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Specific Heat Capacity Extraction of Soybean Oil/MXene Nanofluids Using Optimized Long Short-Term Memory

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ABSTRACT Researchers are turning to nanofluids in PV/T hybrid systems for enhanced efficiency due to nanoparticle dispersion, improving thermal and optical properties over conventional fluids. Three different concentrations of formulated soybean oil based MXene nanofluids are considered 0.025, 0.075 and 0.125 wt.%. Maximum specific heat capacity nanofluids (c_{pNF}) augmentation is 24.49% at 0.125 wt.% loading of Ti_3C_2 in the base oil. The calculation of the c_{pNF} based on the temperature and nanoflakes concentration is very expensive and time-consuming as it should be calculated via the practical test investigation. This study employs a long short-term memory (LSTM) as an efficient machine learning method to extract the surrogate model for calculating the c_{pNF} based on the temperature and nanoflakes concentration. In addition, a couple of other machines learning methods, including support vector regression (SVR), group method of data handling (GMDH), and multi-layer perceptron (MLP), are developed to prove the higher efficiency of the recently proposed LSTM model in the calculation of the c_{pNF} . In addition, the Bayesian optimization technique is employed to calculate the optimal hyperparameters of the developed SVR, GMDH, MLP and LSTM to reach the highest efficiency of the system in predicting the c_{pNF} based on temperature and nanoflakes concentration. Notably, 95% of the recorded data via differential scanning calorimetry (DSC) is used for training machine learning techniques. In comparison, 5% is used for testing and validation purposes of the developed algorithm. The newly proposed optimized SVR, GMDH, MLP, and LSTM are modelled in MATLAB software. The results show that the newly proposed optimized LSTM model can reduce the mean square error in calculating the c_{pNF} by 99%, 99% and 91% compared with SVM, GMDH and MLP, respectively. The proposed methodology can be used to calculate other thermophysical properties of nanofluids.

INDEX TERMS nanofluids, MXene, deep learning, machine learning, specific heat capacity, Bayesian optimization

I. INTRODUCTION

In recent numerical/experimental studies, researchers are attracted to exploring innovative techniques to further efficiency enhancement of PV/T hybrid systems using nanofluid (NF) as a coolant instead of conventional

working fluids since conventional fluids usually suffer from poor thermal and optical characteristics that limit the efficiency of PV/T [1, 2]. NFs are advanced heat transfer fluids with superior thermo-physical characteristics prepared by dispersing nano-sized solid particles (1–100

nm) into conventional pure base fluids such as water, mineral oils and a combination of different fluids or organic chemical fluids. NFs exhibit improved heat transfer characteristics due to advanced properties of nanoparticles dispersed in a base fluid, such as greater heat transfer coefficient, Brownian motion mechanism in colloidal mixture and surface charge of the nanoparticles [3, 4]. Besides, investigations have demonstrated that NFs convey significantly higher thermal conductivity because dispersed nano-sized particles cause a larger surface area than base fluids [5, 6]. Due to the advanced properties of NFs, they are being extensively implemented in solar-based energy conversion systems [7]. The impact of NFs on non-concentrating and concentrating solar collectors has exhibited remarkable augmentation inefficiency of the systems [8].

Nanoparticles, including carbon nanotubes and 2D graphene materials, significantly impact nanofluids' thermal properties [9, 10]. These two-dimensional materials possess exceptional thermal, optical, and electrical characteristics, garnering extensive research attention [11]. In 2011, Drexel University researchers unveiled MXenes, a family of 2D materials comprising carbonitrides, transition metal carbides, and nitrides [12]. MXenes exhibits outstanding thermoelectric, optical, magnetic, and adsorption properties and robust mechanical strength. MXenes are derived from the $Mn+1AX_n$ phase through selective 'A' layer etching, offering diverse applications due to their remarkable chemical and mechanical attributes. Recent studies have explored MXene (Ti_3C_2) particles, revealing significant improvements in energy storage and thermal conductivity [13]. However, their utilization in hybrid PV/T solar systems as nanofluids remains unexplored. Conventional base fluids in solar thermal processes pose environmental threats due to toxicity and non-biodegradability. Researchers are increasingly focusing on alternative, eco-friendly base fluids, such as vegetable oils, known for their non-polluting properties [14]. Various oil-based nanofluids, including thermal, transformer, turbine, and synthetic oil, have been extensively studied [15]. In addition, neural network-based models have been proposed for optimizing solar thermal fluid transfer systems, demonstrating their reliability [16]. Soybean oil, known for its superior heat transfer capacity, wide availability, non-toxicity, and biodegradability, stands out as an effective additive in PV/T solar collectors [17]. Wang *et al.* [18] demonstrated the enhancement of photothermal conversion efficiency (63.35%) of MXene nanofluids, outperforming graphene nanofluids, optimizing the working conditions of direct absorption solar collectors. These findings emphasize the need for continued research in this domain.

c_{pNF} has contradictory results stated in several research articles. However, literature reports that c_{pNF} can be elevated considerably relative to base fluid due to distributed nanoparticles. Hu *et al.* [19] showed that the c_p of salt-based SiO_2 increases at low particle loading (< 1 wt.%) and begins

to decrease at high concentrations. The analogous study conducted by Rodríguez-Laguna *et al.* [20] revealed 18% augmentation in c_p of graphene NF. They attributed the mechanism to negligible flake thickness, nano-layering across the flakes and emerging thermal resistance in the dispersion. Sonawane *et al.* [21] revealed some exciting findings about ATF (aviation turbine fluid) based Al_2O_3 NF. They measured the specific heat of 0.1 vol% of Al_2O_3 , less than pure fluid. However, for higher volume concentrations (0.3 vol% and 0.5 vol%), the c_p was higher than the parent fluid, and for 1 vol% of Al_2O_3 , it again decreased. These results indicate uncertainty of specific heat capacity (c_p) with low to high particle loading.

The idea of machine learning has been implemented in many areas to imitate the complicated plant model, which cannot be modelled using a classical mathematical model [22, 23]. It helps researchers reduce the number of trials in extracting the thermophysical properties of the NFs. The idea of machine learning is to develop a model using the limited experimental dataset to calculate the thermophysical properties of the NFs [24]. Several researchers have used Machine learning methods in NFs to estimate c_{pNF} . Alade *et al.* [25, 26] used a support vector machine (SVR) to estimate the c_{pNF} of metallic oxides/ethylene glycol using temperature (K), c_p of ethylene glycol (J/K.g), the c_p of nanoparticles (J/K.g) and volume fraction of the nanoparticles (wt.%). Their proposed SVR prediction model was one of the pioneer machine learning-based models in estimating the c_{pNF} . They used the Bayesian optimization technique to choose the optimal hyperparameters of the SVR prediction model. Later, Alade *et al.* [27] proposed another SVR prediction model using the volume fraction of the nanoparticles (wt.%) and the c_p of nanoparticles (J/K.g). It should be noted that the simplification (usage of 2 inputs instead of 4 inputs) and usage of a meta-heuristic algorithm for optimization instead of global optimization (genetic algorithm (GA) instead of Bayesian optimization method) is the main differences between their proposed method [27] in comparison with previous method [25, 26]. Hassan and Banerjee [28] employed a multi-layer perceptron (MLP) for the estimation of the c_{pNF} of molten salt-based using temperature ($^{\circ}C$), the mass fraction (wt.%), the specific heat of nanoparticles (J/K.g), and average diameter of nanoparticles (nm) as inputs of the prediction model. Jafari and Fatemi [29] estimate the c_{pNF} of nitride-based using the Monte Carlo method with consideration of nanoparticle sizes (nm), temperature ($^{\circ}C$) and a Mass fraction (wt.%). Alade *et al.* [30] predicted the isobaric c_{pNF} of nitrides/ethylene glycol-based with consideration molar mass of the nanoparticles (g/mol), size of the nanoparticles (nm), the temperature ($^{\circ}K$), and mass fraction of nanoparticles (wt.%) as inputs of the system. Alade *et al.* [31] used SVR and MLP for c_{pNF} of copper oxide prediction with consideration of temperature ($^{\circ}K$), volume fraction (wt.%) and specific heat of nanoparticles (J/K.g) as input vector of the system. They found that the machine

