

Predictive ANN Modelling of Thermorheological Properties of Iron-Oxide Yield Stress Nanofluid

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Abstract

The intent of the research is to find the dependency of the volume fraction of nanoparticle (ϕ) and the temperature on the absolute viscosity (μ_{nf}) of Fe₃O₄ nanoparticles in Carbopol polymer gel. Rheological and stability analysis of the solution is identified. A total of 48 viscosity values has been calculated from experiments using two different base fluid concentrations and two different nanofluid concentrations at eight different temperatures. The data gathered are used for the training of an ANN (Artificial Neural Network) to observe results in a predefined range of two input criteria. It uses a feed-forward perceptron ANN with a temperature input, a volume concentration input, and a viscosity output. The topology was established by trial and error; and the two-layer model having ten neurons in the hidden layer that used the tansig function produced the best results. Ten training functions were utilized to analyze the best result for η_f prediction, and the trainbr algorithm was found to be the best ANN. Due to the trained ANN, the anticipated value of viscosity is obtained from each temperature and volume concentration combination. The best results were witnessed with trainlm algorithm with an MSE value of 5.92e-4 and a R2 value of 0.9988 for forecasting of viscosity. Nanoparticle volume concentration increases with viscosity, while temperature increases cause viscosity to decrease. As the temperature rises from 15°C to 50°C, the shear stress value drops with a corresponding shear rate. The shear stress value of the associated shear rate decreases as the nanoparticle concentration rises.

Keywords: ANN, Viscosity, Shear stress, Stability, Nanofluid, Multi-Layer perceptron

Introduction

Water is an excellent base fluid for thermal management applications available today, and its large heat capacity improves its importance. Water, however, has poor thermal conductivity, so metals in nanosized are added to it to improve the base fluid's thermal conductivity. The metals have high thermal conductivity as compared to non-metals and aqueous solutions, etc [1,2,3]. It is significant from the experiment results that increase in heat transfer rate after adding nanoparticles to the base fluid. Newtonian fluids like DI water, ethylene glycol, etc. have been the subject of numerous experiments, whereas non-Newtonian fluids like Maxwell fluids, dilatant fluids, Rivlin fluids, purely viscous fluids, viscoelastic fluids, Reiner materials, couple stress fluids, power-law fluids, viscoelastic fluids, pseudo-plastic fluids, Casson fluid, micro polar fluid, etc. have received less attention. After research on nanofluids, some of the researchers have concentrated on magnetic nanofluids as it is seen that the magnetic field puts down effect on the heat transfer coefficient [4]. These ferrofluids are made by mixing a non-magnetic suitable solvent with magnetic nanoparticles and stabilizing the combination using a surfactant like oleic acid. Different metal elements, such as iron, cobalt, and nickel, as well as their oxide forms, such as spinel-type ferrites and magnetite (Fe₃O₄), are used to create these magnetic nanofluids in a variety

of shapes and sizes. [5,6].

Researchers are presently concentrating more on the prediction of thermal conductivity, viscosity, and stability of nanofluids to avoid the experimental expense. These methods include curve fitting, ANN (Artificial Neural Network), fuzzy logic, and genetic algorithm. Artificial neural networks, or ANNs, anticipate data using a model that resembles the structure and goals of biological neural networks. Because ANN can forecast the thermal conductivity, viscosity, and other thermophysical properties of nanofluids through nonlinear mapping. For the ANN modeling to forecast viscosity and thermal conductivity, old experimental data have recently been gathered [7,8]. By using ANN modelling, Shahsavar et al. calculated the thermal conductivity of paraffin-Al₂O₃ nanofluid [9]. To predict the rheological behaviour of the water-ethylene glycol/WO₃-MWCNTs nanofluid, Fan et al. created a well-trained artificial neural network (ANN) using the trial approach. [10]. The algorithm showed an R2 value of 0.996 for predicting viscosity and experiments are conducted at 7 different temperatures and 6 different concentrations. Viscosity decreases with an increase in temperature at all volume concentrations. An ANN was modelled by Simon et al. to forecast the μ_{nf} of a nanoparticle colloidal suspension in water/ethylene glycol [11]. The input parameters used

