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Global Modeling and Predicting of Thermal Conductivity of Nanofluids Using an Ensemble of Different Tree-based Gradient Boosting Algorithms

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Abstract

Accurate prediction of the thermal conductivity of nanofluids attracts great interest from scholars, especially with experimental studies being so laborious and expensive, and with the inability of theoretical/ empirical models to achieve the required accuracy. In addition, there is not enough literature targeting the global modeling of thermal conductivity, in other words, the modeling of the mega profile -over various nanofluids- not of the thermal conductivity of a specific nanofluid. In this research, Extreme Gradient Boosting (XGBOOST), Light Gradient Boosting Machine (LGBM), and Multilayer Perceptron (MLP) are implemented and optimized to predict nanofluids' thermal conductivity in a global manner. Therefore, eight parameters; the temperature of nanofluids, size of nanoparticles, nanoparticles' volume concentration, thermal conductivity of the base fluid, thermal conductivity of nanoparticles, nanoparticle density, specific surface area of nanoparticles, and the nanoparticles' shape are chosen as model input variables. 4689 data points -representing various nanofluids and collected from 88 published papers - have been used to train the three mentioned models. Moreover, ten different sub-sets of features were investigated to detect the most important sub-set. The results from the three models as well as from the different subsets were then compared. Furthermore, the feature importance was determined for XGBOOST and LGBM. The results demonstrate a new approach to predict the global thermal conductivity. The best RMSE value on the validation set is 0.0052 for MLP model, 0.011035 for LGBM model, and 0.00695 for the XGBOOST model. Also, the best sub-set includes size, temperature, concentration, thermal conductivity of base fluid, density, thermal conductivity of nanoparticle and shape. In addition, the highest relative importance of the nanofluids thermal conductivity is the thermal conductivity of base fluid. The shape is rarely explored in global prediction of thermal conductivity in literature.

Paper type: Research paper

Keywords: Nanofluids, Thermal Conductivity, MLP, XGBOOST, LGBM**.**

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Introduction

Nanofluids are comprised of diluted formulations of synthesized nanomaterial structures (Saidur,et al, 2011). A nanofluid is a fluid type with nano-sized particles dispersed in a base fluid. These particles, usually made of metal or metal oxide, improve convection besides conduction coefficients, permitting extra heat to be transferred from the coolant. Past investigations have demonstrated that nanofluids have improved thermophysical characteristics, including thermal diffusivity,

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thermal conductivity, viscosity, as well as convective heat transfer coefficients, especially in comparison to common fluids like water or oil (Wong and De Leon, 2010).

The first critical stage in conducting experimental research using nanofluids is the synthesis of nanofluids. Nanofluids are constructed by placing nm-sized solid particles in base liquids like water, oils, ethylene glycol, and similar liquids. Nanofluids are more than just liquid-solid combinations. Several unique characteristics must be met, such as even and stable suspension, long-term suspension, minimal particle agglomeration, no chemical change in the fluid, etc. Agglomeration is a critical issue in the production of nanofluids. There are primarily two main methods for producing nanofluids. These include single-step and two-step approaches (Wang and Mujumdar, 2008).

Extensive research on diverse nanofluids applications has been conducted within the previous few decades. Several review papers addressing residential, industrial, commercial, and transport applications have lately been published. Electronic cooling, welding, engine cooling/vehicle thermal management, nuclear system cooling, lubrication, thermal storage, solar heating, generator cooling, coolant in machining, cooling and heating in buildings, transformer cooling, refrigeration, transportation, energy storage, biomedical applications (including antibacterial activity and Nano drug delivery), space, defense, and marine and many other applications are just a few examples (Yu and Xie, 2012) (Sarkar et al., 2015) (Sun, and Wang, 2021). Large companies like GM and Ford, among several others, have continued nanofluid research initiatives in the transportation industry (Wang and Mujumdar, 2008).

Nanofluids have specific distinct characteristics that distinguish them from mm or μm particle dispersions. Nanofluids have been demonstrated to have more excellent thermal conductivities than typical cooling liquids such as water, kerosene, ethylene glycol, and micro fluids. Improved thermal conductivity, higher heat transfer, with enhanced critical heat flow are three qualities that make nanofluids ideal coolants (Angayarkanni and Philip, 2015). Changes in thermo-physical parameters such as thermal conductivity, viscosity, and specific heat impact convective heat transfer when nanoparticles are incorporated into the base fluid. The parameters of various nanomaterials alter to varying degrees. Some of the primary parameters that significantly impact the thermo-physical characteristics include nanoparticle concentration, clarity level, morphology, but also size of nanomaterial (Gupta et al., 2017) (Mondragón et al., 2012). Many parameters that impact the thermal conductivity of nanofluids were explored in literature, as nanoparticle size (Apmann et al., 2021), nanoparticle shape (Mirmohammadi et al., 2019), nanoparticle concentration (Das et al., 2017), nanoparticle density (Rudyak and Minakov, 2018), nanoparticle specific surface area (Fang et al., 2015), nanoparticle TC (Michael and Shajahan, 2017), base fluid TC (Shekarian et al., 2014), and nanofluid temperature (Mukherjee et al., 2016).

Experimenting with nanofluids to determine their thermal conductivity is a difficult and time-consuming operation. Furthermore, the cost and time required to conduct sufficiently repeatable experiments prevent the measurement of nanofluids' thermal conductivity under all of the desirable operating conditions. As a consequence, diverse theoretical (Maxwell model (Ariana, et al., 2015)) and empirical (Afrand et al., 2016a) Model (Zendehboudi and Saidur, 2019)) correlations linking nanofluid thermal conductivity to clearly verified factors including volume fractions, nanoparticle size and temperature have been developed (Ariana et al., 2015). Regrettably, the accuracy and applicability of current theoretical or empirical models cannot fulfill the demand due to their limitation to take all attributes that affect the nanofluids thermal conductivity. Also, the accurate predictions achieved from these models are only for a limited range of input variables (Zhang et al., 2019).

The extensive literature on the use of machine learning and artificial neural networks (ANN) to model one or more of the thermophysical properties of nanofluids, as well as the corresponding high accuracy results, demonstrates how using computer-aided solutions can significantly outperform many complex empirical formulas by capturing hidden features that may not be measurable by laboratory tools or easy to formulate through human observations (Durgam and Kadam, 2021). However, there is no enough studies on the use of machine learning for the global modeling of thermal conductivity, in other words, for the modeling of the mega profile - over various nanofluids- not of the specific trend of thermal conductivity. Recently, Meijuan (Meijuan, 2021), in his recent comprehensive review of the ANN approach for modeling the thermal conductivity of nanofluids, discussed the most relevant methods in machine learning used for the prediction of nanofluids' thermal conductivity. Precisely, multilayer perceptron (MLP), adaptive neuro-fuzzy inference system (ANFIS), radial basis function neural networks (RBFNN), least square support vector machine (LSSVM), and group method of data handling (GMDH) were significant machine learning approaches used for this task. Based on the conclusion of (Meijuan, 2021), the MLP model occupies the highest percent of applications for predicting the thermal conductivity of a nanofluid; up to 82% of studies used MLP, while ANFIS, RBFNN, and GMDH have 9.8%, 4.9%, and 2.4%, respectively. The optimal structure of MLP depends on the experimental samples and it is considered a challenge to achieve the best performance. The

complex problem needs more hidden layers and neurons. One of the most common ways to decide the good fit of the model is Root Mean Square Error (RMSE) (Meijuan, 2021). Nevertheless, the commentary of the review is that most of the studies designed their model for one type of nanofluid only, while not many studies designed their model based on various types of nanofluids; which means that there are no reliable means to investigate the global effect of the parameters (temperature, size of nanoparticles, volume concentration, and nanoparticles and base fluid thermal conductivity) on the thermal conductivity of nanofluids.

