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3 **Comparative evaluation of AI-based intelligent GEP and ANFIS for model**

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5 **prediction of thermophysical properties of Fe3O4-coated MWCNT hybrid**

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7 **nanofluids for potential application in energy systems**

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## 3 Abstract

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5 Hybrid nanofluids are gaining popularity due to the synergistic effects of nanoparticles,

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8 which offer them improved heat transfer capacities than base fluids and regular nanofluids. The

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10 thermophysical properties of hybrid nanofluids play a crucial role in shaping heat transfer

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12 properties. Hence an in-depth analysis of thermophysical properties is important before its use

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15 in industrial applications. In the present work, a metamodel framework is developed to forecast

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17 the influence of nanofluid temperature and concentration on several thermophysical properties

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19 of Fe3O4 coated MWCNT hybrid nanofluids. Evolutionary gene expression programming

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21 (GEP) and an adaptive neural fuzzy inference system (ANFIS) were employed to develop the

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24 prediction models. The model was trained using 70% of the datasets, with the remaining 15%

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26 used for testing and validation. A variety of statistical measurements and Taylor's diagrams

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28 were used to assess the proposed models. The Pearson’s correlation coefficient (R), coefficient

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31 of determination (R2) was used for regression index, the error in the model was evaluated with

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33 root mean squared error (RMSE). The model's comprehensive assessment additionally includes

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35 modern model efficiency indices such as Kling-Gupta efficiency (KGE) and Nash-Sutcliffe

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38 efficiency (NSCE). The proposed models demonstrated impressive prediction capabilities.

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40 However, the GEP model (R> 0.9825, R2 >0.9654, RMSE = 0.7929, KGE > 0.9188, and NSCE

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42 > 0.9566) outperformed the ANFIS model (R> 0.9601, R2 >0.9218, RMSE=1.495, KGE >

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44 0.8015, and NSCE > 0.8745) for the majority of the findings. The generated metamodel was

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47 robust enough to replace the repetitive expensive lab procedures required to measure

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49 thermophysical properties.

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54 **Keywords:** Thermophysical properties; Nanofluid; Artificial intelligence; Gene expression

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56 programming; ANFIS models

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## 3 Highlights

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5  Predictions of thermophysical properties of Fe3O4 coated MWCNT hybrid nanofluid

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8  AI-based ANFIS and GEP models performed well on statistical indices.

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10  ANFIS and GEP based prognostic models validated and compared with Taylor

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12 diagrams

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## 3 Abbreviations

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5 **AI** Artificial intelligence **KGE** Kling-Gupta efficiency

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1. **ANFIS** Adaptive neuro-fuzzy inference
2. system

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| --- | --- | --- | --- |
| **ANN** | Artificial neural network |  | Multi-walled carbon nanotubes |
| **Al2O3** | Alumina | **NSCE** | Nash Sutcliffe efficiency |
| **CuO** | Cupric oxide | **SiC** | Silicon carbide |
| **EA** | Evolutionary algorithm | **R** | Pearson’s correlation coefficient |
| **ET** | Expression tree | **R2** | Coefficient of determination |
| **Fe3O4** | Magnetite | **RMSE** | Root mean squared error |
| **GEP** | Gene expression programming | **RSM** | Response surface methodology |

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**ML** Machine learning

## MWCNT

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## 3 1. Introduction

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5 The usage of nanofluids, which are nano-sized materials suspended in a variety of

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8 working fluids, increases thermophysical characteristics. It led to significant breakthroughs in

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10 heat transfer applications [1]. Hybrid nanofluids are formed by the dispersion of two or more

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12 distinct nanomaterial combinations in a base fluid or base fluids. They are frequently used in

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15 heat transfer applications due to their higher thermal conductivity than regular nanofluids [2].

