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ARTICLE

Latent Heat Prediction of Nano Enhanced Phase Change Material by ANN Method

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ABSTRACT

Thermal characteristics of phase change material (PCM) are important in design and utilization of thermal energy storage or other applications. PCMs have great latent heat but suffer from low thermal conductivity. Then, in recent years, nano particles have been added to PCM to improve their thermophysical properties such as thermal conductivity. Effect of this nano particles on thermophysical properties of PCM has been a question and many experimental and numerical studies have been done to investigate them. Artificial intelligence-based approach can be a good candidate to predict thermophysical properties of nano enhance PCM (NEPCM). Then, in this study an artificial neural network (ANN) has been developed to predict the latent heat of the NEPCM. A comprehensive literature search was conducted to acquire thermal characteristics data from various NEPCM to train and test this artificial neural network model. Twenty different types of Nano particle and paraffin based PCMs were used in ANN development. The most important properties which are used as the input for the developed ANN model are NP size, density of NP, latent heat of PCM, density of PCM, concentration and latent heat of NEPCM in the range of 1–60 nm, 100–8960 kg/m^3, 89.69–311 kJ/kg, 760 to 1520 kg/m^3, 0.02–20 wt% and 60.72–338.6 kJ/kg, respectively. The output variable was latent heat of NEPCM. The result indicates that the ANN model can be applied to predict the latent heat of nano enhanced PCM satisfactory. The correlation coefficient of the created model was 0.97. This result shows ability of ANN to predict the latent heat of NEPCM.

KEYWORDS

NEPCM; ANN; latent heat; prediction

1 Introduction

Although energy producing technologies have improved, but they do not meet the global energy demands [1]. In addition, the percentage of fossil fuels as primary energy sources in the globe has remained persistently high at 85 percent. The use of these fossil fuels will contribute significantly to greenhouse gas emissions, resulting in global warming, severe weather events, sea level rise, and other long-term consequences [2]. Then, providing the renewable energy to fulfill energy demands of human being has become a crucial necessity in recent years [3]. Many studies have been conducted to find safe, inexpensive, and renewable energy sources [4]. It is stated that the solar energy can be a promising renewable source of energy to successfully fulfill thermal energy demand of society [5]. But inherent intermittent nature of the solar energy is a challenge which should be tackled [6]. The disadvantage of intermittent nature of solar energy can be mitigated using a thermal energy storage (TES) system [7].

The thermal energy storage systems can be classified as sensible heat, latent heat, and thermo-chemical heat TES [8]. Among them latent heat TES which use phase change materials (PCMs) to store thermal energy has been most popular TES for solar thermal energy in recent years [9]. PCMs are materials that absorb and release a significant amount of thermal energy during their phase change process [10]. PCMs have several benefits, including high TES density, a short working temperature range, and a modest volume change during the phase transition [11]. PCMs have been demonstrated to be useful in enhancing the thermal performance and energy efficiency of buildings in particular climatic zones. However, the properties of the PCM are considerably effective on the efficiency of developed TES [7].

PCMs are divided into three categories based on its material: organic, inorganic, and eutectic [1]. Organic materials offer strong thermal and chemical stability, as well as minimal undercooling and high heat of fusion and no corrosive properties. They are also accessible in a wide temperature range and have good compatibility with other components of TES [12]. On the other hand, they have poor thermal conductivity, a lower phase transition enthalpy, are flammable, and have a relatively substantial volume change [13]. Inorganic materials are those that do not contain carbon as one of its constituent elements, and their characteristics include high thermal conductivity, larger phase transition enthalpy, low volume change, and low cost in comparison to others [14]. Inorganic materials, on the other hand, have the drawbacks of undercooling and corrosion, as well as a lack of thermal stability [15]. Eutectic PCMs are the result of different PCMs combination and categorized as organic-organic, organic inorganic and inorganic-inorganic PCMs [16]. The eutectic PCMs have a large volumetric thermal storage density as well as a sharp melting point. However, like other PCMs, eutectic PCMs have certain drawbacks such as low thermal conductivity and corrosion at high temperatures [17].