As a global modeling approach that is much outperforming the best reported score of the other few global techniques, Hemmati-Sarapardeh et al. (2020) used three different models to predict thermal conductivity of 78 distinct nanofluids from 3200 data points: radial basis function neural networks (RBFNN), multilayer perceptron (MLP), and least square support vector machine (LSSVM). Their parameters were size, temperature, volume fraction, and thermal conductivity of base fluid and nanoparticle. They also combined their models' predictions to improve accuracy and conduct final comparisons with the best theoretical and empirical models. The findings revealed that the generated model improved accuracy considerably, with just 0.016 RMSE and 0.87 percent average absolute relative error (AARE).

Ahmadi et al. (2018) discussed the effect of two groups of features on the TC of Al2O3/water and Al2O3/ ethylene glycol. Firstly, temperature and volume fractions were used as input variables, and then the size of nanoparticles was added as the third input variable. The obtained R-squared value is 0.9958.

Recently, the shape of nanoparticles was used as a novel input parameter beside other parameters. The two articles that considered the shape as a feature, predicted the thermal conductivity of TiO2-water nanofluid using relatively small data sets with a specific type of shape (Sharma et al., 2022), they used 228 samples to predict the thermal conductivity by five models: ANN, support vector regression (SVR), decision tree regression (DTR), gradient boosting regression (GBR), and random forest regression (RFR). The size, volume fraction, the shape of nanoparticles (rod, cubic, and spherical), and the temperature of the whole system were used as input variables. The higher accuracy was achieved by the GBR algorithm with an R2 equal to 99 % and 2×10-4 MSE. The beneficial result of the study was that nanoparticles' shape had a lower effect on the thermal conductivity of nanofluid compared with the other parameters included in the data set (Sharma et al., 2022).

This research aims at building machine learning models for global prediction of the thermal conductivity of nanofluids in order to simulate the mega trend of the thermal conductivity based on various nanofluids not only on a specific nanofluid as in literature. Also, the work investigates the importance of every possible feature in the models (size, temperature, concentration, thermal conductivity for base fluid, density, thermal conductivity for nanoparticle, shape and specific surface area), especially the added new features in global prediction (shape and specific surface area and density). Mainly three predictive models are used in this research which are multi-layer perceptron (MLP), extreme gradient boosting (XGBOOST) and light gradient boosting machine (LGBM). All of the developed models were applied to a collected dataset that contained 4689 data points. Furthermore, this research proposed 10 feature combinations to explore the effect of the various features in predicting the thermal conductivity of nanofluids.

1 Materials and Methods

1.1. Research dataset

1.1.1. Dataset Description

To develop a reliable predictive model -with a wide range of applicability and comprehensivity- for the global prediction of the thermal conductivity of nanofluids, a large dataset with a variety of nanofluids is required. For this purpose, 4689 experimental data points (more than 110 different nanofluids) have been collected from 88 published papers papers from 2005 to 2020 ((Patel, et al., 2010), (Agarwal et al., 2016), (Timofeeva et al., 2007), (Raja et al., 2015), (Vajjha and Das, 2012), (Abdolbaqi et al., 2016), (Duangthongsuk and Wongwises, 2010), (Keyvani et al., 2018), (Milanese et al., 2016), (Mariano et al., 2015), (Al-Waeli et al., 2017), (Esfahani et al., 2017), (Vajjha et al., 2010), (Warrier and Teja, 2011), (Jiang et al., 2015), (Zhang et al., 2007), (Dehkordi et al., 2017), (Omrani et al., 2019), (Alrashed et al., 2018), (Said, et al., 2016), (Sundar et al., 2015), (Liu et al., 2006), (Zhao and Li, 2017), (Vajjha and Das, 2009), (Abdolbaqi et al., 2016), (Sharifpur et al., 2017), (Tshimanga, et al., 2016), (Abdolbaqi et al., 2016), (Wei, et al., 2017), (Godson et al., 2010), (Yu et al., 2011), (Sabiha et al., 2016), (Hussein et al., 2013), (Longo and Zilio, 2011), (Longo and Zilio, 2013)., (Reddy and

Rao, 2013), (Kumar and Sonawane, 2016), (Xing et al., 2015),(Li et al., 2016a), (Li et al., 2016b), (Afrand, et al., 2016a), (Sundar et al., 2013a), (Sundar et al., 2013b), (Sundar et al., 2016a), (Sundar et al., 2016b), (Sundar et al., 2016c), (Chougule and Sahu, 2015), (Asadi and Pourfattah, 2019), (Suganthi, et al., 2014), (Satti, et al., 2017), (Duangthongsuk and Wongwises, 2009), (Yiamsawasd, et al., 2012), (Tertsinidou et al., 2017), (Akilu et al., 2017), (Li et al., 2015), (Das et al., 2016), (Agarwal, et al. 2016), (Fedele, et al., 2012), (Żyła, 2017), (Akilu et al., 2019), (Jiang et al., 2014), (Wan et al., 2015), (Beck et al., 2010a), (Beck et al., 2010b), (Chiam et al., 2017), (Soltanimehr and Afrand, 2016), (Abdul Hamid et al., 2016), (Lee et al., 2012), (Karimi et al., 2015), (Kim et al., 2007), (Mostafizur et al., 2014), (Mariano et al., 2013), (Pastoriza-Gallego et al., 2014), (Li and Zou, 2016), (Rohini Priya et al., 2012), (Pastoriza-Gallego et al., 2011), (Banisharif et al., 2020), (Ranjbarzadeh et al., 2019), (Buonomo et al., 2015), (Poongavanam et al., 2019), (Kumar et al., 2018), (Krishnakumar et al., 2019), (Khedkar et al., 2012), (Sharif et al., 2016), (Redhwan et al., 2017), (Shima, et al., 2010)).

The collected dataset covers the main parameters that influence the thermal conductivity of nanofluids. The dataset includes therefore eight features, where seven of them are numerical features and one categorical feature.

These features are the temperature measured in Kelvin (K), particle volume concentration measured as a percentage (%), particle size (size) measured in nanometer (nm), nanoparticle thermal conductivity measured in Watt/Kelvin-meter (W/m.K), base fluid thermal conductivity measured in Watt/Kelvin-meter (W/m.K), shape which is a categorical variable (represented as spherical, cylindrical, rod, and cubic), particle density measured in Kilogram per cubic meter (Kg/m^3), and particle specific surface area measured in squared meter per gram (m2/g).