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17 Another motivation for combining nanoparticles to form a hybrid nanofluid is to allow the

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19 physio-chemical properties of the individual nanomaterials to synergize. Consequently, a

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21 nanofluid with higher thermal conductivity and rheological properties than their thermal

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24 conductivity is created [3]. The improved thermal transfer performance has resulted in a smaller

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26 heat exchanger, needing fewer materials and energy. A modest number of nanoparticles floating

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28 in the base fluid in energy storage systems or automotive radiator technology may cool and

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31 disperse heat faster than a huge volume of traditional fluid without nanoparticles. This has a

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33 huge impact on renewable energy systems and vehicle design since heat exchangers/radiators

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35 of smaller sizes may be constructed with less weight, saving space and money while boosting

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38 system efficiency [4][5][6].

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40 The thermophysical characteristics of the test nanofluids play an important role in

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42 determining heat transfer efficiency. To evaluate heat transfer capabilities, researchers are

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44 interested in exact measurements of thermal conductivity, density, viscosity, and specific heat.

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47 Thermal conductivity and viscosity were the two thermo-physical parameters of nanofluids that

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49 scientists were most interested in. A couple of them looked at other factors like as density and

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51 specific heat. Thermal conductivity and viscosity alone are insufficient to theoretically estimate

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54 heat transfer coefficients. Heat transport information also requires density and specific heat.

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56 These qualities must be calculated precisely since they have a significant impact on nanofluid

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58 flow and heat transfer characteristics. Many restrictions exist in the experimental assessment of

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3 nanofluid characteristics, such as challenges in producing monodisperse suspensions,

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5 concentration, systematic issues in measuring particle size, and solution inhomogeneity. As a

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8 result, the range of variables studied is constrained.

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10 Various heat transfer augmentation tactics and flow conditions, on the other hand, have a

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12 non-linear influence on the thermophysical properties of nanofluids. Many influencing

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15 elements, nonlinearity, and rationales make nanofluid research challenging and limit its

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17 potentially significant applications. In this context, machine learning (ML) approaches based

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19 on artificial intelligence (AI) are proving to be particularly effective in nanofluid research for

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21 predicting thermophysical characteristics and their performance in energy systems [7][8]. The

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24 continual growth in computational power, along with the introduction of powerful AI & ML

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26 approaches for regression and model prediction [9][10], has enabled reliable prediction of the

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28 highly non-linear behavior of hybrid nanofluids characteristics [11]. AI-based approaches are

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31 proven to be increasingly valuable as alternatives to established procedures or as elements of

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33 integrated systems. They have been utilized to tackle complex practical problems in a range of

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35 sectors and are growing increasingly popular at the time. AI approaches can train from patterns;

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38 they are highly reliable in the notion that they can accommodate noisy data; they can handle

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40 non-linear problems; and, once learned, they can do generalization and estimate at high speeds

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42 [12]. Several studies have reported the efficient use of ML approaches for the model prediction

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44 of hybrid nanofluid properties. For example, the ANN [13][14][15][16][17], random forest

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47 regression [18][19], Bayesian regularization network [20], Multivariate adaptive regression

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49 splines [21], genetic algorithm [22][23], and particle swarm optimization [24][25] was used for

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51 mapping and predicting the thermophysical properties of hybrid nanofluids. The literature

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54 survey reveals extensive use of ANNs for model prediction in the domain of nanofluid

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56 characterization. Malika and Sonawane [26] estimated the thermal conductivity ratio of Fe2O3

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58 doped SiC in water base fluid employing a combination of response surface methodology

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3 (RSM) and artificial neural network. It was concluded that as the ultrasonication time,

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5 temperature, and nanoparticle concentration were increased, the thermal conductivity ratio

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8 improved. Even though the RSM-ANN hybrid strategy yielded second-order correlation

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10 equations, the ANN outperformed the RSM in model prediction. Kumar et al. [27] investigated

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12 the thermophysical properties of hybrid nanofluids as a function of temperature. An ANN-based

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15 model was developed using the experimental data. The thermophysical properties of hybrid

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17 nanofluids were predicted using the ANN technique with high efficiency.

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19 ANFIS is a hybrid intelligence technique that combines a sharp decision-making ability

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21 of fuzzy methods with the good training ability of neural networks. In essence, ANFIS

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24 combines the advantages of these two models (ANN and FIS) into a cohesive solution for

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26 addressing scientific and technical difficulties [28]. ANFIS has been widely used for complex

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28 system modeling [29]. To solve some of the shortcomings of ANN, like poor speed and poor

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31 adaptiveness, the ANFIS employs a hybrid approach with input clustering [30]. To model

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33 predict the thermophysical properties of reduced graphene oxide/cobalt tetraoxide (rGO/Co3O4)

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35 hybrid nanofluids, Said et al. [31] used an adaptive neuro-fuzzy inference system (ANFIS).