learning method (MLP) is able to reach more accurate results compared to a classical method (SVR). Jamei *et al.* [32] developed the hybrid model with a combination of Gaussian process regression and Radial basis function network to reach a higher accuracy in predicting c_{pNF} based on temperature ($^{\circ}\text{K}$), solid volume fraction (wt.%), mean diameter of nanoparticle (nm) and c_p of nanoparticles (J/K.g). Their proposed method [32] shows higher accuracy in the prediction of c_{pNF} in comparison with random forest (RF) as the suitable candidate for the classical method. Later, Jamei *et al.* [33] investigated the estimation of c_{pNF} of molten salt-based using two novel ensemble machine learning methods, including extra tree regression and AdaBoost regression. These two models are validated using RF and a boosted regression tree. It should be noted that the inputs of the proposed algorithms are solid mass fraction (wt.%), temperature ($^{\circ}\text{K}$), c_p of base fluid, mean diameter (nm), and density of nanoparticle (ρ). Adun *et al.* [34] investigated the influences of volume concentration (wt.%), mixture ratio and temperature ($^{\circ}\text{K}$) on the c_{pNF} of $\text{Fe}_3\text{O}_4\text{-Al}_2\text{O}_3\text{-ZnO}$ /water ternary hybrid synthesis. They [34] proposed the Hybrid machine learning-based prediction model to calculate the c_{pNF} based on pre-investigated parameters. Their proposed method is the combination of GA and SVR as well as MLP. Their proposed GA-based SVR prediction model beat the MLP in calculating c_{pNF} with higher accuracy than the MLP prediction model. Assad *et al.* [35] reviewed the influence of different parameters in c_{pNF} . They found that properties of solid structures, concentration (wt.%) and temperature have the considerable influence in c_{pNF} [35]. Zobeiry *et al.* [36] used MLP to solve the heat transfer equation in engineering applications and advanced manufacturing. They validated their extracted results for one- or two-dimensional case of a heat transfer partial differential equation by finite element models. Recently, reinforcement learning is used by Wang *et al.* [37] in order to control the heat transfer parameters of the indirect-contact heat exchangers. Their proposed method shows the higher efficiency in the existence of higher disturbances.

In order to eliminate the time-consuming and expensive practical extraction of the thermophysical properties of the soybean oil/MXene NFs, machine learning methods are used to calculate the requested outcomes. However, the above-reviewed literature [25-37] shows a lack of comprehensive investigation to extract the most efficient method for calculating the thermophysical properties of soybean oil/MXene nanofluids. This study aims to develop a methodology to extract the efficient machine learning method to calculate the c_{pNF} based on the temperature and nanoflakes concentration. In detail, the research gaps and contributions can be categorized as follows:

- For research gaps:
 - 1) Limited exploration of advanced machine learning techniques, such as LSTM, for predicting the c_{pNF} .

- 2) Lack of clarity on which machine learning method is currently the most effective for c_{pNF} prediction.
- 3) Insufficient information on the impact and effectiveness of Bayesian optimization in improving the performance of c_{pNF} prediction models.
- 4) Lack of quantification regarding time and cost savings is achieved by eliminating practical tests for the determination of thermophysical properties.
- For research contributions:
 - 1) Introduction of advanced machine learning methods, including SVR, MLP, GMDH, and LSTM, for estimating c_{pNF} based on temperature and nanoflakes concentration.
 - 2) Utilization of Bayesian optimization to enhance the performance of machine learning models.
 - 3) Elimination of the need for time-consuming and expensive practical tests in determining thermophysical properties of soybean oil/MXene nanofluids.

It should be noted that the Bayesian optimization method, as one of the most efficient global optimization methods with higher accuracy and lower computational load, is employed in this study to calculate the hyperparameters of the proposed machine learning techniques to increase the model's performance [38, 39].

In the next Section, the design of the experiment from producing soybean oil/MXene NFs until the extraction of the dataset is explained. Section III explained the proposed methodology of this study, including the investigation of the investigated and newly proposed machine learning methods with a combination of Bayesian optimization. MATLAB software verifies and validates the investigated methods in Section IV. The most remarkable outcomes are explained, and the consequence is concluded in Section V.

II. Materials and Experiments

The thermophysical properties of the NF are composed of viscosity, thermal conductivity, c_p , and thermal diffusivity. It is not hard to exaggerate the importance of thermal conductivity compared to other thermophysical properties. In total, 95% of studies are based on investigating thermal conductivity NFs because of the importance of these thermophysical properties. In addition, the c_{pNF} received less attention than the other 5% of thermophysical properties investigation of the NF. Despite this, the investigation of the c_{pNF} is essential for calculating the solar collector's performance. In addition, understanding the c_{pNF} is the key to calculating the heat transfer rate between different fluids. Due to good heat transfer properties, Soybean oil (Sigma Aldrich, USA) is selected as the base fluid. Soybean oil is a vegetable oil with a chemical composition of long-carbon chained triglycerides and several lipids.

A. Preparation of $\text{SO}/\text{Ti}_3\text{C}_2$ nanofluids

Our previous research used the MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) synthesis process [40]. A two-step technique is applied to synthesize Soybean oil-based Ti_3C_2 NF, considering this method is convenient for large-scale production and most economical. However, stability is a major challenge in formulating NF in this method. Firstly, synthesized Ti_3C_2 powder was dispersed to the base Soybean oil at three different weight fractions ranging from 0.025 to 0.125 wt.%. After adding Ti_3C_2 , two stabilization techniques were used to develop stable NF. Firstly, NF samples were stirred for 30 min at 700 rpm by a magnetic stirrer and concurrently heated at 70 °C temperature to make the mixture homogenous into the base fluid. The sonication process was conducted for 30 min using an ultrasonic probe sonicator (FS-1200N) to agitate the intermolecular forces between Ti_3C_2 nanomaterials and disperse them uniformly.

B. Characterization

The c_p measurement of the developed soybean oil-based MXene nanofluids is processed using differential scanning calorimetry (DSC), DSC-1000/C (Linseis, Germany) [40]. According to our research study [40], the acquired experimental results exhibited good accuracy by the provided results by the supplier. In addition, a uniform measurement process was another advantage of ensuring the precision of the measure c_p results.

III. Methodology

This paper aims to predict the c_{pNF} of the soybean oil/MXene NF based on temperature and nanoflakes concentration. The employed data in machine learning methods is obtained via a DSC for 0.025, 0.075 and 0.125 (wt.%) of soybean oil/MXene NF. High-advanced machine learning methods, including SVR, GMDH, MLP and LSTM, are employed in predicting c_{pNF} . Then, it is worth mentioning that this work is the first to use a comprehensive machine learning study to calculate the NF's c_{pNF} . The reason for using highly advanced machine learning such as LSTM is the highly nonlinear behavior of the c_{pNF} behavior of the soybean oil/MXene NF based on the temperature and nanoflakes concentration. The high power of the LSTM because of the existence of memory cells inside the structure of this network is the main reason for achieving the task compared with other machine learning methods such as SVR, GMDH and MLP.