to forecast viscosity include temperature, nanoparticle diameter, and base liquid characteristics. By measuring the stability and thermophysical characteristics of a Fe₃O₄-coated MWCNT hybrid nanofluid, said et al. created an artificial intelligence (AI) interface to forecast the density, thermal conductivity, viscosity, and specific heat using the temperature and mixture concentration as input data [12]. The correlation coefficient for the model is between 0.9938 to 0.9999. In order to forecast the thermal conductivity and viscosity of a non-Newtonian hybrid nanofluid in which CNT/Fe₃O₄ nanoparticles are embedded, Shahsavari et al. undertook an experimental research and ANN modelling [13]. Temperatures between 25 and 55 °C, Fe₃O₄ volume concentrations between 0.1 and 0.9 %, and CNT concentrations between 0 and 1.35 % are used to assess the thermal conductivity and viscosity. The fluid exhibits non-Newtonian behaviour with a declining viscosity trend in the rising shear rate. Experimental research by Bahiraei et al. showed that both thermal conductivity and viscosity have a non-linear relation with concentration when they were examined at various concentrations and temperatures. The Levenberg-Marquardt approach, which is based on Bayesian regularisation, was selected for the training of ANN [14]. To anticipate both thermal conductivity and viscosity, Shahsavari et al. carried out experimental research on a liquid paraffin Fe₃O₄ and combined modeling of the GMDH neural network. The fundamental indices used to assess the model correctness are Root mean square (RMS), root mean square error (RMSE), mean absolute deviation (MAE), and coefficient of determination (R²) [15]. In Fe₃O₄ hybrid nanofluids, Said et al. experimentally studied water and water/ethylene glycol mixture-based nanodiamonds [16]. In a 60:40 W/EG mixture, the thermal conductivity increased to 12.79 percent at the same =0.2 percent, but it increased by 17.76 percent in a water-based nanofluid. Multivariate linear regression (MLR) and Multivariate linear regression with interaction (MLRI) models are used to statistically analyze the experimental data. The thermal conductivity of an alumina-silica hybrid nanofluid was predicted using the ANN approach by Boobalan et al. [17].

After going through a series of research paper modelling, ANN is preferred by the researchers as it reduces time-consuming experiments and costs of operating related to it. In this research the μ_{nf} of Carbopol-Fe₃O₄ solution in which two different concentrations of Carbopol polymer, two different concentrations of Fe₃O₄ nanofluid, and eight different temperatures through a series of experiments. These results helped to train the ANN network in a defined range of two input parameters. For which a feed-forward perceptron with two input parameters (T and ϕ) and a output parameter of viscosity (μ_{nf}). It is a two-layered network with ten neurons in the hidden layer following the tansig function for best results. The network prepared is checked by ten training methods of which the best algorithm obtained by the mean square error and correlation coefficient value.

Nomenclature Subscript

ANN Artificial Neural Network of Nanofluid
 μ Viscosity of Base fluid
 ϕ Nanoparticle concentration μ_{np} Nanoparticle
 ANN Artificial Neural Network
 MSE Mean square error
 T Temperature
 R² Regression coefficient
 DI Deionized
 NaOH Sodium Hydroxide

Experimental Preparation of Nanofluids

There are two steps to prepare the nanofluids i.e., a one-step method and a two-step method. In a one-step method, the nanoparticles are prepared and mixed in the same time in the base fluid. The two-step method is more practiced due the formation of nanoparticles and adding it to base-fluid are two different steps. The Fe₃O₄ nanoparticles are procured and mixed in the DI water by a marine blade stirrer. The nanoparticle of concentration 0.05 and 0.1 wt.% are considered for experiment. The samples are kept under an ultrasonicator for about 60 min. Anhydrous Carbopol Ultrez 30 (purchased from Lubrizol, Belgium) powder is allowed to pass through a fine mesh to avoid the effect of agglomeration. The prepared DIW- Fe₃O₄ nanofluids are stirred constantly at around 1000 rpm [18,19]. The passed Carbopol is added gently to the stirring nanofluid at its vortex area in the center. The Carbopol are 0.1 and 0.05 wt.%. The stirring continues till homogeneity establishes. The disappearance of lumps formed shows the homogeneity of the solution and the complete hydration of Carbopol powder. An aqueous solution of 18 wt.% NaOH added dropwise to neutralize the colloidal solution and stirred at 300 rpm. The gel forms and reduces the speed of the stirrer. The colloidal solution formed is kept for two days in a sealed container and under a controlled environment. The formed yield stress nanofluids are complex due to their unusual rheological behaviour. The pH of the solution is maintained at 7.0 ± 0.2 . Fig.1 shows the yield stress gel formation from an Iron-Oxide nanoparticle.