The main challenge with application of PCM based TES is their low thermal conductivity [18]. Then, various method has been studied to improve the thermal conductivity of PCMs. One of this method which has been popular in designing of TES is developing nano enhanced PCMs [19]. NEPCM which is a mixture of PCM and nanoparticles are introduced to improve thermophysical properties of PCMs. The thermal conductivity of nanoparticles is significantly higher than PCM and it is proved that adding nanoparticles to PCM can increase thermal conductivity of PCM which is then called NEPCM [20]. The high value of latent heat for PCM makes them a suitable candidate for TES but low thermal conductivity of these materials has forced scientists to use NEPCM. Although some researchers found that the presence of nanoparticles reduces the latent heat of PCM, there are others that state the presence of an optimal particle loading will increase the latent heat [21].

The thermophysical properties of the developed NEPCMs from different PCM and nano particles has been a question for scientists [22,23]. Then, numerous studies have been conducted to find these properties for various NEPCMs. The results of these studies showed that the thermophysical properties of NEPCMs is different from each other and for each PCM and nano particle should be investigated individually [24]. This means innumerable studies are required to find thermophysical properties for most of the NEPCMs. Moreover, these get harder when it reveals that different loading value or percentage of nano particle is also an effective parameter on the thermophysical properties of developed NEPCM [25]. Therefore, scientists utilized numerical methods to predict the thermophysical properties of NEPCM [7]. Although, the numerical models are useful in prediction of the thermophysical properties of NEPCM, there is some limitation for these models. First, most of the numerical models are valid only for liquid phase of NEPCM, secondly, they includes too many terms and the information about many parameters is required in the model [7]. Then, artificial intelligence (AI) based models were introduced as appropriate approach to predict the thermophysical properties of NEPCM [26].

In AI based models, some of the properties of PCM and nano particle are used to predict some of the thermophysical properties of NEPCM [27]. The NEPCMs are classified as nano fluid in most of the literature however these materials experience a phase change process and are not utilized in liquid phase only. Nevertheless, there is many AI based models for nanofluid but they are not valid for NEPCMs and just few studies can be found in the literature for modeling of NEPCM by AI models. For instance, artificial neural network which is the base of AI is used to predict the thermal conductivity and viscosity of nano encapsulated PCM slurry [27]. They used temperature of the NEPCM and the nano particle concentration as the predictor in their model.

Based on the literature review, there is not any AI based study to predict the latent heat of paraffin based NEPCM. Then, the aim of this study is prediction of the latent heat of NEPCM with various concentration and type of nano particles for paraffin based NEPCM. An ANN model has been developed for 20 different types of nano particles (Graphene, expanded graphite, TiO_2, Fe_3O_4, CUO, ZnO, SiO_2, Graphite, CNF, GNP, MWCNT, Al_2O_3, CB, Si_3N_4, NG, GN, Ag, magnetite, xGnP, CNT) mixed with Paraffin as PCM. Data are collected from literature to develop ANN model. Finally, the performance of the model will be evaluated by correlation of determination of the model.

2 Methodology

2.1 Data Collection

The important considerations for training of a reliable and general ANN model is the quantity and quality of the data [28]. Then, a comprehensive literature review has been conducted by the authors of the current study to find appropriate data for ANN model. Based on this literature review, appropriate data to develop the ANN model were extracted from different studies (Table 1) and totally 196 samples were collected. The concentration of the NP in NEPCM is introduced as important factor on the latent heat of NEPCM. Then, the concentration of the NP for various studies which have been used for data collection is shown in the Table 2. As it can be seen in this table, different types of the NPs with different concentration have been found in the literature and have been used in this study.

Table 1: The range of the extracted data for different properties of NPs, PCMs and NEPCMs

Property	Unit	Min	Max
NP size	nm	1	60
Density of NP	(kg/m^3)	100	8960
Latent heat of PCM	(kJ/kg)	89.69	311
Density of PCM	(kg/m^3)	760	1520
Concentration	wt%	0.02	20
Latent heat of NEPCM	(kJ/kg)	60.72	338.6

The other important factor on the effect of the PCM to develop NEPCM is the latent heat of the PCM. Mixing NP with PCM will change latent heat of the PCM and the result will be latent heat of NEPCM [29]. Then, obviously the latent heat of the NEPCM is a crucial property to predict the latent heat of NEPCM. The latent heat of PCMs which have been used in this study to develop ANN model are presented in the Table 3. As it can be seen in this table, all of the data which have been collected are for different types of Paraffin. In addition, the source for this data are mentioned in the tables.