Figure 1 shows the schematic structure of the proposed method in this study, from the production of the soybean oil/MXene NF to the calculation of the c_{pNF} . The proposed method started with producing the NF using pure, 0.025, 0.075 and 0.125 (wt.%) concentrations. Then, the produced materials are tested via a DSC, and the dataset is saved using .csv format. The recorded dataset is employed in a pre-processing block to eliminate the out-of-range data, normalized and divided to train and test datasets. The Bayesian optimization method calculates the optimal indexes of the four investigated machine learning techniques. The

validation process halts training when the validation error rate on a non-training subset increases continuously for more than 6 epochs to prevent overfitting. After extracting the optimal indexes of the proposed machine learning techniques, the final models, which are known as Opt-SVR, Opt-GMDH, Opt-MLP and Opt-LSTM, are compared with each other using the extracted dataset to extract the most accurate model among the four investigated machine learning methods.

A. Datasets

Figure 2 represents the c_{pNF} of SO/ Ti_3C_2 NF at different particle loading of Ti_3C_2 nanoparticles. Results show that c_{pNF} of the NF improves with the increment of weight fraction of Ti_3C_2 particles and evaluated temperatures from 25 to 80 °C. The uncertainty measurement of c_{pNF} in the present investigation is approximately 2.5% for the working temperature range. c_{pNF} exhibited significant enhancement with the addition of Ti_3C_2 particles. The achieved data reveals that the maximum c_{pNF} increment is found to be approximately 24.49% for 0.125 (wt.%) ($c_{pNF} = 2.06$ J/g K) compared to Soybean oil ($c_{pNF} = 1.65$ J/g K) at 25 °C. The higher heat absorption capacity of two-dimensional Ti_3C_2 particles and interface attractions in surface area between pure Soybean oil and MXene atoms are attributed to the cause of c_{pNF} augmentation of the NF. The formed interaction between these molecules and the homogenous dispersion of nanoflakes in the pure oil can cause improved c_{pNF} of SO/ Ti_3C_2 NF. At elevated temperature, particles tend to store more energy as extra heat leads to vibrational energy and enhances the average energy of the molecules. For negligible surface thickness (< 10 nm) of 2D materials, c_{pNF} of the NFs can be enhanced due to emerging phonon modes (Rodríguez-Laguna *et al.*, 2018). The results suggest the prominent heat storage capability of SO/ Ti_3C_2 NF. Therefore, it can be stated that developed NF can be a potential substitution for conventional fluids in the PV/T system to improve the overall c_{pNF} of the system. In addition, Table 1 summarizes the extracted datasets from the above-explained experimental study to clarify the understanding of the input parameters (including Temperature °C and wt.%) and output parameter (c_{pNF}). However, we should mention that the actual dataset is consists of 3348 different Temperature (°C) for each concentration, including pure, 0.025, 0.075, and 0.125 Cp (J/(g K)). Then, it can be concluded that the training/validation/testing dataset is 13,392.

B. Pre-Tuning of Algorithm

The pre-processing of the dataset is utilized to reduce the system's complexity during the training process of the network to reach higher accuracy. It starts with eliminating the out-of-range data because these data dramatically decrease the accuracy of the network. The main source of these data is the fault in measuring systems. Normalization $\mathbf{n}_{x_i}$ and standardization σ_{x_i} can be used to allocate the mean

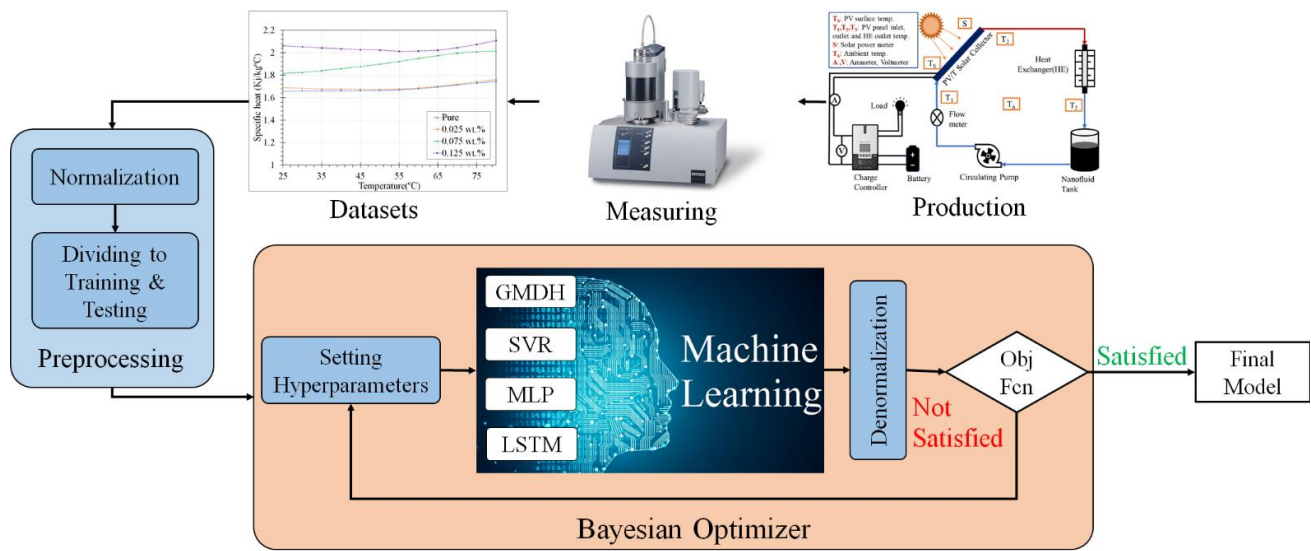


FIGURE 1. The graphical representation of the proposed method in this study from producing the NFs until the evaluation of the investigated machine learning methods.

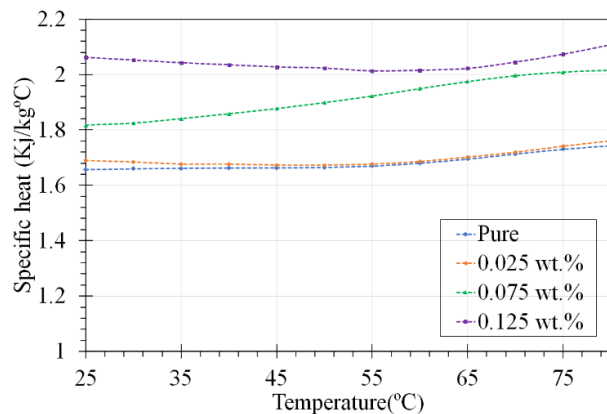


FIGURE 2. c_p variation of Soybean oil and SO/Ti₃C₂ NFs at increasing temperature.

TABLE 1
THE SAMPLE OF THE EXTRACTED DATASET FROM THE EXPERIMENTAL STUDY INCLUDES INPUTS (TEMPERATURE °C AND WT.%) AND OUTPUT (C_{PNF}).