Figure 1: Fe₃O₄-Yield stress gel preparation

Rheological Measurement

Before the rheological measurement, the yield stress fluid is kept in a low-pressure place to remove the trapped air bubbles. The rheological measurement is performed in Strain controlled Anton Paar MCR-92 rheometer. Stress ramps and oscillating sweep both are used in the analysis. The cone and plate tool are used for the oscillating test, whereas rotational tests are conducted in a concentric cylinder of diameter 5cm with a cone angle of two degrees. Peltier heating and cooling system are used for controlling temperature. The rheological studies are carried out in the temperature range of

15-50 °C. After loading the sample, it is kept for a few minutes to attain thermal equilibrium. It is presheared for about 30 seconds at a shear rate of 1 s⁻¹ and then waited for about 30 s. The rotational tests are conducted in a shear rate range of 0.01-100 s⁻¹. Each test fluid is loaded cautiously and smoothly to avoid bubble entrapment. The measurement of each sample is conducted twice for maintaining the accuracy and precision. Table 1 represents the wt.% of nanofluid and Carbopol in the aqueous solution and its notation as A0, A1, A2, A3, A4, A5.

Table 1

Representation	Carbopol wt.%	Iron-Oxide wt.%
A0	0.05	0
A1	0.05	0.05
A2	0.05	0.1
A3	0.1	0
A4	0.1	0.05
A5	0.1	0.1

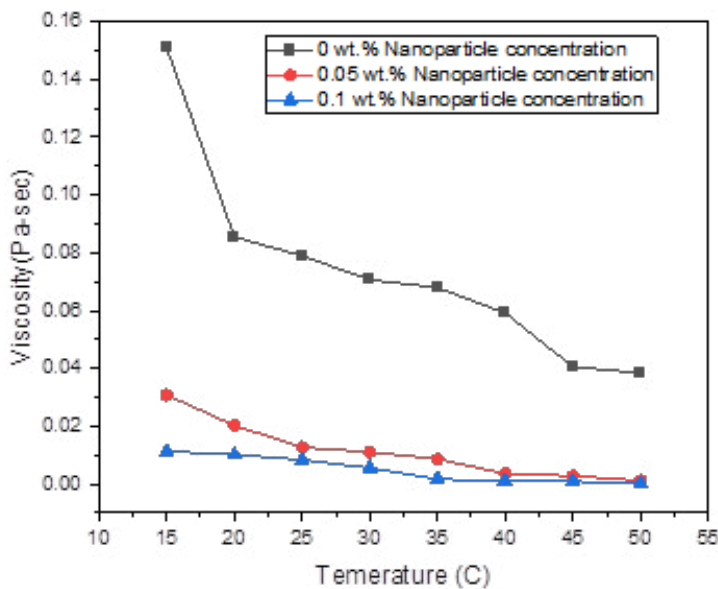


Figure 2: Carbopol polymer of 0.05 wt.%

Fig.2 shows the plot of viscosity of Carbopol polymer of 0.05 wt.% at eight different temperatures. It is evident from the plot that Carbopol polymer without any nanoparticle concentration has the highest viscosity as they behave as viscoplastic in nature. When nanoparticles are added to the Carbopol gel, the viscosity decreases with an increase in concentration because the nanoparticle fractures the gel's polymer chain. An rise in temperature increases the kinetic and thermal energy, which promotes ion mobility and a decrease in binding energy and viscosity. This has the opposite impact on viscosity. The graph of viscosity vs. temperature for two distinct concentrations of nanoparticles in 0.1 weight percent of Carbopol polymer is shown in Fig. 3. It is clear from the graph that viscosity decreases as temperature rises, both with and without the

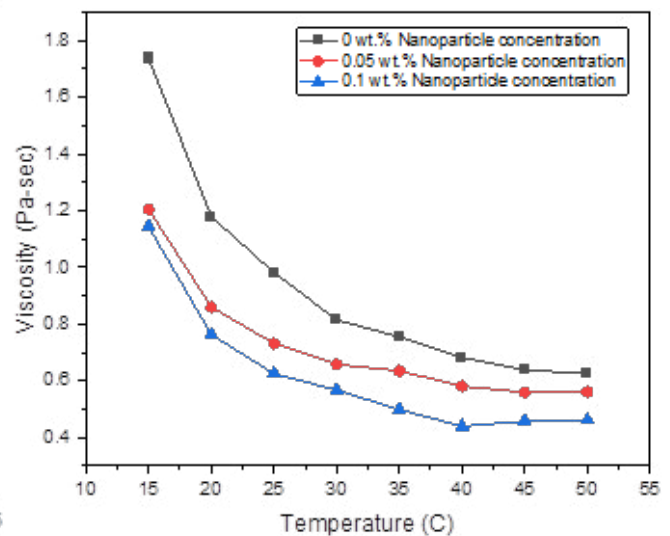


Figure 3: Carbopol polymer of 0.1 wt.%

addition of nanoparticles at varying quantities.