Table 2: Properties of the NPs which used to develop ANN model

NP type	Concentration range (wt%)	Reference
Graphene	0, 0.10, 0.15, 0.20, 0.30	[30]
Expanded graphite	2, 4, 7, 10	[31]
TiO_2	0, 0.1, 0.3, 0.5, 0.2, 3	[32]
CuO	5, 0.1, 0, 0.2, 0.3	[33]
SiO_2	0, 0.5, 1, 2	[33]
Graphite	5, 7.5, 10, 2.5	[33]
GNP	2, 5	[34]
MWCNT	0, 0, 1, 0, 5, 1, 2, 10	[34]
Al_2O_3	1, 0, 2, 4, 6	[35]
Si_3N_4	0, 1, 2, 3, 4, 5, 10	[36]
NG	0.02, 0.06, 0.1	[37]
GN	0, 0.1, 0.5, 1, 2, 3, 4, 5	[38]
Ag	0, 0.1, 0.5, 1, 2, 3, 5	[38]
Magnetite	0, 10, 20	[39]
xGnP	0, 1, 4, 5	[40]
CNT	0, 1, 3, 5	[40]

Table 3: Properties of the paraffine PCM which used develop ANN model

PCM type	Latent heat (kJ/kg)	Reference
RT 22 HC	168.99	[30]
PARAFFIN	194.6	[31]
PARAFFIN	137	[32]
PARAFFIN	207.22	[33]
PARAFFIN	119.3	[34]
RT20	117.78	[41]
RT25	133.52	[41]
PARAFFIN	209.33	[35]
PARAFFIN	143.8	[37]
PARAFFIN	188	[36]
RT20	184.181	[38]
RT22 HC	169.02	[38]
PARAFFIN	134.9	[39]
PARAFFIN	165.6	[39]

2.2 ANN Model Development

Based on the conducted literature review, size (nm), density (kg/m^3) and concentration of nano particle (wt%) and density (kg/m^3) and latent heat of PCM (kJ/kg), phase change process (solidification or melting) were selected as the input for the developed ANN model. The MATLAB software was used to develop ANN model. The ability to understand intricate nonlinear correlations between dependent and independent parameters, the ability to detect all conceivable interactions between predictor variables, and the availability of multiple training datasets are all advantages of neural networks [28].

The ANN type which was used in this study is multilayer perceptron (MLP). This type of ANN is developed by interconnection of artificial neurons. The main important properties of MLP ANN neurons, layers, learning algorithm and transfer function [42]. Neuron is the main component of MLP which is basically an arrangement of these neurons in different layers. The working procedure for ANN is shown in the Fig. 1. In this figure the X_j is the jth input of the model and i represents the neurun number and W_{ij} is the weight f neurn from neuron j to I [43]. This conection of neuron in ANN can be written mathamtically as follows [44]:

$$f_i = \sum_{j=1}^{n} W_{ji} X_j \tag{1}$$

$$y_i = \varphi(u_i + b_i) = \varphi\left(\sum_{j=0}^{n} X_j W_{ij} + b_i\right) \tag{2}$$

where the y_i, φ and b_i represent the output, activation function and bias.

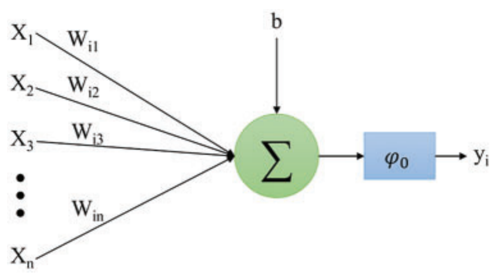

Figure 1: An artificial neuron structure

The activation function is an important component of the ANN which determine how the output of a neuron is transferred to the other neuron [45]. Then, generally for a three-layer ANN (input layer, hidden layer and output layer), there is two activation function, one form input to hidden layer and the other from hidden layer to output [46]. Different type of the activation function can be used in ANN but in this study three type of activation functions were used, namely, Pureline, Tansig and Logsig. These functions are as follows [47]:

$$Pureline(X) = X \tag{3}$$

$$Tansig(X) = \frac{2}{1 - e^{-2X}} - 1 \tag{4}$$

$$Logsig(X) = X \tag{5}$$

The minimum required layer for an MLP ANN is three layers [48]. Input layer which the number of the neuron in this layer is equal to the inputs of the model. Next layer is the hidden layer which contain hidden neurons and they called hidden neuron because their input and output is not shown [49]. Their inputs come from input layer and their output will be directed to output layer. Number of the neuron in hidden layer depends on the complexity of the problem. The last layer is the output layer which number of its neurons is same as the number of the outputs of the model [26]. More information about activation function and learning algorithm can be found in the [50,51]. The structure of the developed model is shown in the Fig. 2.