TEMP (°C)	C_p (J/(G K))			
	PURE	0.025 WT.%	0.075 WT.%	0.125 WT.%
25	1.656833	1.689561	1.81698	2.061926
30	1.659902	1.684547	1.824393	2.052467
35	1.661488	1.677129	1.840338	2.04233
40	1.662575	1.677094	1.858106	2.035072
45	1.663308	1.673066	1.876944	2.027286
50	1.665074	1.673056	1.898761	2.022955
55	1.669391	1.676841	1.922448	2.012461
60	1.68013	1.686066	1.949505	2.015223
65	1.694943	1.702049	1.974919	2.02169
70	1.713314	1.719549	1.996323	2.044691
75	1.73043	1.741267	2.009633	2.073444
80	1.74357	1.760389	2.016403	2.108299

and std of the dataset in the rational range and decrease the system's complexity for the network. It has been calculated as follows:

$$n_{x_i} = \frac{x_i - \underline{x}}{\bar{x} - \underline{x}} \quad (1)$$

$$\sigma_{x_i} = \frac{x_i - \bar{x}}{\sigma_x} \quad (2)$$

where $\underline{x}$, $\bar{x}$ and $\tilde{x}$ are the minimum, maximum, and mean values of the dataset. Also, x_i , n_{x_i} and σ_{x_i} are i th raw, normalized, and standardized data. It should be noted that the normalization/standardization process is implemented for input and output data separately. The final step of the data pre-processing is dividing data into training and testing samples.

C. Group Method of Data Handling

GMDH, introduced by Ivakhnenko [41], is a modelling method for complex nonlinear systems. It selects, combines, and generates neurons to adapt to system complexity without relying on a precise physical model, making it a valuable tool for modelling and prediction tasks.

The methodology of GMDH revolves around selecting essential neurons in a network to minimize prediction errors and extract an ideal neural structure. This process includes continuously choosing, combining, and generating new neurons until a new generation fails to outperform the previous ones. GMDH adapts to the complexity of nonlinear systems through the regeneration of filtered neurons, their combination, and the extraction of next-layer neurons. This

iterative process continues until the best model is obtained. Regarding mathematical representation, GMDH employs Volterra-Kolmogorov-Gabor (VKG) polynomial components in a self-organized network. This network captures relationships between inputs and outputs through polynomial terms, with coefficients determined during the modelling process.

GMDH consists of multiple neural layers, with each neuron having two inputs and one output. The Ivakhnenko polynomial calculates the neuron outputs, effectively modelling the relationships between input variables.

D. Support Vector Regression

SVR, introduced by Cortes and Vapnik [42], is a powerful technique for handling linear and nonlinear time-series data. It seeks an optimal hyperplane with strong generalization capabilities, making it particularly useful in financial applications and other fields. The method minimizes a specific function with constraints and utilizes a mapping function to handle nonlinear data effectively. SVR aims to find an optimal decision hyperplane that maximizes the margins between two sample classes, demonstrating strong generalization ability. It is well-suited for small-sized and nonlinear datasets and finds use in various fields, including approximation.

In SVR, data is typically represented as a set of pairs (x, T) , where x represents attributes and T represents labels for linear functions. The regression function in SVR is expressed as $f(x) = \langle w|x \rangle + b$. The goal of SVR is to minimize a specific function $\Phi(w, \xi)$ that includes a regularization term and a term related to errors. This function is minimized concerning the support vector (w) and a cost parameter (C). Slack variables (ξ) are used to account for errors in predictions. SVR employs a loss function to reduce errors between the predicted and actual labels. In this context, the ϵ -insensitive loss function is commonly used. Solving the optimization problem in SVR involves constraints related to the ϵ -insensitive loss function, and it is typically done using Lagrange multipliers and the Karush-Kuhn-Tucker conditions. To handle nonlinear data, SVR employs a mapping function Ψ , which maps the data into a feature space, facilitating better regression.

E. Multi-Layer Perceptron

The Multi-layer Perceptron (MLP), initially introduced by Rosenblatt [43], is a learning network that employs backpropagation and features multiple hidden layers. Typically, MLP comprises three layers: hidden, input, and output. Nonlinear activation functions are utilized for all neurons, excluding those in the input layer. MLP is a versatile tool used predominantly for regression tasks as a supervised learning method, but it can also handle classification tasks. MLP adjusts its parameters, including biases and weights, during training based on the provided input and output datasets. The primary objective is to

minimize the error between predicted outputs and target values.

Validation parameters such as the mean square error (MSE) or root mean square error (RMSE) are employed via the backpropagation algorithm to achieve this error minimization. Notably, the backpropagation algorithm employs gradient descent as a stochastic method to propagate the biases and weights backward throughout the network. During training, the j th output node in the n th data point is represented as the difference between the actual (d) and predicted (y) values:

$$e_j(n) = d_j(n) - y_j(n) \quad (3)$$

The weights are extracted by minimizing the error across all actual and target values of the system:

$$\varepsilon(n) = \frac{1}{2} \sum_j e_j^2(n) \quad (4)$$

Gradient descent is then used to calculate the weight variations as follows:

$$\Delta w_{ij}(n) = -\eta \frac{\partial \varepsilon(n)}{\partial v_i(n)} y_i(n) \quad (5)$$

where v_i , y_i , and η represent the local induced field, the previous neuron's output, and the learning rate, respectively. The learning rate affects the convergence speed of the network. The derivative of the weight concerning the local induced field can be expressed as:

$$-\frac{\partial \varepsilon(n)}{\partial v_i(n)} = e_j(n) \phi'(v_j(n)) \quad (6)$$

where ϕ' represents the derivative of the activation function, and it remains constant with respect to variations in the local induced field and weights. Furthermore, the derivative of the weight for the hidden neuron is determined by considering the derivative of the activation function (ϕ') and the influence of the k th node's weight (output layer) on the hidden node's weight variation, thus defining the activation function's backpropagation [44].

F. Long Short-Term Memory

LSTM is used in machine learning and deep learning as a highly advanced artificial neural network model [45]. Unlike the MLP, LSTM has a feedback connection to decrease errors. The LSTM model can efficiently handle a lengthy list of data samples using its memory blocks. Memory blocks are employed in the LSTM model to handle the complexity of a long sequence dataset. Using LSTM, input is defined based on the history of the signal, and the output is the signal's actual future (next time-step). LSTM comprises three units, including the input, output, and forget. Every unit combines the sigmoid function and dot product to generate gradient information regarding elimination, control, and distortion of the information flow. The proposed LSTM model for c_{pNF} of the soybean oil/MXene NFs comprises an input generator unit, a normalization unit, and a sequence input layer,

followed by a variable number of hidden layers and units, a fully connected layer, and regression output. It is noteworthy that during the training process of the model, the inputs and outputs of the model are defined on the basis of the history of the motion signal.

The LSTM model, which consists of input, output, and forgets gates, with each gate derived from the sigmoid function and dot product to defend the gradient information from deletion or distortion and regulate the flow of information, is made learning-friendly by the forgotten historical information and updated memory units. The LSTM indexes are chosen based on the Bayesian optimization method to get the most effective outcomes in regenerating the optimal input motion signal for the motion simulator user. It should be noted that the proposed algorithm is modularly designed to support the definition of LSTM or BiLSTM as well as consideration or non-consideration of the dropout layer, which is normally used to avoid the overshooting problem of the data during training and testing. The trained LSTM is used to predict the c_{pNF} of the soybean oil/MXene NFs.

There are two training methods in the LSTM, including real-time recurrent learning (RTRL) and truncated backpropagation through time (BPTT) with respect to gradient descent optimization. The summation of the square of the errors is defined as a loss function. The exploitation of the linear constant error carousel of the memory cell shortens the error. The error discharges from the cell and decreases exponentially inside the carousel of the memory cell.