Stability

The electrokinetic characteristics of nanofluid in an aqueous solution provide stability and hence improve heat transfer efficiency. The nanoparticle consists larger charge density which generates a stronger repulsive force as same as charged particles. The stability of nanoparticles is usually measured by the Zeta potential which works on the principle of calculating the potential difference between the base fluid and the nanoparticle. As the surface of a nanoparticle has less charge density it attracts the ions of opposite charge to coat it and creates a double layer of ions which is carried away by the liquid in nanoparticles. As a result, the nanopar-

ticles moving in the solution can be viewed as a coating in the medium's original stationary layer. Zeta potential is the electric potential value at the boundary of the created dual layer, between the slab grasped by the nanoparticle and the solution. The stable range of the zeta potential value is $\pm 30-40\text{mV}$ whereas more than

$\pm 40-60\text{mV}$ is considered highly stable. A potential value less than $\pm 30\text{mV}$ leads to poor stability as in such condition nanoparticles lead to settle down and at such zeta potential values nanoparticles feel it difficult to withstand the forces which help in mixing it with base fluid.

Table 2

Sample	U0	U1	U2	U3	U4	U5
mV	-27.3	-44.8	-49.2	-28.1	-47.1	-50.2

Table.2 shows the zeta potential values of different samples. The sample with zero nanoparticle percentage is highly unstable as there is no charged particle present in the base solution for the generation of electro potential which results in a low electro-kinetic potential value. It is evident from the value that with the addition of nanoparticle concentration the stability is increasing as the charge density is increasing but it will increase to a certain percentage, with further increase in number leads to sedimentation and settling of nanoparticles and hence results in lowering of stability. With the increase in Carbopol concentration stability increases as the intermolecular bond gets strengthened due to gel nature. Stability is also checked manually by taking photographs each week and comparing them with previous one.

ANN configuration

An artificial Neural network (ANN) is a modern tool used by researchers for the optimization and prediction of data in widespread scientific and engineering problems in different fields. ANN works

on the basic structure of the human brain and neurons act as transferring signals from one end to the other end and the configuration of artificial neurons are prepared from several weighted elements. The weights build the relationship between inputs and outputs of neurons. There are 2 classes of ANN according to morphology. One of the group is Feed-forward-network and the other one is the recurrent network. The static data formed by the experimental work emphasizes a feed-forward perceptron ANN, but the input and output results showcase non-linearity. For the non-linearity we use Multilayer perceptron ANN which works on 2 layers with non-linear equations. Among many training methods, the Back-propagation algorithm is more effective and capable. In this project, we have compared various training methods and compared their performance and we have checked different ANN with different neuron numbers and transfer functions. A lot of 10 neurons in the 2nd layer with hyperbolic tangent function show the best performance. Fig 4 shows a multilayer perceptron ANN with different inputs and outputs.

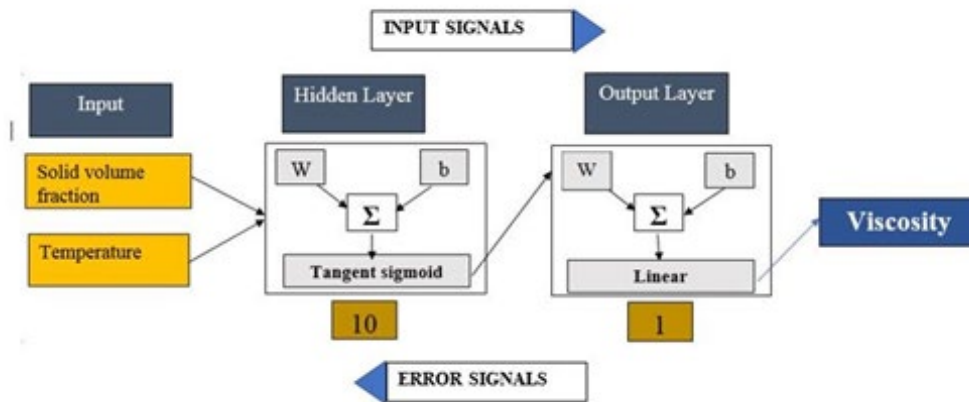


Figure 4: Multilayer perceptron ANN with input and output

For the training purpose of ANN, a database of experimental or simulation results is created for the learning of the algorithm. A total of 48 different samples versus temperature and ϕ were prepared for Carbopol-Fe3O4 nanofluid. Out of 48 samples, 70% of the data is used for the training whereas the other 30% is divided into equal parts 15% for validation and 15% for testing. The validation result protects the neural network from overtraining using early stops and concludes the ANN results. Table 3 shows the viscosity