1.1.2. Data Preprocessing

1.1.2.1 Data Preparation

Several preprocessing operations have been done to render the collected data appropriate for training. At first, the acquired dataset has been checked for duplicate samples, all duplicates have been eliminated. Such an operation resulted in removal of 9 samples in total from the dataset to reach 4680 data points.

The shape variable is presented as a categorical feature in the acquired dataset. However, machine learning algorithms in general deal only with numerical variables. To overcome this problem, the shape variable has been converted from the categorical form into the numerical form via the one-hot encoding. This method allows for representing each categorical variable in a numerical format by converting each category in the attribute into a standalone feature which takes values of 0 or 1. For any data point, if a certain category is present in this data point it takes the value of 1, while the remaining features take 0 values. For example, spherical shape has a label of 0001, while cylindrical shape represented by 0010.

In addition, as the values of the dataset variables differ significantly in their values, such a situation can affect the performance of trained algorithms. To overcome this problem, all numerical variables in the dataset have been standardized via the standard scaling method to bring all variables into a unified scale and to provide homogeneity for the dataset, by making the mean of our data equal to zero and the variance equal to 1.

1.1.2.2. Features Combinations and Sub-Datasets Selection

The present work follows the strategy of the investigation of the effect of features via different features' combinations to train the models. To elaborate more on this, the implemented models have been trained on 10 different overlapped selected sub-datasets as given in table 1. This process of selection helps in exploring how the model's performance varies according to the various feature combinations, hence in determining the importance of features in the models. Consequently, one of the selected sub-datasets is used to train the models on all features, while the other nine sub-datasets are used to train the models on nine different combinations of features.

In order to successfully achieve the previous step (selection of suitable sub-datasets), the missing data should be tackled in the originally collected dataset. The selection mechanism has therefore been performed as follows: (1) all features in the collected dataset which have no missing values are kept in all selected sub-datasets. These features are the size, temperature, concentration, and thermal conductivity for the base fluid. (2) every selected sub-dataset contains those "constant" features as well as additional features issued from the dataset points where those additional features are not missing. For example, the first combination contains only the previously

mentioned four features; while in the second combination, those four features are combined along with the density feature from the points where the density feature is not missing, and so on. The process of combination generation including new features continues until all features are included. However, it is worth noting that this process is conducted on the expense of the number of data points used for each combination. Meaning that, each time a new feature -that has missing values- is included, all the data points -related to those missing values- are removed from the dataset to create the new sub-dataset (to reduce the effect of missing values).

As a result, 10 partitions were obtained where one of them contains four features, four of them contain five features, three of them contain six features, one of them with seven features and one of them covers all features in the dataset. **Table 1** summarizes the created combinations as well as the number of data points for each combination after removing the missing ones.

Table 1. Summary of studied features combinations and corresponding numbers of data points after the removal of the missing ones.

Code	Features combination	Data Points
Comb.1	Size, temperature, concentration, thermal conductivity of base fluid	4680
Comb.2	Size, temperature, concentration, thermal conductivity of base fluid, density	3444
Comb.3	Size, temperature, concentration, thermal conductivity of base fluid, thermal conductivity for nanoparticle.	3431
Comb.4	Size, temperature, concentration, thermal conductivity of base fluid, shape	3116
Comb.5	Size, temperature, concentration, thermal conductivity of base fluid, specific surface area	990
Comb.6	Size, temperature, concentration, thermal conductivity of base fluid, thermal conductivity of nanoparticle, shape	2380
Comb.7	Size, temperature, concentration, thermal conductivity of base fluid, thermal conductivity nanoparticle, density	2512
Comb.8	Size, temperature, concentration, thermal conductivity of base fluid, density, shape	2093
Comb.9	Size, temperature, concentration, thermal conductivity of base fluid, density, thermal conductivity for nanoparticle, shape	1842
Comb.10	Size, temperature, concentration, thermal conductivity of base fluid, specific surface area, density, shape, thermal conductivity of nanoparticle	524

1.1.2.2. Elimination of Outliers

Eventually, outliers have been detected by examining the box-plots of all variables in the acquired dataset. All data points which had extreme values have been removed from the dataset.

1.2. Experimental Setup

1.2.1. Creation of Data Folds and Cross-validation

After the complete data preprocessing, the dataset has been split into training and testing dataset. Rather than creating fixed training and test splits, K-Folds Cross validation method has been employed in this research. Clearly, K-Fold cross validation allows for splitting the data into equivalent training and testing splits. Each split is then used for training where in each training round a single split is

employed as testing split while the remaining splits K-1 splits are used for training. The choice of cross-validation folds is set to five folds for all algorithms training schemes as it provided the best result. In addition, the shuffling option is allowed when creating the splits to avoid exposing the models to a variety of training examples in a single batch rather than having similar ones in the same batches.

1.2.2. Set-up of Implemented Models

1.2.2.1. Multi-layer Perceptron Setup

A special MLP architecture is designed for the sake of this research project, which in total consists of six layers arranged as an input layer, four hidden layers, and an output layer. The first layer consists of 8 neurons that will receive the input from the features with linear activation function. For the hidden layer, the first and second layers hold 128 neurons each, while the third layer consists of 64 neurons, and the fourth layer consists of 32 neurons. In addition, each of the hidden layers is controlled by a Rectified Linear Unit (ReLU) activation function. Lastly, the output layer consists only of a single neuron which has a linear activation function. In total, this design results in around 28,000 parameters that would be responsible to fit the data. **Table 2** summarizes the specifications of the designed multi-layer perceptron model.

Table 2. Summary of the implemented Multi-layer perceptron MLP design specifications.

Layer	Number of neurons	Number of parameters per Layer	Activation function
Input layer	8	0	Linear
Hidden layer 1	128	1152	ReLU
Hidden Layer 2	128	16512	ReLU
Hidden layer 3	64	8256	ReLU
Hidden layer 4	32	2080	ReLU
Output layer	1	33	Linear

With respect to the hyper-parameters of the MLP algorithm, RMSProb (Hinton, et al., 2020) optimizer was employed in this research along with a learning rate value of 0.001, epsilon value of 1e-7 for numerical stability and a momentum value of 0.9 for weights update. Eventually, MLP training has been run for 10000 training epochs, while Mean Absolute Error MAE was used as loss function. It is worth noting that these hyper-parameters values have been obtained by experimentation. **Table 3** summarizes the MLP model hyper-parameters.

Table 3. Summary of MLP training hyper-parameters.

Hyper-parameter	Optimizer	Learning rate	Epsilon	Momentum	Epochs	Loss function
Value	RMSProb	0.001	1e-7	0.9	10000	MAE

2.2.2.2. XGBoost and LGBM Setup

For both XGBoost and LGBM models, a part of the training parameters has been specified via Optuna hyper-parameters optimization packages (minimum child weight, number of leafs and regression lambda hyper-parameters). Optuna is an automatic hyperparameter tuning library, particularly built for machine learning and deep learning frameworks. The remaining parameters have been specified experimentally. Hence, the learning rate was set to the value of 0.1, the number of decision trees to build was set to 10000, the early stopping rounds was set to 50, and the loss function was set to MAE. **Table 4** summarizes the fixed hyper-parameters of XGBoost and LGBM models.