G. Bayesian Optimization method

Bayes' theorem, invented by Thomas Bayes, is based on statistical methods to calculate the probability of the incident [46]. A Bayesian optimization can be categorized into constrained optimization while minimizing the objective function [47]. The cost function is defined in this study to minimize the MSE and RMSE while maximizing the correlation coefficient (CC) using the stochastic method. Also, the state can be continuous reals, categorical, or integers. In this study, we used the Bayesian optimization method for the automatic tuning of our proposed machine learning methods because of the tremendous advantages of this constrained-based optimization method. The tuning of the machine learning method is often a black art that needs expert knowledge to reach high performance. The Bayesian method works through an iterative development of the global statistical model of the unknown objective function. The optimization starts with a likelihood and prior over functions. A posterior distribution is calculated according to each iteration's previous objective function evaluation. The elements in the Bayesian optimization method are a Gaussian model of the cost function, Bayesian's updating procedure, and acquisition function. An acquisition function assesses the location of the state using the posterior distribution function.

The Bayesian optimization method extracts the GMDH, SVR, MLP and LSTM hyperparameters. The proper cost function definition is essential in calculating the relevant results based on the system's needs. The modular definition of the sequencing block and MLP model is used inside the Bayesian optimization method. Then, the model is trained and evaluated using the predefined values via the optimization algorithm. The cost function is defined to decrease prediction error. Then, the MSE between the actual c_p and predicted $\hat{c}_p$ during the testing process is defined as the cost function for the Bayesian optimization algorithm.

$$J = \frac{1}{n} \sum_{i=1}^n (T_i - \hat{T}_i)^2 \quad (7)$$

where T_i and $\hat{T}_i$ are the i th output and the i th predicted value.

IV. Results and Discussions

Four investigated machine learning methods, including SVR, GMDH, MLP and LSTM, have been modelled in MATLAB to discover the most efficient model in predicting the soybean oil/MXene NFs using temperature and nanoflake concentration. The Bayesian optimization method is employed to extract the optimized model of each machine learning method shown as Opt-SVR, Opt-GMDH, Opt-MLP and Opt-LSTM. The combination of the verification and validation subsections structured this Section.

A. Verification

GMDH is designed regarding the explained model in Section III.C. SVR is designed regarding the described model in Section III.D. MLP is prepared based on the presented mathematical model in Section III.E. LSTM is prepared based on the presented mathematical model in Section III.F. The Opt-GMDH, Opt-SVR, Opt-MLP and Opt-LSTM have been prepared according to the presented mathematical model in Sections III.G. MATLAB software's `fitrsvm`, `feedforwardnet` and `trainNetwork` functions are used to design the SVR, MLP and LSTM models. In addition, the GMDH algorithm is developed based on the provided model by Kalami Heris [48]. The proposed methods in the previous Section are coded in MATLAB software, and outputs are visualized using the `plot` function. In addition, the `bayesopt` function of MATLAB is used to develop a Bayesian optimization method.

B. Validation

Five parameters have been used to validate our proposed method compared with the traditional methods, including CC, MSE, RMSE, normalized root mean square error (NRMSE), and R2. These validation parameters are calculated as follows:

$$CC = \frac{\sum_{i=1}^n (x_i - \bar{x})(T_i - \bar{T})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 (T_i - \bar{T})^2}} \quad (8.a)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (T_i - \hat{T}_i)^2 \quad (8.b)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (T_i - \hat{T}_i)^2}{n}} \quad (8.c)$$

$$NRMSE = \frac{RMSE}{\bar{T}} \quad (8.d)$$

$$R^2 = 1 - \frac{\sum (T_i - \hat{T}_i)^2}{\sum (T_i - \bar{T})^2} \quad (8.e)$$

where n , x_i , $\bar{x}$ and $\bar{T}$ are the number of samples, the i th input, the mean of inputs and the mean of outputs.

The investigated Bayesian optimization method is employed four times for extracting the optimal hyperparameters of GMDH, SVR, MLP and LSTM. The extracted hyperparameters of MLP and LSTM are shown in Table 2 using the Bayesian optimization method. The extracted hyperparameters are defined inside the initial definition of the proposed and investigated machine learning parameters, such as Opt-SVR, Opt-GMDH, Opt-MLP, and Opt-LSTM, to be trained via the implementation of 95% of the datasets. At the same time, 5% is used for validation and testing purposes of the methods. Increasing the validation error rate on a non-training subset for more than 6 epochs is employed to terminate the training process and prevent the networks from facing overfitting problems.

In addition, Table 3 shows the testing samples of the investigated methods for 20 trials. It includes the inputs (Temperature °C and wt.%) and actual output (c_{pNF}) captured via the experimental investigation.

In order to show the influence of the Bayesian optimization method on the proposed and investigated machine learning methods (GMDH, SVR, MLP, and LSTM), the models are developed using the extracted optimized and trial-and-error hyperparameters. Table 4 shows the extracted outcomes with/without implementing the Bayesian optimization method. As represented in Table 4, the efficiency of GMDH, SVR, MLP, and LSTM increased by 0.73%, 1.25%, 0.59%, and 0.59% using the CC as the evaluation parameter, respectively. Also, Table 4 shows that the implementation of the Bayesian optimization method can reduce the MSE of GMDH, SVR, MLP, and LSTM by 28.07%, 65.96%, 36.08-times, and 592.22-times, respectively. In addition, the NRMSE reduces using the

TABLE 2
THE EXTRACTED OPTIMAL HYPERPARAMETERS USING THE BAYESIAN OPTIMIZATION METHOD FOR MLP AND LSTM.

METHOD	ADJUSTMENT PARAMETERS
GMDH	MAXIMUM NUMBER OF LAYERS=10; MAXIMUM NUMBER OF NEURONS=100; TRAINING RATIO=0.7; SELECTION PRESSURE=0
SVR	GAUSSIAN KERNEL FUNCTION; AUTOMATIC KERNEL SCALE; STANDARDIZE THE DATA.
MLP	NUMBER OF LAYER=2; NUMBER OF NEURONS=11; LINEAR RATE=0.0959
LSTM	NUMBER OF LAYER=10; NUMBER OF NEURONS=321; INITIAL LEARNING RATE=5×10-4; L2REGULARIZATION=1.0825×10-10

TABLE 3
THE TESTING SAMPLES FOR EVALUATION OF THE FOUR INVESTIGATED MACHINE LEARNING METHODS.

N	TEMP (°C)	WT.%	C_{pNF} (J/G °K)	N	TEMP (°C)	WT.%	C_{pNF} (J/G °K)
1	68.2805	0.125	2.04	11	82.7700	0	1.75
2	83.3962	0.075	2.02	12	63.5959	0.025	1.70
3	36.6116	0.075	1.85	13	89.6680	0.025	1.79
4	47.1150	0	1.66	14	73.7205	0.025	1.74
5	28.6824	0	1.66	15	92.7611	0.125	2.20
6	85.2578	0.125	2.15	16	79.3697	0	1.74
7	68.4706	0.125	2.04	17	29.8299	0	1.66
8	45.0176	0.025	1.67	18	57.4651	0.025	1.68
9	69.8175	0.075	2.00	19	87.3806	0.025	1.78
10	87.2807	0.025	1.78	20	39.2977	0.075	1.86

Bayesian optimization method by 1.34-times, 0.97-times, 5.39-times, and 23.05-times using GMDH, SVR, MLP, and LSTM methods, respectively.