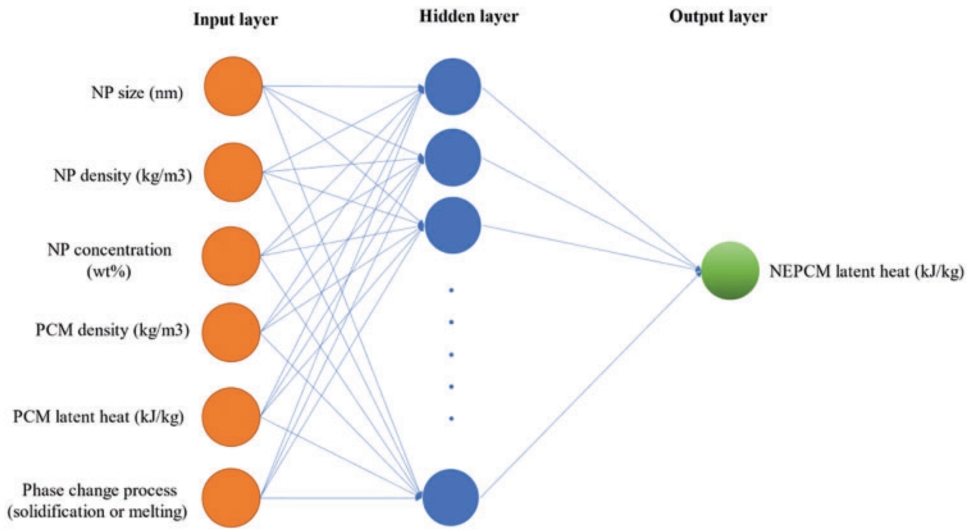

Figure 2: Schematic of developed ANN model

The training process of the ANN is shown in the Fig. 3 [52]. The minimum required mean squared error (MSE) (Eq. (9)) and the maximum epoch number are two important criteria which should be decided before training of the network [53]. MSE is a measure of the accuracy of the network and epoch is a training cycle which during that all the data have been introduced to the network. Basically, the training of ANN means determine the value of the weights and biases which predict the output of the network satisfactory [47]. This training process starts with selection of some random values for weights and biases of the network. Then, the values for outputs will be calculated based on the introduced values to the network for the inputs. Next, mean square error (MSE) for output of the network and experimental values which is also introduced to the model, will be calculated. This MSE will be calculated for all three data sets including train, validation, and test data sets [54].

The network is trained by training data set and validation data set is being used to prevent over-fitting of the network. The overfitting of the network means the neuron in the network will memorize the input-output relationship instead of learning that. Then, the validation data is introduced to the network, the data which network is not using for training or in other words the output is not shown to the network [28]. If the calculated MSE for train data is almost constant or even decreasing but the MSE of validation data is increasing, then overfitting is occurred and the performance of the network to predict test data will not improve anymore. Training of the network will continue until it reaches the minimum MSE, or maximum epoch or overfitting is detected. The test data will be used in the last step of the ANN training and the performance of the network should be evaluated by MSE and other statistical measures such as R-squared for test data [26].