Table 4: Summary of XGBoost and LGBM training fixed hyper-parameters.

Hyper-parameter	Learning rate	Early stopping rounds	Number of trees	Loss Function
Value	0.05	50	10000	MAE

1.2. Training Environment Setup

All training efforts have been accomplished on Google Colab Platform which provides its users with A TESLA K80 GPU accelerator which has a 12 GB RAM. In addition, TensorFlow along with its high-level interface were utilized to implement the multi-layer perceptron codes. Further, LightGBM library is employed for Light Gradient Boosting Machine code implementation, while XGBOOST library is employed for Extreme Gradient Boost implementation code. Moreover, Optuna Library is employed to find the best hyper-parameters for the features sub-set combination under investigation. Finally, all research coding efforts have been developed via Python programming language version 3.7.13.

1.3. Evaluation Metrics

There are numerous evaluation metrics that can be used for regression tasks such as the one in hand. Some of these metrics are best used when a large gap between the true and predicted target values is expected such as root mean squared logarithmic error (RMSLE). This metric is less intuitive, but produces much smaller absolute values compared to other metrics like Root Mean Squared Error (RMSE) or Mean Absolute Error (MAE) due to the employment of the logarithmic operation. Nevertheless, other evaluation metrics are appropriate when the gap is smaller such as in the present work. Hence two evaluation metrics are reported herein, including RMSE and MAE.

It is worth noting that both RMSE and MEA are error values, which means that the lower the value of these measures the better performance and the higher prediction capabilities. In addition, despite reporting both RMSE and MEA in our results, only RMSE value is used for analysis as it is more precise in penalizing the large errors.

2. Results and Discussion

Figure 1 gives a close view on the RMSE measure for the validation set. It can be clearly seen that MLP model gives the least RMSE value in predicting the nanofluid's thermal conductivity when trained on the ninth combination (comb.9) which contains seven features as given in Table 1 with an RMSE value of 0.00203 on the training set and of 0.0052 on the validation set. This indicates that the MLP model ability to correctly predict the nanofluid's thermal conductivity is best achieved under this combination.

Following that, the seventh combination (comb.7) ranks as the second best performing feature combination -for training the MLP model- which contains six features. More clearly, despite the fact that (comb.7) provided very close performance to comb.9 on the training set (RMSE: 0.00204), the RMSE value on the validation set (0.00739) is relatively higher than comb.9 although it contains more data points (1236).

In addition, the tenth combination (comb.10) which includes all features in the dataset comes in fifth position with an RMSE value of 0.00791 on the training set and 0.01079 on the validation set. Although this combination has only (488) data points, it manages to give a relatively good performance as compared to the other combinations.

The first combination (comb.1) provides the worst performance against the other combinations with RMSE values of 0.02111 on the training set and 0.03264 on the validation set. It is worth noting that despite the fact that comb.1 has the highest number of data points which is 3970, it gives the least performance in predicting the thermal conductivity of the nanofluid. This can be attributed to the number of features it contains which is only restricted to four features: size, temperature, concentration, and thermal conductivity for base fluid.

The performance of MLP models shows a substantial improvement with those combinations that contain more features such as comb.9 and comb.7 and less prediction accuracy when few features are used such as comb.1 even they have lower number of data points. This means that feature inclusion is more critical to the performance than the number of data points.

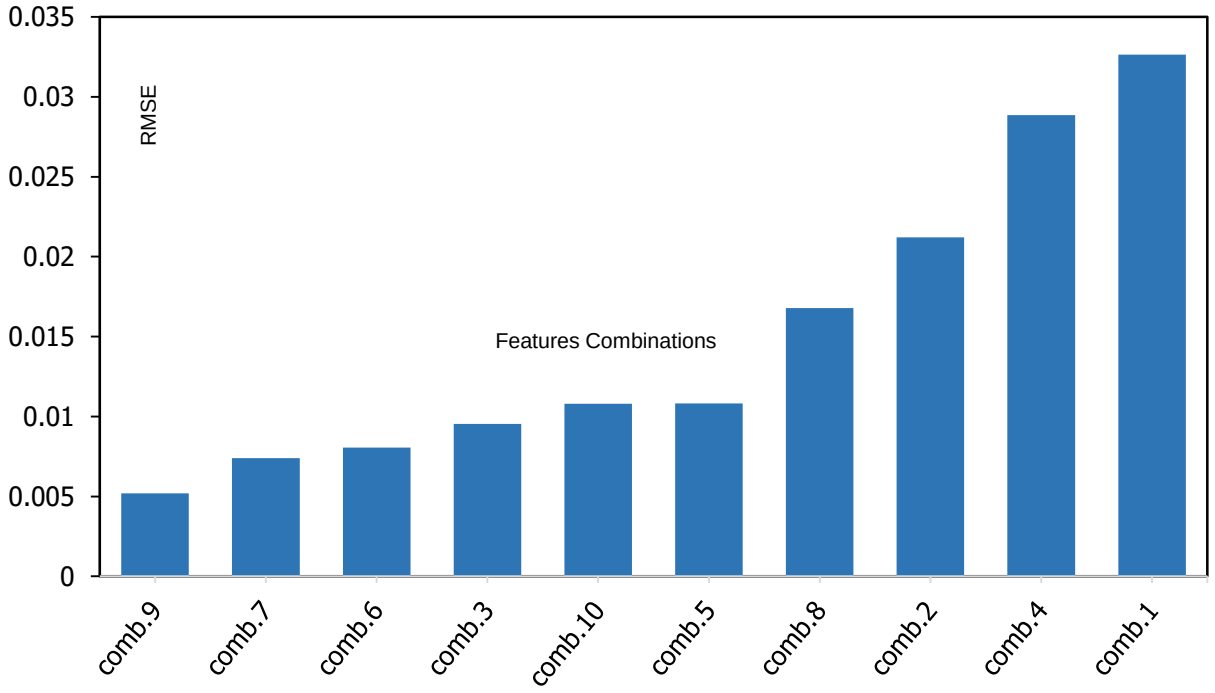

Fig. 1. Summary of RMSE measure for MLP mode according to the different combinations (for validation set).

Figure 2 summarizes the RMSE performance measures on the validation set for LGBM algorithm (according to all combinations). It can be clearly observed that the ninth combination (comb.9) shows also the best performance in predicting the thermal conductivity for the nanofluid with an RMSE value of 0.00732 on the training set and an RMSE value of 0.01035 on the validation set.

Furthermore, both of the seventh (comb.7) and the sixth combination (comb.6) show also a very close performance to comb.9 and hence stand at the second and the third positions respectively (on the validation set) according to the RMSE measures which are 0.01121 and 0.01171, respectively. This means that both comb.7 and comb.6 can also be considered as best performers if we tolerate the amount of the error they achieve as compared to comb.9. In addition, the tenth combination (comb.10), that includes all features, ranks the fourth as compared to the other combinations when trained using LGBM model with an RMSE value of 0.00114 on the training

set and 0.0158 on the validation set. In comparison to MLP model, comb.10 ranked the fifth against the other combinations (Validation RMSE: 0.01079). However, the level of RMSE error achieved for the same features combination (comb.10) by LGBM is higher.