Figure 3 represents the target and predicted c_p of the soybean oil/MXene NFs based on temperature and nanoflakes concentration using optimized GMDH, SVR, MLP and LSTM. Based on the presented results in Figure 3, the CC between the actual and predicted c_p using GMDH, SVR, MLP, and LSTM are -0.0008, -0.0428, 0.9998 and 0.9999. The higher CC using LSTM compared to GMDH, SVR, and MLP is because of the highest power of this

TABLE 4
THE EXTRACTED RESULTS OF PROPOSED AND INVESTIGATED MACHINE LEARNING METHODS, INCLUDING GMDH, SVR, MLP AND LSTM, WITH/WITHOUT USING THE BAYESIAN OPTIMIZATION METHOD DURING THE IMPLEMENTATION OF TESTING DATASETS.

METHOD	GMDH	SVR	MLP	LSTM	METHOD	GMDH	SVR	MLP
PROCESS	TRIAL-AND-ERROR	OPTIMIZED	TRIAL-AND-ERROR	OPTIMIZED	PROCESS	TRIAL-AND-ERROR	OPTIMIZED	TRIAL-AND-ERROR
MSE	0.073	0.057	0.078	0.047	MSE	0.073	0.057	0.078
RMSE	0.581	0.239	0.531	0.216	RMSE	0.581	0.239	0.531
NRMSE	0.304	0.130	0.231	0.117	NRMSE	0.304	0.130	0.231
CC	-0.0081	-0.0008	-0.1373	-0.1248	CC	-0.0081	-0.0008	-0.1373
ERROR MEAN	0.024	0.001	0.025	0.010	ERROR MEAN	0.024	0.001	0.025
ERROR STD	0.423	0.246	0.326	0.221	ERROR STD	0.423	0.246	0.326
R ²	0.114	0.057	-0.169	-0.125	R ²	0.114	0.057	-0.169

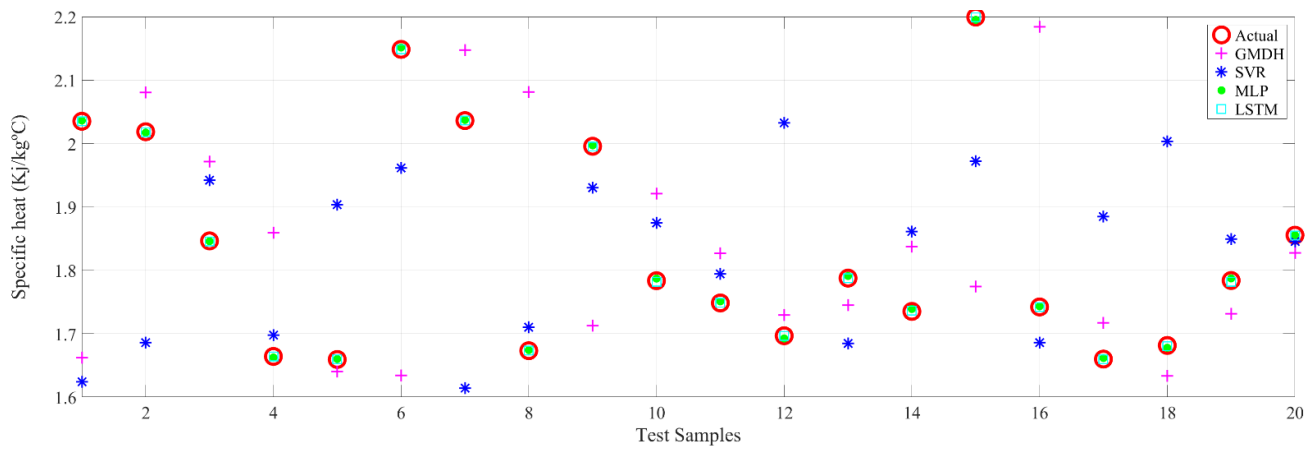


FIGURE 3. The actual and predicted c_{pNF} of soybean oil/MXene NFs based on temperature and nanoflake concentration using Bayesian optimization-based GMDH, SVR, MLP and LSTM machine learning methods.

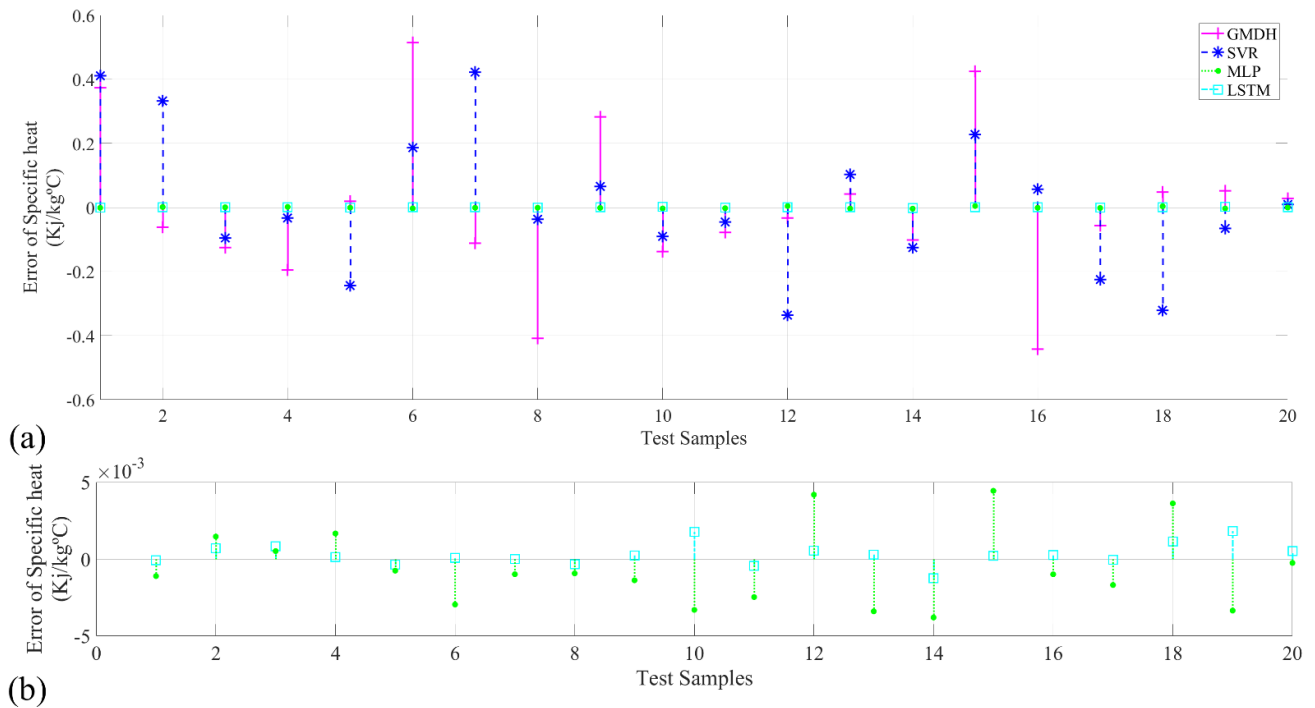


FIGURE 4. The error between the actual and predicted c_p of soybean oil/MXene NFs based on temperature and nanoflake concentration using (a): Bayesian optimization based GMDH, SVR, MLP and LSTM machine learning methods; (b): Bayesian optimization based MLP and LSTM machine learning methods.

machine learning technique in handling nonlinear systems.