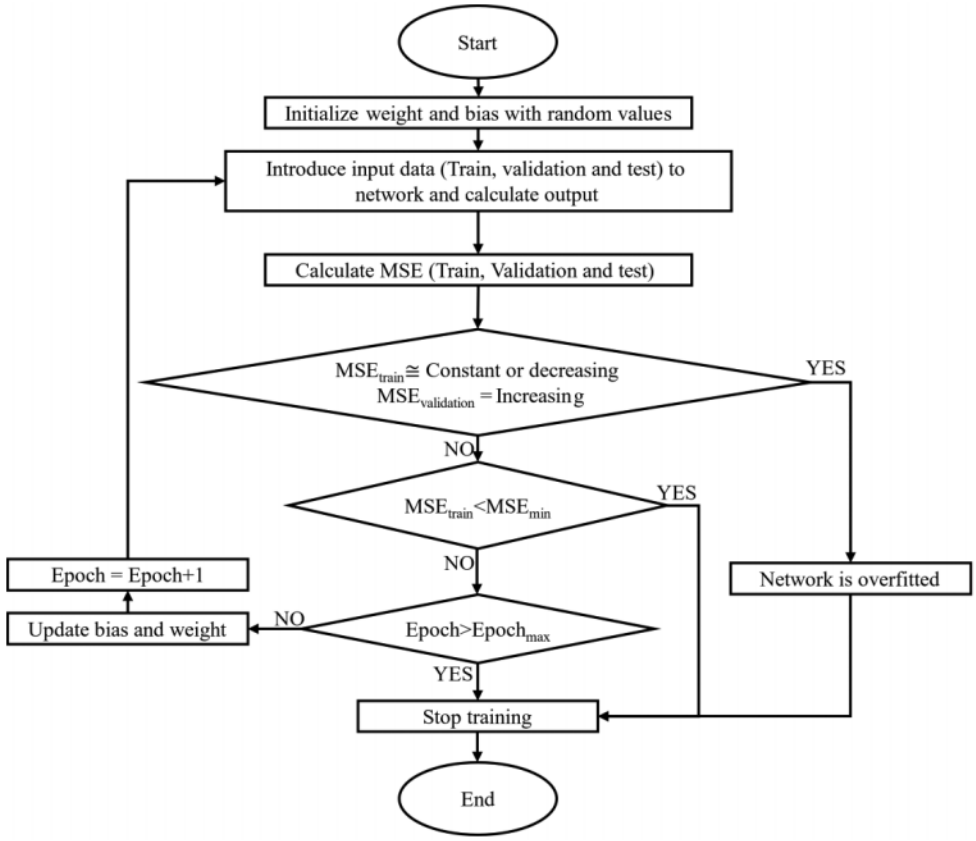

Figure 3: The training process of the ANN

The updating of the weight and biases in the ANN is based on a minimization of error process. This optimization process is carried out using learning algorithm. In other words, learning algorithm can be any optimization method for minimizing the error between the predicted and experimental data. The learning algorithm of the model in this study is Levenberg–Marquardt (LM) Feed forward which is a popular type of learning algorithm for ANN model development [55]. LM will modify the weight and biases to minimize the error function which is the MSE between predicted and experimental values. In this algorithm the θ is defined as follows [56]:

$$\theta = \{W_{ij}, b_j\} \tag{6}$$

$$\theta_{K+1} = \theta_K - (J_K^T J_K + \mu I)^{-1} J_K^T E_K \tag{7}$$

$$E_K = \sum_{j=1}^{N} (d_j - y_j)^2 \tag{8}$$

where d and y are predicted and experimental values, N is the number of samples, J is the error vector Jacobian matrix E_θ and J^T is its transpose, I represent the identity matrix with same dimension of Hessian matrix J^TJ, $J^TE(\theta)$ repress the error function E gradient respect to $\theta = \{W_{ij}, b_j\}$, the μ (initially equal to 0.001) which represents the damping factor is changed for each iteration to guide the optimization process. The adjustment factor β is used to justify the damping factor. Damping factor is increased or decreased by multiplication by adjustment factor or division to it, respectively. This rise and drop in the damping factor will be repeated until error decreases and then current epoch or iteration stop [57]. This process will be repeated for next epoch until one of the training stop criteria is reached, e.g., minimum MSE, maximum epoch and overfitting [58].

Two statistical parameters were used to evaluate performance of the ANN model. Mean squared error (MSE) and R (correlation coefficient). These two are given as follows:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_t - y_o)^2 \tag{9}$$

$$R = \sqrt{1 - \frac{\sum_{i=1}^{n}(y_t - y_o)^2}{\sum_{i=1}^{n}(y_t - \bar{y}_t)^2}} \tag{10}$$

where y_t, y_o, $\bar{y}_t$ and n are target value, predicted value, average of target value and number of samples, respectively [44].