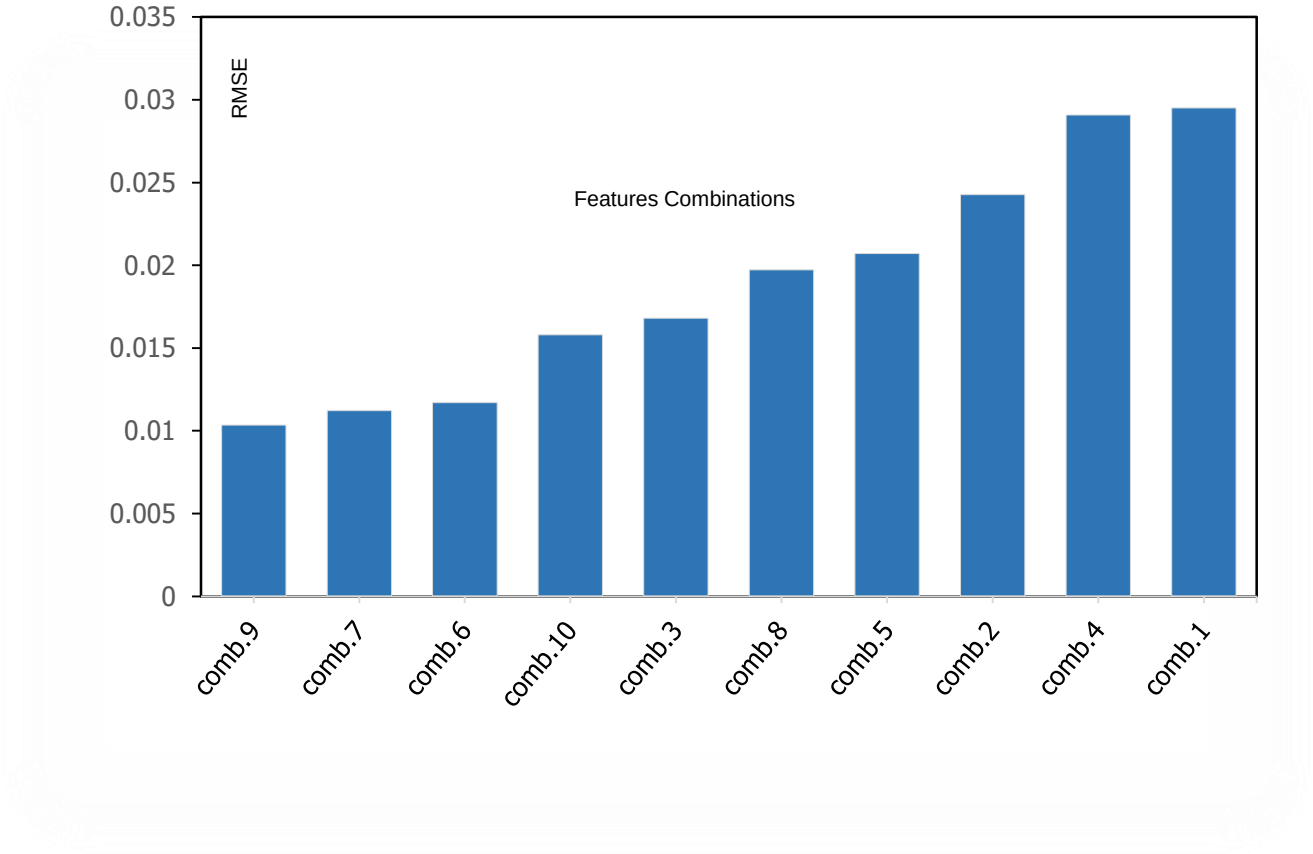

Fig. 2. Summary of RMSE measure for LGBM model according to the different combinations (for the validation set).

The first combination (comb.1) provides also the worst performance in predicting the thermal conductivity for the nanofluids with an RMSE value of 0.02431 on the training set and 0.02951 on the validation set. In addition, the fourth combination (comb.4) provides also a very close performance to comb.1 with respect to the RMSE which is 0.02321 on the training set and 0.02909 on the validation set. However, comb.4 provides a slightly better performance in comparison to comb.1.

Overall, the same trend of the MLP results can be observed in the LGBM results in regard to the effect of various features combinations as well as the number of data points. In other words, those combinations with higher number of features tend to show better performance even though they have a lower number of data points.

Figure 3 shows the RMSE values on the validation set. It is obvious from **Fig 3** that comb.9 provides also the best performance when trained under the XGBOOST algorithm with an RMSE value of 0.00099 on the training set and 0.00695 on the validation set. In addition, comb.7 and comb.6 rank in second and third positions on the training set, with RMSE values of 0.00084 and 0.00091, respectively. On the other side, they have a very close performance to each other on the validation set with an RMSE value of 0.00815 for comb.7 and 0.00824 for comb.6.

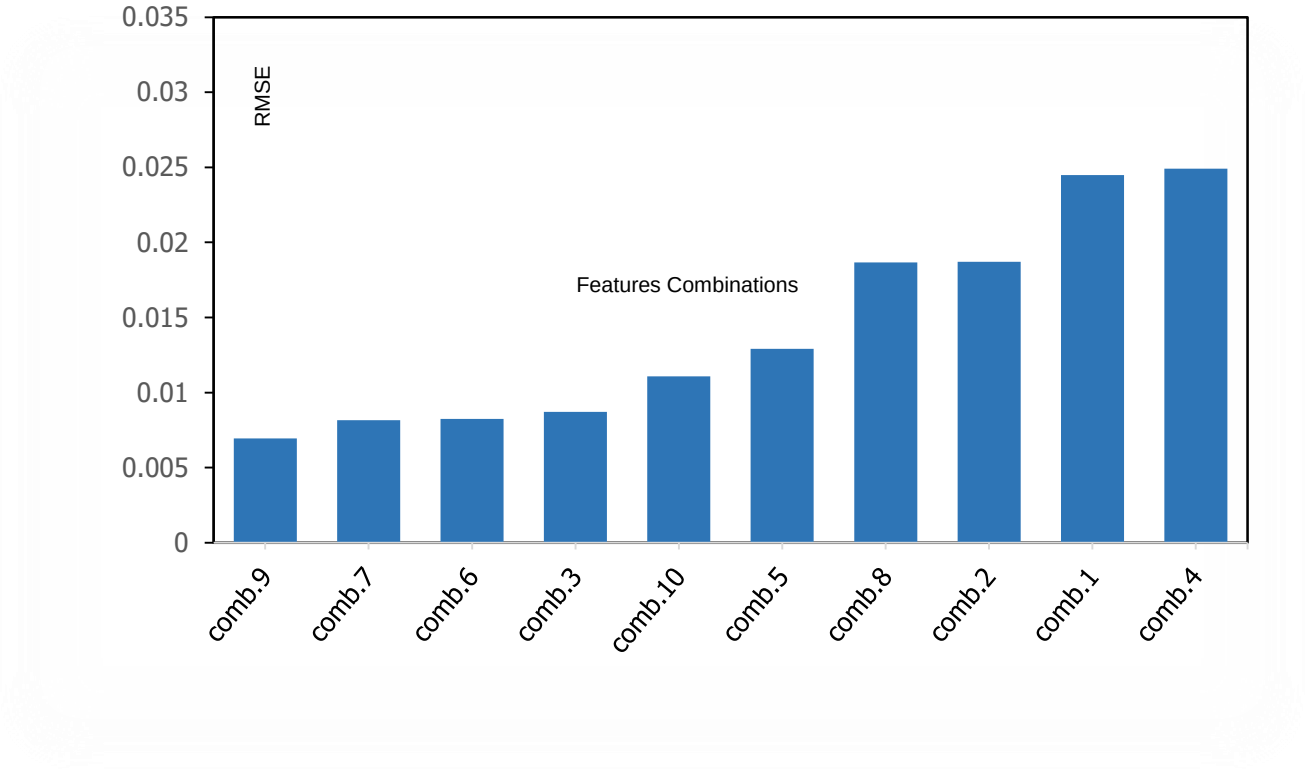

Fig. 3. Summary of RMSE measure for XGBOOST model according to the different combinations (on the validation set).