value used for the learning of the ANN. Due to the unevenness in weights of ANN each network is trained 20 times with each training algorithm. The algorithm with the best results is considered the algorithm for the system. We got the best outcome at ten neurons in the second layer with hyperbolic sigmoid function and straight equation in the output layer. Table 4 gives the idea about the configuration of the network.

Table 3: μ nf of Carbopol – Fe₃O₄ nanofluid

Temp/Viscosity	15	20	25	30	35	40	45	50
U0	0.1509	0.0855	0.072	0.0706	0.0679	0.0391	0.0406	0.0117
U1	0.0308	0.0203	0.0127	0.0111	0.0086	0.0036	0.0087	0.0093
U2	0.0113	0.0102	0.0084	0.0056	0.0017	0.0011	0.0059	0.0062
U3	1.2054	0.8602	0.7321	0.6585	0.6355	0.5813	0.5598	0.5613
U4	1.7376	1.1789	0.9824	0.8155	0.7554	0.6821	0.6387	0.6261
U5	1.1445	0.7632	0.6256	0.568	0.4988	0.4405	0.4581	0.4621

Table 4: Network Configuration

Network Parameter	Data
ANN study	Multi-Layer-Perceptron
Network Type	Feed-forward
Training Method	Back-propagation
No of Train Data	34
No of Validation Data	7
No of Test Data	7
No of Hidden Layer	1
Best Training Method	trainbr
Error Criteria	Mean square error
Function in hidden layer	tansig
Function in output Layer	linear

A Feed-forward-network in a Multi-Layer-perceptron is considered in the study of Artificial Neural networks. A feedforward type network is the simplest model of an Artificial network in which information passes in one direction from the input node followed through the hidden nodes and finally came out through the output node. The Back-propagation algorithm is the best method as it reduces the training time and helps to train all neural network frameworks. Table.5 describes the various training algorithms considered for the comparison of data training, validation, and testing. The R² value of trainbr is 0.999 is the highest among all other

algorithms. The tansig hyperbolic sigmoid function followed in the hidden layers with an output ranging from -1 to +1 and Purelin linear transfer function for the output layer. Neurons in the hidden layer play a vital role in the performance of the network due to which different combination of neurons in a medium layer is checked with the trial and error technique and the best performance is obtained at ten neurons in the hidden layer following tangent sigmoid function. The ANN possesses random nature for training weights for which each network is trained random wise more than 20 times by all training techniques.

Training Techniques

Table 5: Error value and R² comparison in different training algorithm in MATLAB software

MSE	Acronym	Algorithm	Description	R ²
0.00059	LM	trainlm	Levenberg-Marquardt	0.998
0.0842	BFG	trainbfg	BFGS Quasi-Newton	0.85
0.014	RP	trainrp	Resilient Back propagation	0.967
0.013	SCG	trainscg	Scaled Conjugate Gradient	0.988
0.087	GDX	traingdx	Variable Learning Rate Back propagation	0.752
0.015	GDA	traingda	Gradient descent with adaptive learning rate	0.96
6.07E-05	BR	trainbr	Bayesian regularization backpropagation	0.999
0.00051	CGB	traingcb	Conjugate Gradient with Powell/Beale restarts	0.988
0.0013	CGF	traingcf	Fletcher-Powell Conjugate Gradient	0.9918
0.029	CGP	traingcp	Polak-Ribiere Conjugate Gradient	0.845

Our main focus is to find the best training technique to get more accurate predictions with high performance in μnf estimation. A feed-forward perceptron ANN following various training techniques using MATLAB software. The error value and the R2 related to each technique along with its MATLAB function name and description are also presented in Table 4. The full comparison of error values at various training methods is shown in a 3-D bar graph in Figure 5. The error criterion used in every training algorithm situation in which the average of the square of the difference between the predicted and actual values of the data are reported