Figure 4a-b presents the error between the actual and predicted c_p of the soybean oil/MXene NFs based on temperature and nanoflakes concentration using four investigated methods (GMDH, SVR, MLP and LSTM) and two investigated methods (MLP and LSTM) for 20 trials during the testing session, respectively. Based on the represented result in Figure 4a, MLP and LSTM are able to decrease the MSE, RMSE, and NRMSE more than 8260-, 107- and 111-times compared to GMDH and SVR for 20

trials of a testing session, respectively. Also, Figure 4b shows that LSTM is able to decrease the MSE, RMSE and NRMSE between the actual and predicted c_p of the soybean oil/MXene NFs 95.08%, 78.00% and 76.67% compared with MLP for 20 trials of the testing stage, respectively. As a result, the higher accuracy of MLP and LSTM compared with GMDH and SVR is the first revealed information regarding the represented results in Figure 4a. Also, the higher accuracy of the LSTM compared with MLP is the second revealed information based on Figure 4b. In the

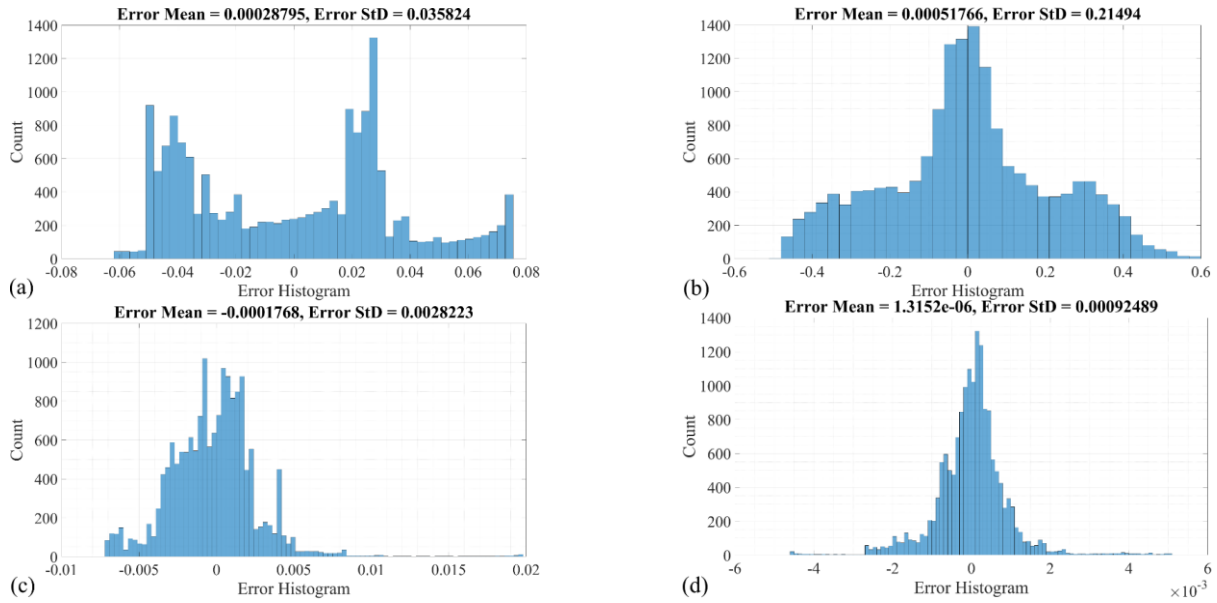


FIGURE 5. The error histogram of the data using all data, including all data (training and testing) using optimized based (a): GMDH; (b): SVR; (c): MLP; (d): LSTM.

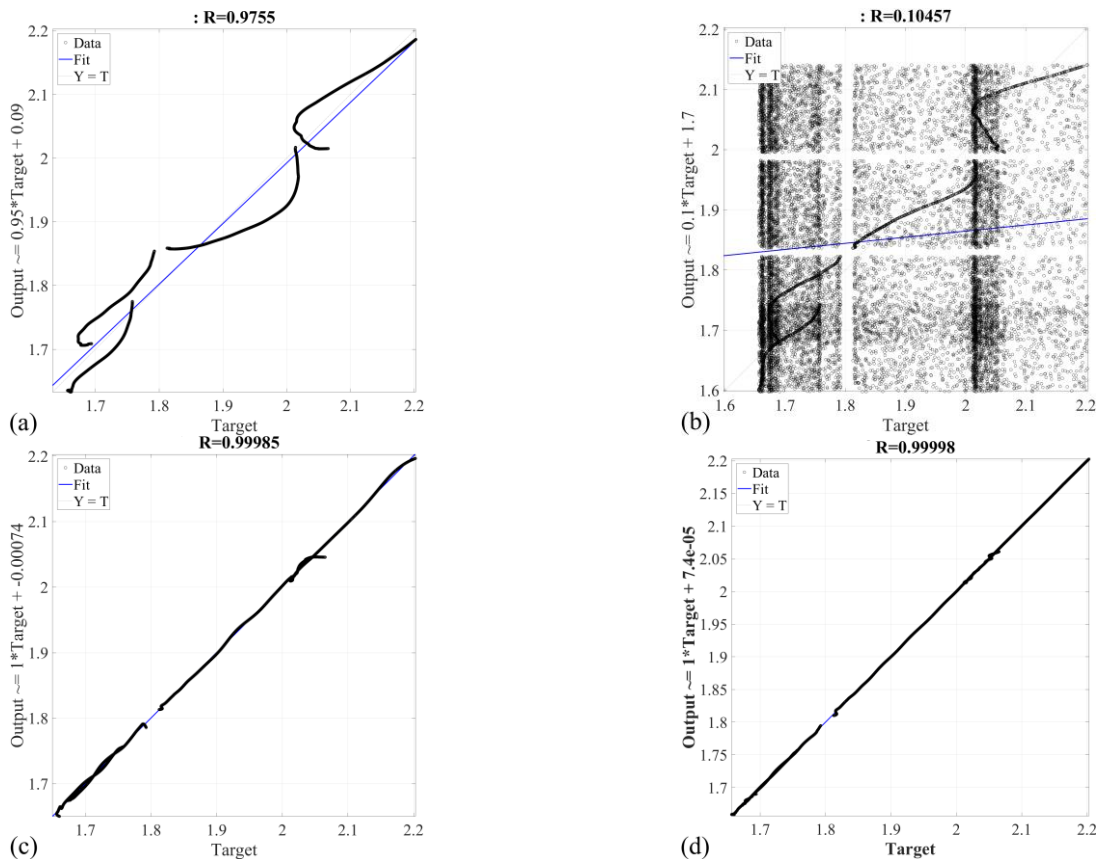


FIGURE 6. The regression of the data during all data (training and testing) using optimized based (a): GMDH; (b): SVR; (c): MLP; (d): LSTM.

following the error histogram and regression of the investigated machine learning methods with the cooperation of Bayesian optimization technique is shown in Figure 5-6.