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38 Subsequently, the ANFIS model’s output was optimized utilizing a marine predator algorithm.

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40 The hybridization strategy produced more accurate modeling and optimization. In another study

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42 by Said et al. [32], ANFIS was employed to predict the thermophysical characteristics of nano

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44 diamond-water nanofluids. The experiential data was collected for modeling at various

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47 temperatures and concentrations. The optimizer confirmed that the ideal values of the

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49 thermophysical properties could be achieved even when no nanomaterial was utilized in the

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51 multi-objective method and that the optimal temperature was determined to be 59.48 °C. The

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54 literature survey shows that ANFIS can provide superior prediction performance with less

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56 computing time. The literature in the realm of nanofluid characterization is overloaded with the

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58 usage of ANNs. There is numerous published research that employs ANNs for model

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3 prediction. Despite their advantages, ANN-based computational intelligence models are black

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5 boxes. Black boxes are weight matrices with some difficult to interpret biases [33]. The issues

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8 mentioned above can be resolved by generating explicit mathematical relations that may be

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10 understood and employed in practical works. Evolution-based Gene expression Programming

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12 (GEP) is one such machine learning method that improves upon the shortcomings of neural

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15 networks. The GEP model may be shown as expression trees, which can be readily translated

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17 to metathetical expressions. The key advantage of the GEP model is that it transmits its result

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19 as an expression tree and an easy link between the design variables and the intended outcome.

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21 Unlike many optimization strategies, which need prior knowledge of the relationship between

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24 the model parameters and the output parameter. As a result, many optimization approaches'

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26 rigors in establishing the model parameter combination that will produce the best outcomes

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28 have been overcome [34][35]. GEP had been used effectively in the model prediction of

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31 complex engineering problems such as combustion-emission modeling of biodiesel-powered

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33 engines [36][37], modeming of green concrete properties [38], and model prediction of

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35 meteorological data [39]. Despite being a very effective prognostic tool, GEP's prediction

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38 potential has yet to be completely realized in the realm of hybrid nanofluid characterization. As

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40 a result, the current initiative aims to fill a critical research gap in the rapidly developing study

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42 domain of hybrid nanofluids. The primary goals of this research are as follows:

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44 • Creating a prediction model using GEP and comparing it with benchmark ANFIS

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47 • Modern statistical performance criteria like as Nash-Sutcliffe efficiency (NSE) and

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49 Kling-Gupta efficiency (KGE), among others, were used to compare ANFIS with GEP

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51 models.

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54 • Graphically using Taylor diagrams to compare prediction models.

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## 3 2. Methodology

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5 The primary objective of employing soft computing techniques was to develop a

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8 regression model between input and output. In this work, the volume percent nanoparticle

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10 concentration in hybrid nanofluids and the nanofluid temperature were employed as input

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12 variables. The output variables were thermal conductivity, density, specific heat, and viscosity.

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15 The prediction model was developed using the evolutionary GEP approach and the Neuro-

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17 Fuzzy based ANFIS. Four distinct prediction models were created, one for each output and a

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19 wide range of temperature and mixture concentrations.

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## 24 2.1 Data for modeling

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26 The data for the modeling came from lab-based observations of the thermophysical

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28 properties of nanofluids. Thermal conductivity, viscosity, density, and specific heat were

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31 measured in 5 oC increments throughout a nanofluid temperature range of 20 oC to 60 oC. Data

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33 was collected in a similar manner for different nanofluid concentrations, namely 0% (only base

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35 fluid), 0.05% (0.05% hybrid nanoparticles + 99.95% base fluid), 0.10% (0.10% hybrid

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38 nanoparticles + 99.90% base fluid), 0.20% (0.20% hybrid nanoparticles + 99.8% base fluid),

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40 and 0.30% (0.30% hybrid nanoparticles + 99.7% base fluid). There was a total of 45 data points.