Result and Discussion

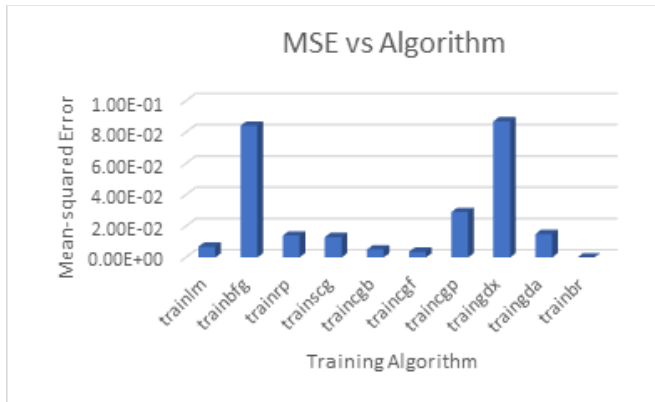


Figure 5: Mean Squared error vs training algorithm using MATLAB

The performance graph, which shows the fluctuation of MSE versus training stages, is one of the most essential indicators for displaying an ANN's training status. Fig.8 shows the viscosity performance curve for Carbopol-Ultrez gel and Iron-Oxide Nanoparticle in which MSE is plotted on the vertical axis and the training repetition on the horizontal axis of the curve called Epochs. This graph shows three different types of data training, validation, and testing, which represent MSE for the training validation and test points respectively. The MSE value is largest in the training stage where the network has random weights, and it reduces after increases in

is a mean squared error. Fig 6 shows the 3-D bar graph of the comparison of R² values in different training methods. R2 value indicates the goodness of the fit of the defined model and how well the regression value approximates with the predicted one. In this paper, it is evident that the trainbr algorithm has the best results among all other nine different algorithms in the case of both the Mean squared error value as well as the R2 regression value.

$$\text{MSE} = 1/n \sum_{i=1}^n (\bar{Y} - X)^2 \quad \bar{Y} = \text{predicted value, } X = \text{Observed value, } n = \text{no of data point}$$

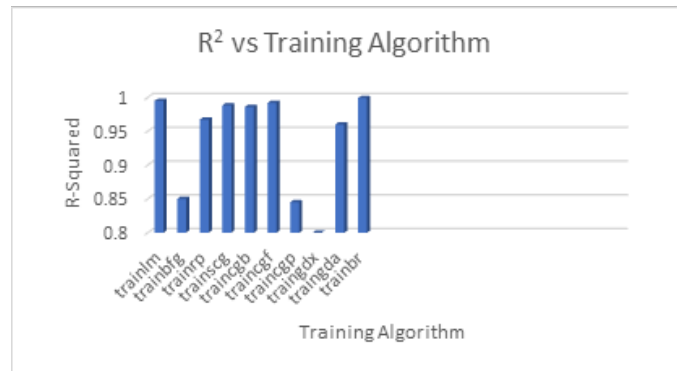


Figure 5: R² vs Training algorithm using MATLAB neural network

training cycles. At the end of the iteration, the MSE value of the training data is substantially lower than that of validation and test data. This is the result of the early stop technique which presents the untrained fresh points have a higher MSE value than that of trained points given to the system. The green circle indicated in the graph shows the best stop time for the best performance, with the lowest MSE among alliteration. As each training scheme utilized 30 distinct ANNs, the network with the lowest MSE was chosen as the optimal solution for estimating the viscosity for each combination of input.