3 Results and Discussion

Different structure for MLP ANN were tested and finally the model with 10 neurons in hidden layer was selected as the appropriate model for prediction of NEPCM latent heat. The change in the number of neurons in hidden layer has not changed the performance of the model. Same results is stated for ANN prediction of thermal conductivity prediction for CuO–water/EG nanofluid [43]. Performance of the model need to be checked during training to make verify learning process of the model [49]. The training performance for the model was evaluated by MSE of the model for different data sets and in different epochs. As it can be seen in the Fig. 4, as the number of the epochs is increased, MSE of the model for all the data set is reduced until epoch number 21. In this epoch, MSE of the model for validation and test data starts to rise. This means the model at this epoch starts to overfitting and learning process is stopped after epoch 21. This is one criterion for stop of the learning process of the model as well. After this epoch, however the MSE of the model for training data set may become lower but it is due to overfitting and not increase in the network performance.

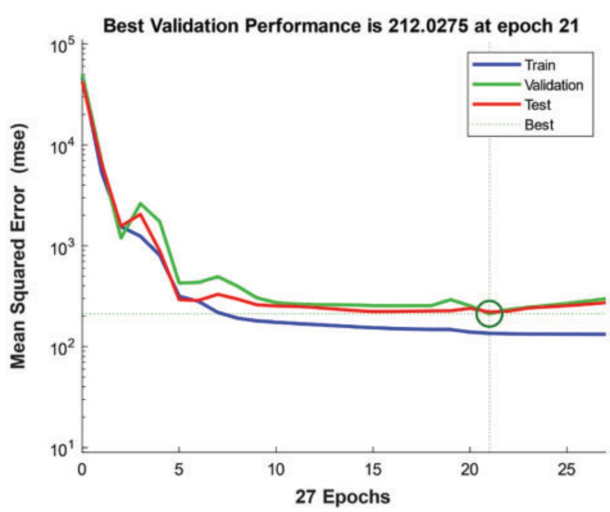

Figure 4: Model performance evaluation in different epochs

It should be noticed that the model performance must be checked for unseen data (test and validation) and not the training data [59]. Although overfitting of the model is undoubtedly important, the underfitting of the model should not be overlooked as well [60]. The curve for test data in the Fig. 4 shows the underfitting is not occurred at selected epoch based on overfitting criteria. This is clearer in the Fig. 5 which shows the R for test data is not far from the R value of training data set. It is normal that the R value for test data be lower than that for train or even validation data set [26]. This is due to: 1. The number of samples for training of the model is much higher than that for testing of the model (70% for train and 15% for test data); 2. The weight and biases are updated in each iteration to increase the performance for prediction of the output of training data set not test dataset [61].