For comb.10 that includes all features, XGBOOST performance ranks the fifth against the other features combinations with an RMSE value of 0.00556 on the training set and 0.01108 on the validation set; which represent a better value on the training set and a worse value on the validation set as compared to MLP results for the same combination despite having the same ranking (fifth position). However, it provides lower RMSE value when compared with LGBM model (0.01580) in which comb.10 ranks fourth under this model.

Finally, as different than MLP and LGBM, comb.4 shows the worst performance in predicting the thermal conductivity for the nanofluids with RMSE values of 0.00723 on the training set and 0.02491 on the validation set. Nevertheless, comb.1 that ranked last in MLP and LGBM- shows in XGBOOST a relatively close performance to the worst combination **(comb.4)** with RMSE values of 0.0746 on the training set and 0.02449 on the validation set. Moreover, it is worth noting that although comb.4 has a worse performance than comb.1 on the validation set in XGBOOST, it performs better on the training set.

In general, we can observe that XGBOOST performance with respect to the ten combinations -in the validation set- follows the same order found by the MLP algorithm except for the last two combinations where the order is reversed in XGBOOST as compared to MLP but with very close errors for comb. 1 and comb. 4 in XGOOST model.

Figure 4 compares the performance of the best combinations for MLP, LGBM and XGBOOST models. First of all, it can be observed from the previous analysis that all models agree that the best performance is achieved when we use comb.9 for predicting the thermal conductivity for the nanofluids; which indicates a consistency in the results.

With respect to the performance comparison, we can see clearly that the MLP algorithm provides the best performance as compared to LGBM and XGBOOST with an RMSE value of 0.0052 on the validation set. XGBOOST performance comes in the second position with an RMSE value of 0.00695 on the validation set, while LGBM gives the worst performance as compared to both MLP and XGBOOST with an RMSE value of 0.01035 on the validation set.

In total, this means that the MLP results should be given the highest priority when predicting thermal conductivity for a nanofluid followed by XGBOOST, while the lowest priority should be given to the LGBM results.

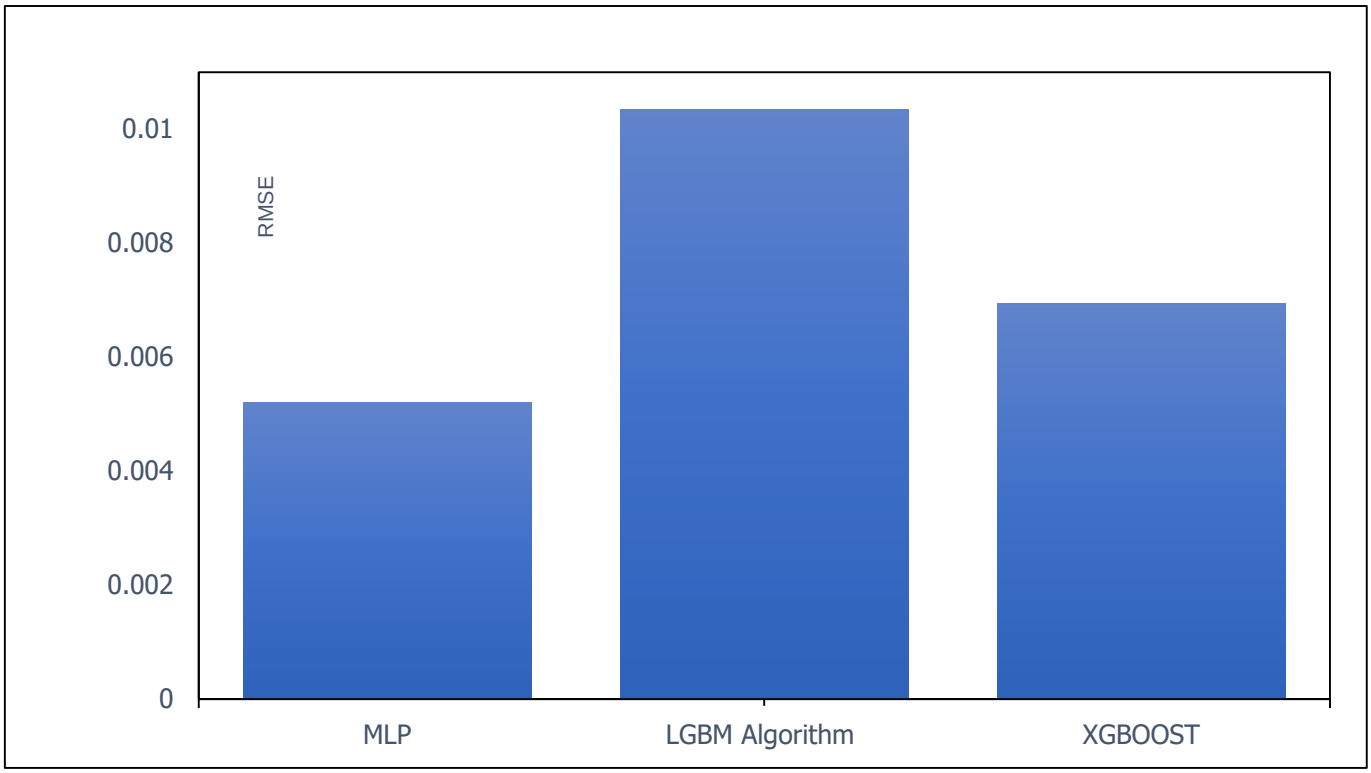

Fig. 4. Comparison of the implemented models in regard to the best achieved RMSE

There is a consent that combination 9 which includes size, temperature, concentration, thermal conductivity for base fluid, density, thermal conductivity for nanoparticle, and shape (does not include specific surface area) gives the best performance with respect to all models. This indicates that the features that constitute this combination are the most effective features for the global prediction of the thermal conductivity for the nanofluids. However, to gain more clear insights about the individual importance of each feature, there is a need to examine the quantitative contribution of each feature. This kind of analysis is performed only for both XGBOOST and LGBM algorithms and excluded for MLP algorithm. This is because the internal algorithm of MLP model does not have the capability to accomplish such an analysis.