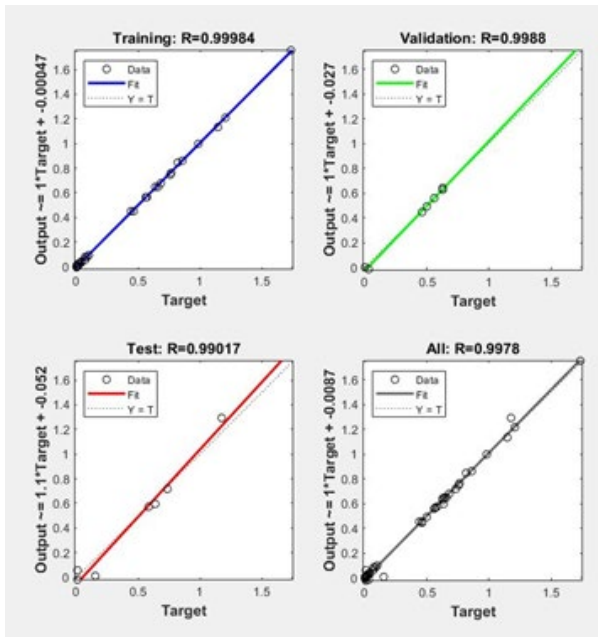


Figure 7: Regression diagram of μ_{nf} output

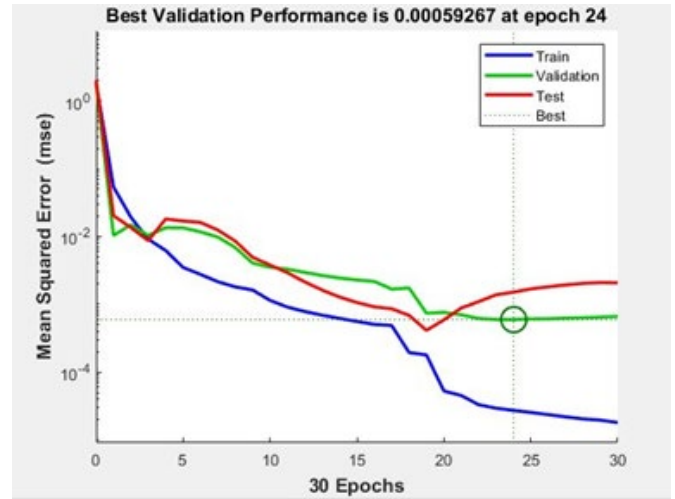


Figure 7: Performance diagram of μ_{nf} output

Other markers for determining the ANN training state include regression diagrams and data correlation coefficients. The relationship of real network outputs (the vertical axis) and target values (the horizontal axis) is shown in Fig.7 for viscosity (μ_{nf}) (the horizontal axis). Three separate parameters are important in this diagram. The correlation coefficient value (R), slope value (M), and bias value (B) are some of these measures (B). The output of an ideal network must match the target values, and the correlation

value and slope are both 1 in this case, and the bias value should be zero. The trend may be noticed in all four graphs. The regression line's slope is nearly equal to 1, therefore it can be determined. that the outcomes are network output values that are satisfactory accuracy and are close enough to the desired values Furthermore, the point scattering style is kept to a minimal, and all the points are connected and located on the plane's bisector.