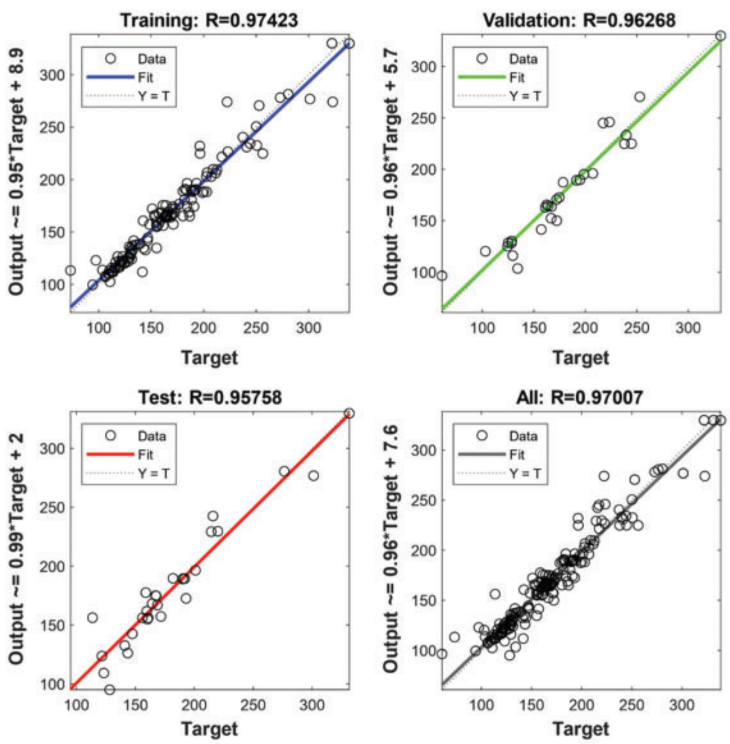

Figure 5: ANN modelling regression

The corelation coefficient of the developed model for different data sets are shown in the Fig. 5. As it can be seen in this figure, R for all the data set is higher than 0.95 which is quite satisfactory. The high value of R for training data set shows provided data have been successfully used by model for training [44,49]. Moreover, validation of the model has been done successfully which show the model has not memorized the input and output relation and it has learnt this relationship [45]. Finally, the high value of R for test data (0.96) implies the ability and generalization of the model to predict the latent heat of NEPCM [62]. The MSE of training, validation and test data were 370.44, 272.66 and 170.21, respectively. However, there is not any optimum value for MSE in different ANN modeling studies but the lower MSE is more desirable [47]. The MSE in this study can be improved by removing of some of the data which seems to be outliar but the generality of the model will be lower. This is always a challenge to find a trade-off between genrality and accuracy of the model [62]. Then, in this study it has been tried to keep the generality of the model with small penalty in its accuracy. It should be noticed that only the latent heat of paraffin based NEPCM were used in this study to increase the accuracy of the model as well. This shows an ANN model for prediction of NEPCM latent from different type of PCM is more challenging and need significantly larger database.

The predicted (output) data and target (experimental) data for all the data points are shown in the Fig. 6. As it can be seen the model has predicted most of the data point closely. The trends and each data point of the predicted data is approximately same as the trends and values for target data however this is not an unexpected result. High value of R already has approved the ability of the developed model for prediction of the latent heat of the NEPCM. This shows how much is the capability of the ANN model to predict the latent heat of NEPCM [51]. As it can be seen in the Fig. 6, the performance of the model in prediction of NEPCM latent heat for high and low is weaker than that for medium (150 to 250 KJ/Kg). This is due to this fact that the ANN model is extremely dependent on the number of provide samples [63]. The performance of the model can be improved by preparing more sample from experimental study.

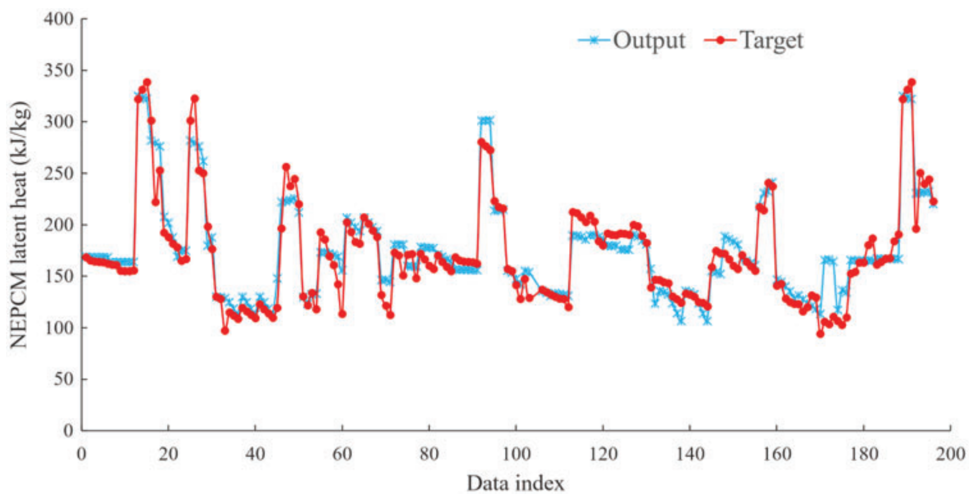

Figure 6: The output of model and target data

4 Conclusions

In this study an ANN model has been developed to predict latent heat of NEPCM and based on the results of the study following conclusions can be stated:

- The ANN can successfully be used to predict the latent heat of paraffin based NEPCM.
- The important properties which need to be used in the ANN model to predict the latent heat of NEPCM are size (nm), density (kg/m^3) and concentration of nano particle (wt%) and density (kg/m^3) and latent heat of PCM (kJ/kg), phase change process (solidification or melting).
- The reported latent heat in literature for different PCM or NEPCM is based on the different phase change process and result of this study reveals that the type of phase change process for latent should be included in the ANN model. Furthermore, all experiments for the measurement of the PCM or NEPCM latent heat should include the phase change process during this measurement.
- The reported properties for nano particles which are added to the PCM should be mentioned for any experimental NEPCM development.

- Although, the R for developed model was satisfactory (higher than 0.95), it can be improved by increasing of the amount of data for ANN modeling of NEPCM latent heat. Then, it is recommended that more experimental data be provided for ANN model in future.
- The model in this study is valid only for paraffin based NEPCM and similar model for other type of PCM can be developed.

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