Figure 5 shows the features importance according to the XGBOOST algorithm. It is obvious from Figure 5 that the most important feature according to XGBOOST model is the thermal conductivity for the base fluid which contributes by approximately 0.85 to the relative importance of all features. Following that, cubic shape of nanoparticle comes as the second most important feature with nearly 0.08 relative importance. Lastly, each of the thermal conductivity for the nanoparticle, size, density, concentration, temperature and spherical shape of the nanoparticle have relative importance less than 0.05.

Figure 6 depicts the relative importance of features when trained using LGBM algorithm. According to Figure 6, temperature of nanofluid is the most important feature which contributes by around 0.95 to the relative importance of all features, while the thermal conductivity for the base fluid ranks the second with a relative importance score of 0.6. The concentration feature appears to be a critical feature according to the LGBM model that holds an importance score of 0.4. In addition, each of the size, thermal conductivity for the nanoparticle and the density features hold relative importance scores around 0.15. Lastly, the shape of the nanoparticle (either cubic or spherical) has the least relative importance.

A last word on the relative importance scores, it can be observed that XGBOOST prediction depends mainly on one features to deduce the thermal conductivity for the nanofluids, while LGBM considers six features as important features to make correct predictions. As XGBOOST is able to make better prediction than the LGBM model, this leads us to the conclusion that some of the features may hurt the performance of the models. It also leads us to an important conclusion that the exclusion of the shape feature is essential.

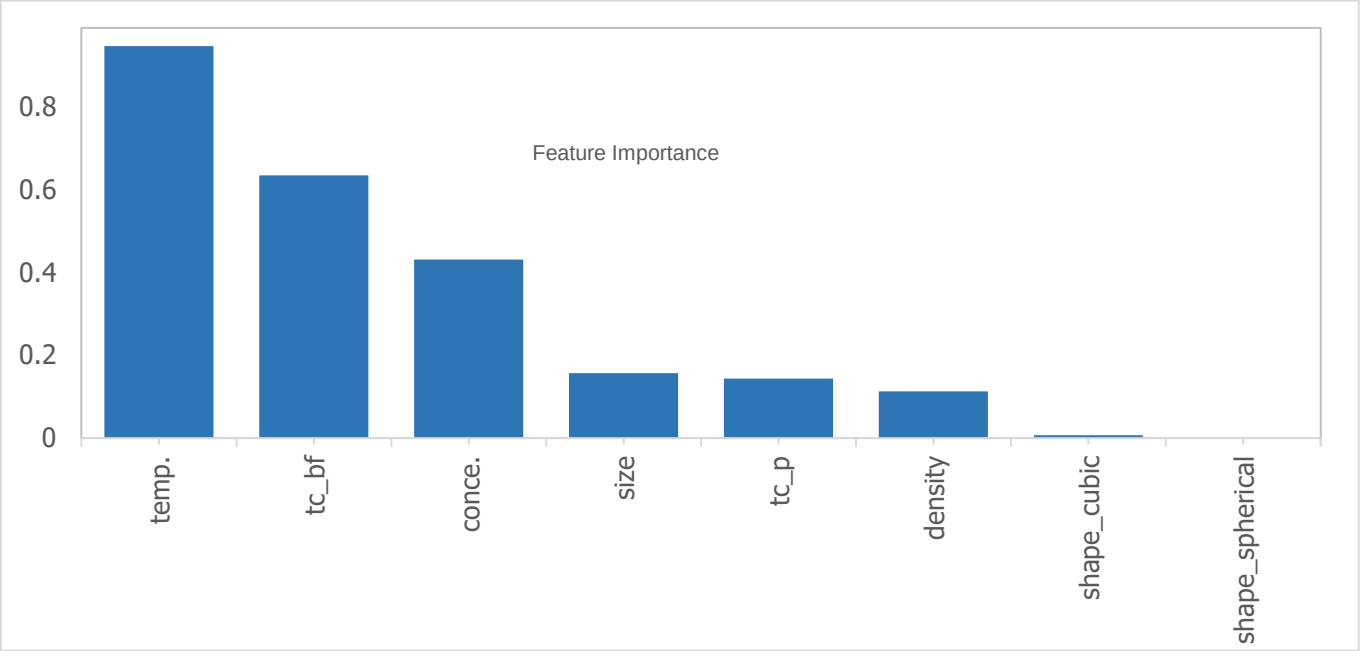

Fig. 5. relative importance according to XGBOOST algorithm.

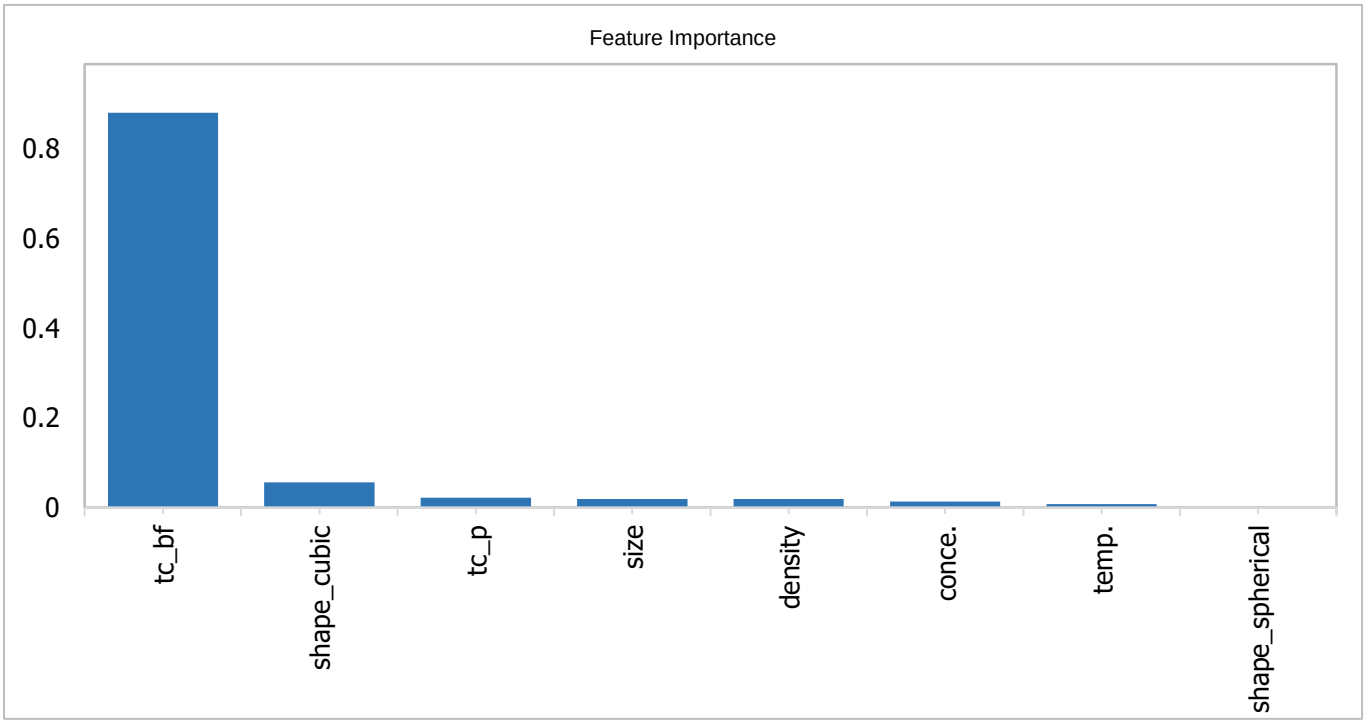

Fig. 6. Features relative importance according to LGBM algorithm

3. Interpretation of Results from Nanotechnology Perspective

Experimental studies have shown that the thermal conductivity of nanofluids is affected significantly by several parameters: size of nanoparticles, concentration of nanoparticles, thermal conductivity of nanoparticles and base fluid, shape of nanoparticles, density of nanoparticles and temperature of nanofluid.

