuO & Al₂O₃), the specific heat capacities of the nanoparticles, specific heat capacity of ethylene glycol and temperature.

The model was trained on 151 experimental datasets (80% of the dataset) and the remaining 38 experimental datasets (20% of the dataset) for testing the generalizability of the SVR model proposed. The model proposed has a high correlation coefficient and low root-mean-square error of 99.53 % and 0.0127, respectively. Furthermore, we applied the existing analytic model to predict the specific heat capacity of the nanofluids. It was revealed that the model based on the thermal equilibrium between the nanoparticles and base fluid (Model II) has good agreement with experimental data while the model based on simple mixing rule overestimated the values of the specific heat capacity of the nanofluids. The significance of our results was highlighted by comparing it to the analytical models. Remarkably, the proposed model was twice more accurate than model II as seen from the AARD values of 0.4043 and 0.8157 for the BSVR and model II, respectively.

Declarations

Author contribution statement

Ibrahim O. Alade, Mohd A. A. Rahman, Tawfik Saleh: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Aliyu Bagudu, Zulkifly Abbas, Yazid Yaakob: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Funding statement

This work was supported by King Fahd University of Petroleum and Minerals and the Ministry of Higher Education Malaysia fundamental research grant scheme (FRGS/1/2017/TK04/UPM/02/5).

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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