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42 Thirty-one (70%) of the 45 datasets were used to train the model, with the remaining used for

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44 testing and validation.

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## 49 2.2 Gene expression programming

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51 Ferreira [40] proposed the GEP method as an advancement over genetic programming

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54 (GP). GEP is an evolutionary algorithm (EA) that is based on the notion of biological evolution.

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56 Evolutionary algorithm-based computing is an approach for engineering optimization in which

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58 solutions are developed through processes modeled after Darwinian evolution rather than being

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3 built from fundamental principles. Heuristic search, often known as trial and error, is an

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5 example of evolutionary computation. In EA, "trials" are alternative solutions, and "error" is

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8 the measurement of how far a trial is from the anticipated conclusion. The error is used to

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10 determine which trials will be used to generate new trials. GEP is recognized as superior to

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12 other approaches. Since simple mathematical equations define GEP's output, it is more adaptive

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15 and accurate [41]. GEP has a one-of-a-kind, multi-genic nature that allows for creating more

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17 complicated programs. The GEP consists of two main components: chromosomes and

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19 expression trees (ET). Each chromosome is composed of a set of mathematically represented

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21 genes. A gene contains two parts: a head and a tail. The head is made up of mathematical

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24 functions, variables, or constants. The tail of a gene consists of terminal symbols such as a fixed

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26 value or variables that determine the terminal. A head connects the several gene terminals and

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28 generates an encoding formula using arithmetic operators or mathematical functions [42][43].

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31 The selection, crossover, and mutation are the main functions. The mutation improves the

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33 chromosomes during the GEP optimization procedure. For greater fitness functions, crossover

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35 operators are used. The GEP flowchart is shown in **Fig .1**.

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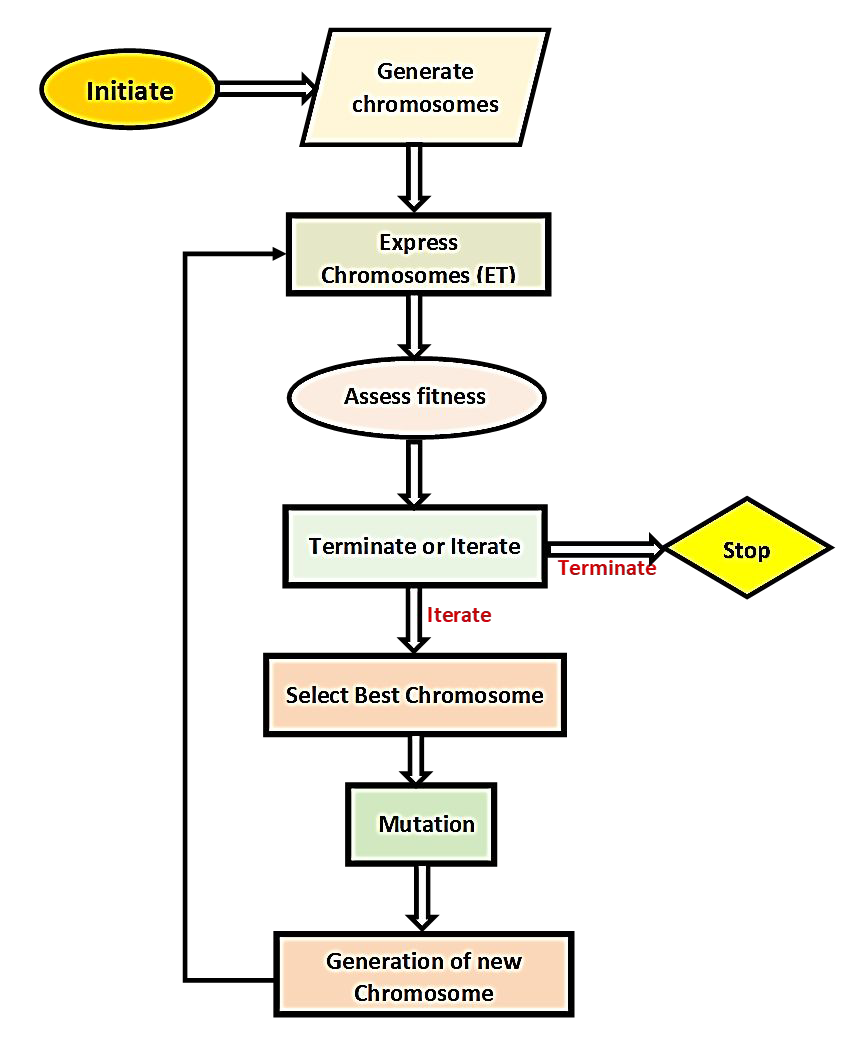
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44 **Fig. 1.** Flow chart for gene expression programming