Table 5: ANN error rates for viscosity

Desired Output	Low error %	High error %	MSE
Viscosity	-2.83	+2.47	5.90E-04

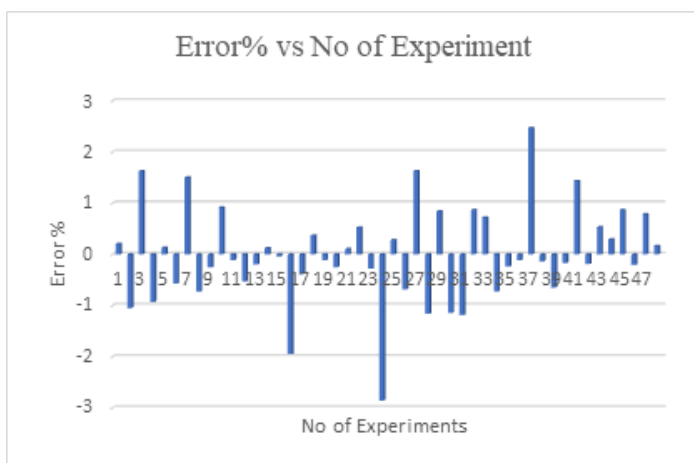


Figure 9: Error % with Experimental data

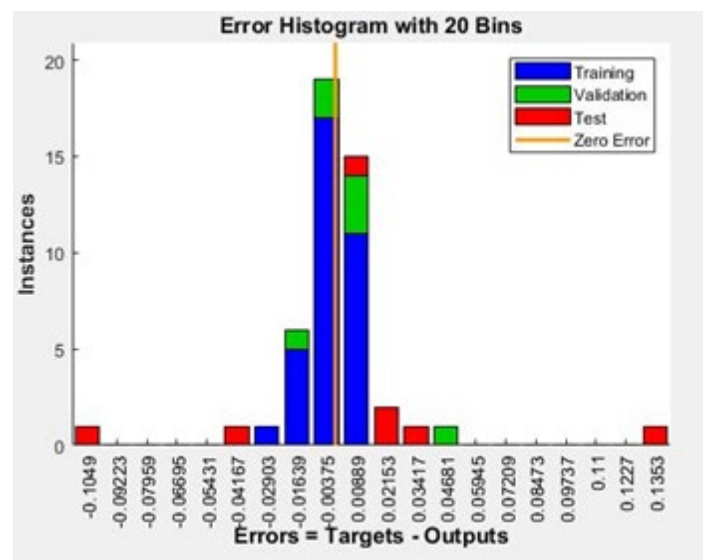


Figure 9: Error histogram of ANN for μ_{nf}

The error value of trained ANNs for viscosity is shown in Table 5. It is observed that the error value are quite small and falls within the allowed margin. The frequency of zero-range error values is exceptionally high, as evidenced by the error diagrams for various experimental data in Fig.9 for μ_{nf} , demonstrating that the network is well-trained and generates reliable estimates. Another key indicator for a well-trained ANN is the error value histograms, as shown in Fig. 10 for viscosity. This bar chart shows the frequency of error percentage between the actual and predicted value of all 48 experiments on the horizontal axis. As a result, the frequency or counts of errors on the vertical axis are compared with different error margin values on the horizontal axis, with the more near-zero frequencies on the vertical axis. The zero-error line is highlighted in red in this diagram. Most of bins with a high intensity of errors tend to group around this line, indicating a good choice of training strategy and a satisfactory result. Fig.11 compares the actual output with the neural network outputs. Thus, it is seen that experimental and ANN output coincides with an excellent regression value and best fits with the trainbr algorithm. We may conclude that a well-trained ANN can be used as an approximation function for estimating the μ_{nf} based on all the diagrams shown for the trained ANNs. Furthermore, volume concentration (ϕ) has a significant effect on viscosity in contrast to temperature which has a minor effect on viscosity.

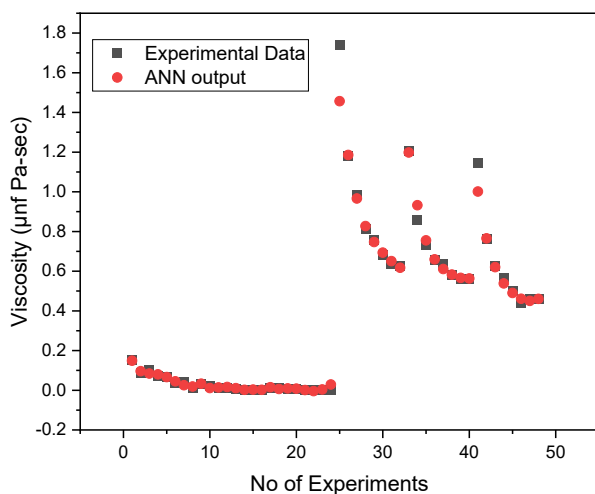


Figure 11: Comparison of ANN output with Experimental Data

Conclusions

The effect of volume concentration and temperature on the viscosity of Iron-oxide nanofluid in Carbopol Ultrez gel was investigated experimentally in this study. As a result, the viscosity of 48 samples has been determined through a series of tests, which included a combination of 8 different temperatures and 6 different samples of nanoparticle and base fluid concentration. In order to generalise the results for the two input parameters of temperature and volume concentration within predetermined bounds, an ANN was trained using these data. As a result, a feedforward Perceptron ANN was utilised, with two input result i'e (T and ϕ) and with one output viscosity (μ_{nf}). The optimum ANN structure

was discovered through trial-and-error method in a two-layered network with 10 neurons in the hidden layer following the tansig function produced the best results. The effectiveness of training procedures on the performance of viscosity prediction was also investigated using ten different training functions, and the best ANN was created when the trainbr was used as a training function. The trained ANN functions are used as a prediction function of μ_{nf} for every combination of temperature and nanoparticle fraction. The results are as follows:

- A suitable ANN with an MSE value of $5.92e-4$ and a correlation coefficient of 0.998 was created using the trainlm algorithm to forecast viscosity (μ_{nf}).
- It has been observed that by adding nanoparticles to gel solutions, the viscosity reduces with an increase in nanoparticle concentration and with a rise in temperature from 15°C to 50°C . This is because of the randomness of the nanoparticles which results in rising of thermal energy.
- Error diagrams and error histograms used to illustrate the ANN's appropriateness as a tool for assessing the competency of the training processes used in founding viscosity.
- Viscosity has a significant change with the increase in the concentration of Carbopol polymer as the viscosity increases with an increase in base gel concentration.
- Stability of the samples is also recorded with an increase in nanoparticle concentration from 0.05wt.% to 0.1wt.% it becomes more electrokinetically stable.

Declaration of the paper

We declare that the work included in the above paper is original and is an outcome of the research carried out by the author indicated in it.

Conflict of Interest

We declare there is no conflict of interest.

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