Agarwal et al. (2016) investigated the thermal conductivity of Al_2O_3 nanoparticle dispersed in two base fluids; (water and ethylene glycol). The result shows the importance of choosing the base fluid correctly, in other words, the base fluid can affect significantly the rate of thermal conductivity enhancement. By selecting the water as a base fluid, the nanofluid thermal conductivity percentage increased to 13%, while it was 7% for ethylene glycol based-nanofluid at 0.25% concentration. When the concentration becomes 2%, the percent increase in the thermal conductivity of Al_2O_3/ water and Al_2O_3/ ethylene glycol were 15% and 9%, respectively. Similar outcomes were reported by other experimental work. From this purpose, we can conclude that the thermal conductivity of base fluids come in the top of the priority in order to enhance the nanofluids thermal conductivity, which it matches perfectly with the features importance to the XGBOOST, which considered that the thermal conductivity of base fluid has the major contribution on the thermal conductivity of nanofluids, while for LGBM come on the second stage of importance.

Maheshwary, et al. (2017) studied the impact of nanoparticle concentration, size, and shape (cubic, rod, and spherical) on the thermal conductivity of TiO_2/water nanofluids. The analysis demonstrate that the greatest influence is for the nanoparticles concentration, while the size contribute for around 25% and the shape plays a minor role in the thermal conductivity enhancement. Signifying that the aforementioned parameters have a various levels of impact on the thermal conductivity of TiO_2/water nanofluids, which deal with the results of the features importance for LGBM.

Patel, et al. (2010) investigated in an experimental study the thermal conductivity of metallic and oxide nanoparticles suspended in different base fluids. They reported that Cu, Al, Al_2O_3, and CuO have 383, 204, 27, and 18 (W/m.K) thermal conductivity values. The nanofluid of Cu/water (at 20°C, 80 nm, K_{bf} = 0.5984 (W/m.K), spherical, and 0.5% concentration) have a 7% thermal conductivity enhancement, while the Al/water nanofluid at the same conditions have a 5% enhancement. Also, the thermal conductivity enhancement of Al_2O_3/water studied for 3 sizes; 11 nm, 45 nm, and 150 nm (at 20°C, K_{bf} = 0.5984 (W/m.K), spherical, and 0.5% concentration) were 6%, 2%, and 1.5%, respectively. Meaning that, the thermal conductivity and the size of nanoparticles play a relatively important role in the enhancement of nanofluids thermal conductivity.

Furthermore, the effect of nanoparticles concentration has been studied by Ranjbarzadeh et al. (2019). They studied the stability and thermal conductivity of SiO_2/water nanofluid as a function of tempreature and concentration, and reported that by increasing the concentration of SiO_2 nanoparticles in the base fluid, the thermal conductivity of nanofluid increased. However, there are reported drawbacks for the increase of nanoparticles concentration in base fluid such increasing the nanofluid viscosity and the instability of the nanoparticle in the base fluid. These drawbacks make the concentration of nanopartcles not crucial factor.

Many studies claimed that the temperature of nanofluids does not play a vital role in the thermal conductivity enhancement of nanofluids ((Hemmat Esfe et al., 2015a), (Hemmat Esfe, et al., 2015b), (Karimipour et al., 2018), (Afrand, et al. 2016b)). Hemmat Esfe et al. (2015a) concluded in their experimental study on MgO/water-ethylene glycol nanofluid thermal conductivity (as a function of nanoparticle concentration and temperature of nanofluid) that the temperature did not affect significantly the thermal conductivity at low concentration of nanoparticles. In other words, the effect of nanofluids temperature on the thermal conductivity enhancement can be neglected.

Conclusions

The main outcomes of this research showed that Combination.9 (size, temperature, concentration, thermal conductivity of base fluid, density, thermal conductivity of nanoparticle, shape) acts as the best combination for predicting the thermal conductivity of nanofluids under each of MLP, XGBOOST and LGBM models. Singularly, the RMSE value on the validation set for combination.9 is 0.0052 for MLP model, 0.011035 for LGBM model, and 0.00695 for the XGBOOST model. The results showed that those combinations which has greater number of features provides better performance than the other combinations with less features. Undoubtedly, MLP algorithm

provides the best performance on the validation set as compared to the other models followed by XGBOOST and LGBM that comes last. The feature importance analysis showed that the thermal conductivity for the base fluid is the most important feature.

Nomenclature

AARE	= Average Absolute Relative Error.	**[—]**
Al	= Aluminum.	**[—]**
Al_2O_3	= Alumina.	**[—]**
ANFIS	= Adaptive Neuro-Fuzzy Inference System.	**[—]**
ANN	= Artificial Neural Networks.	**[—]**
Comb.	= Combination.	**[—]**
Conce.	= Nanoparticle volume concentration.	**[%]**
Cu	= Copper.	**[—]**
CuO	= Copper Oxide.	**[—]**
Density	= Nanoparticle density	**[**Kg/m^3**]**
DTR	= Decision Tree Regression.	**[—]**
GBR	= Gradient Boosting Regression.	**[—]**
GMDH	= Group Method of Data Handling.	**[—]**
LGBM	= Light Gradient Boosting Machine.	**[—]**
LSSVM	= Least Square Support Vector Machine.	**[—]**
MAE	= Mean Absolute Error.	**[—]**
MgO	= Magnesium oxide.	**[—]**
MLP	= Multilayer Perceptron.	**[—]**
NF	= Nanofluid.	**[—]**
RBFNN	= Radial Basis Function Neural Networks.	**[—]**
ReLU	= Rectified Linear Unit.	**[—]**
RFR	= Random Forest Regression.	**[—]**
RMSE	= Root Mean Square Error.	**[—]**
RMSLE	= Root Mean Squared Logarithmic Error.	**[—]**
SiO_2	= Silicon Dioxide.	**[—]**
Size	= Nanoparticle size	**[**nm**]**
SSA	= Specific Surface Area.	**[**m^2/g**]**
SVR	= Support Vector Regression.	**[—]**
TC	= Thermal Conductivity.	**[**W/m.K**]**
tc_bf	= Thermal Conductivity of Base Fluid.	**[**W/m.K**]**
tc_p	= Thermal Conductivity of Nanoparticle.	**[**W/m.K**]**
Temp.	= Temperature of Nanofluid.	**[**K**]**
TiO_2	= Titanium Dioxide.	**[—]**
XGBOOST	= Extreme Gradient Boosting	**[—]**

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