Figure 5a-d shows the error histogram of the optimized-based GMDH, SVR, MLP and LSTM during the implementation of all data (including training and testing

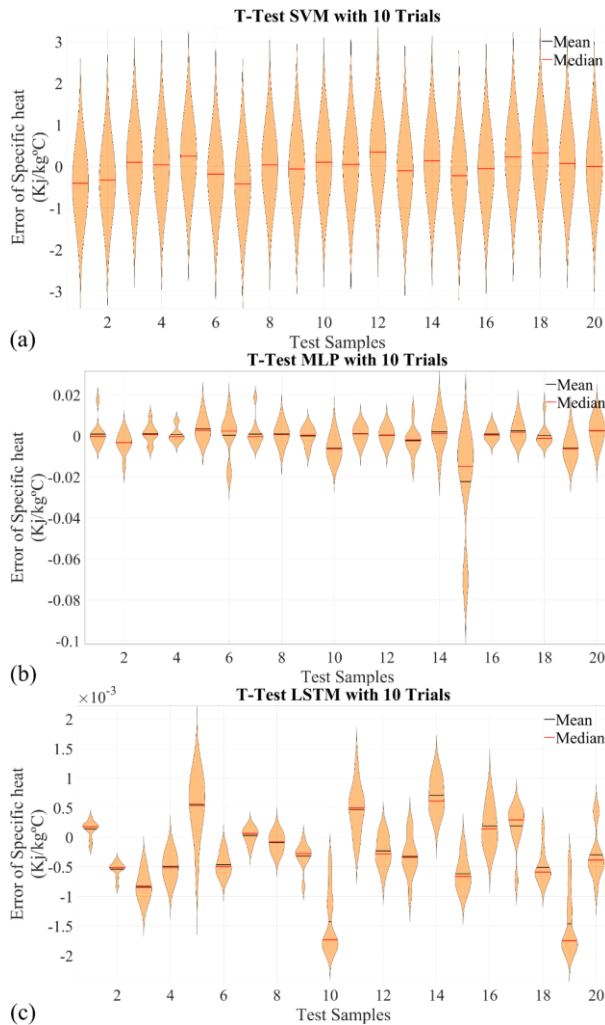


FIGURE 7. The results of the T-test after 10-time trials for proposed optimized machine learning methods, including (a): SVM; (b): MLP; (c): LSTM.

dataset), respectively. Regarding the represented outcomes in Figure 5a-d, the mean of the error between the actual and predicted c_p of the soybean oil/MXene NFs using optimized LSTM is 219-, 393- and 134-times lower than the optimized

GMDH, SVR and MLP methods. The lower mean of the error between the actual and predicted c_p of the soybean oil/MXene NFs using the LSTM method compared to GMDH, SVR and MLP methods proves the efficiency of this investigated machine learning method. Also, the variation of the error, which is used to show the robustness of the model using LSTM, is 39-, 237- and 3-times lower than GMDH, SVR and MLP methods. Then, in the point of error variation, the robustness of the model can be ordered as LSTM, MLP, GMDH and SVR, respectively. Also, the order of the models based on the lower error is LSTM, MLP, GMDH, and SVR. It should be concluded that the LSTM is the most reliable model, while the SVR is the weakest model in predicting the c_p .

Figure 6a-d represents the regression of the developed GMDH, SVR, MLP and LSTM for prediction of the soybean oil/MXene NFs c_p during the training and testing stages of the algorithms, respectively. The vertical and horizontal axes in Figure 6 represent the actual and predicted c_p of the soybean oil/MXene NF. The R^2 of optimized GMDH, SVR, MLP and LSTM during all data processes (including testing and training) are 0.9755, 0.10457, 0.99985 and 0.99998, respectively. It shows the 2.45%, 89.54% and 0.01% improvement of the R^2 using optimized LSTM compared with those of optimized GMDH, SVR and MLP, respectively.

The statistical representations of Figure 3-6 are shown in Table 5. It shows the outcomes during the training, testing and all processes of the four optimized investigated techniques, including GMDH, SVR, MLP and LSTM. Based on the demonstrated results, LSTM is the strongest technique among all investigated machine learning methods during the training and testing stage of the data. LSTM can reach better results compared with those of GMDH, SVR and MLP in terms of lower MSE, RMSE, NRMSE, average of error and variation of error.

In order to study the accuracy and repeatability of the proposed method, the T-test is implemented in all four machine learning methods with 10-times trials. Figure 7a-c shows the violin plot for 10-times trials of the SVR, MLP

TABLE 5
THE EXTRACTED RESULTS OF PROPOSED AND INVESTIGATED MACHINE LEARNING METHODS, INCLUDING GMDH, SVR, MLP AND LSTM, WITH/WITHOUT USING THE BAYESIAN OPTIMIZATION METHOD DURING THE IMPLEMENTATION OF TESTING DATASETS.

Method	GMDH			SVR			MLP			LSTM		
Process	Training	Testing	All	Training	Testing	All	Training	Testing	All	Training	Testing	All
MSE	0.001	0.057	0.001	0.046	0.047	0.046	1.0×10^{-5}	1.2×10^{-5}	1.0×10^{-5}	8.6×10^{-7}	5.9×10^{-7}	8.6×10^{-7}
RMSE	0.036	0.239	0.036	0.215	0.216	0.215	3.2×10^{-3}	3.5×10^{-3}	3.2×10^{-3}	9.3×10^{-4}	7.7×10^{-4}	9.2×10^{-4}
NRMSE	0.020	0.130	0.019	0.116	0.117	0.116	1.7×10^{-3}	1.8×10^{-3}	1.7×10^{-3}	5.0×10^{-4}	4.2×10^{-4}	5.0×10^{-4}
Error Mean	-1.8×10^{-4}	0.001	-1.9×10^{-4}	5.1×10^{-4}	0.010	5.2×10^{-4}	1.0×10^{-4}	9.8×10^{-4}	1.1×10^{-4}	9.5×10^{-7}	3.0×10^{-4}	1.3×10^{-6}
Error Std	0.036	0.246	0.036	0.215	0.221	0.215	3.2×10^{-3}	3.4×10^{-3}	3.2×10^{-3}	9.3×10^{-4}	7.2×10^{-4}	9.2×10^{-4}
R^2	0.967	0.057	0.967	0.103	-0.125	0.103	0.9991	0.9984	0.9991	0.9998	0.9984	0.9998

and LSTM methods, respectively. It should be noted that there is no need to evaluate GMDH because it always reaches the same results. However, the error of the GMDH is quite noticeable besides the robustness of the results. Regarding the demonstrated outcomes in Figure 7a-c, the accuracy and repeatability of the results using LSTM are noticeably better than SVR and MLP methods.

The demonstrated outcomes in Section IV prove the higher performance of our newly proposed optimized LSTM in comparison with those of optimized GMDH, SVR and MLP in terms of higher R2 and CC as well as lower NRMSE, RMSE, MSE, mean error and variation error.

V. Conclusion

Researchers are exploring nanofluids for more efficient PV/T hybrid systems due to their superior thermal properties. MXenes, a class of 2D materials, show promise for improving energy storage and thermal conductivity, while eco-friendly vegetable oils, like soybean oil, are considered for PV/T solar collectors. This study addresses research gaps in thermophysical properties estimation of soybean oil/MXene nanofluids, emphasizing machine learning techniques to replace expensive practical tests. Identified gaps include limited exploration of advanced machine learning methods like LSTM for c_{pNF} prediction, lack of clarity on the most effective approach, and insufficient understanding of Bayesian optimization's impact on c_{pNF} prediction. Contributions include introducing advanced machine learning methods (SVR, MLP, GMDH, LSTM) for c_{pNF} estimation, using Bayesian optimization to enhance model performance, and demonstrating feasibility of eliminating costly practical tests while improving prediction accuracy. The main finding is successful implementation of machine learning methods, including LSTM, SVR, MLP, and GMDH, in predicting c_{pNF} of soybean oil/MXene nanofluids based on temperature and nanoflakes concentration. Results show optimized LSTM model significantly reduces mean square error in c_{pNF} calculation compared to SVM, GMDH, and MLP, achieving reductions of 99%, 99%, and 91% respectively. This approach offers a promising solution for efficiently estimating thermophysical properties and can be extended to predict others. However, proposed method's reliance on data quality may limit generalizability to other fluids, requiring better data and transferability solutions, explored in future studies using conventional neural networks and transfer learning.

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