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48 **Fig. 2** illustrates the model developed with GEP in the form of an expression tree (ET).

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51 It shows a total number of three trees for each model, and their addition forms the model. This

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53 model is used to predict output using the entire range of input conditions. A higher degree of

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1. correlation observed between input and output indicates a robust prediction model.

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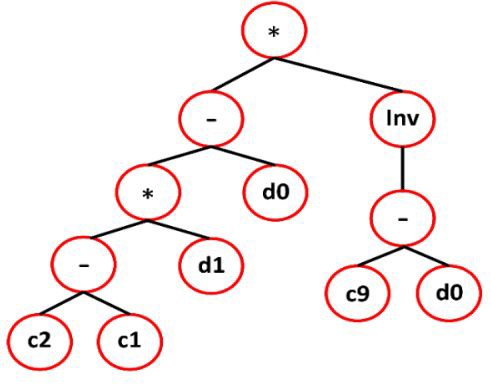
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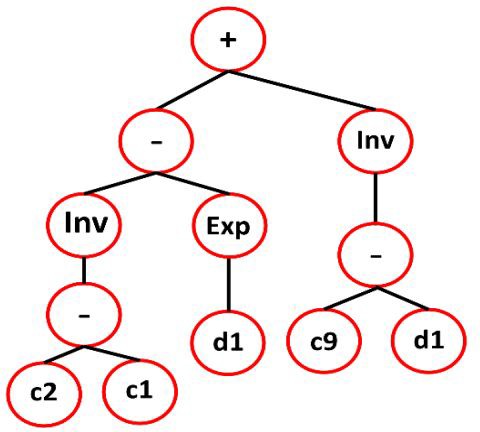
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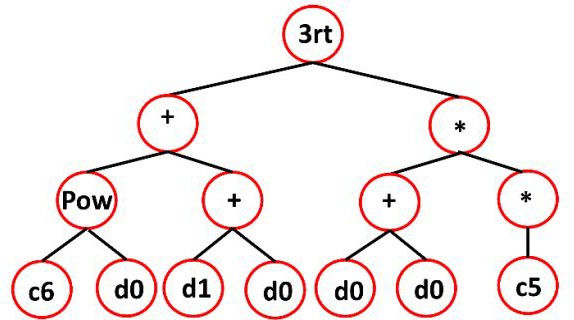


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**Sub-ET 2**

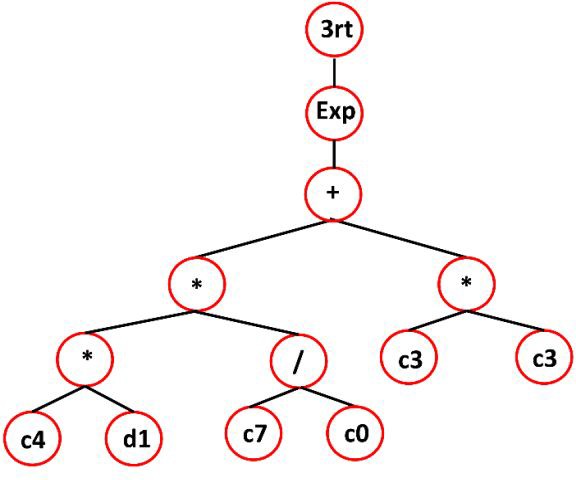


**Sub-ET 3**



**Sub-ET 1**

**Sub-ET 2**



**Sub-ET 3**

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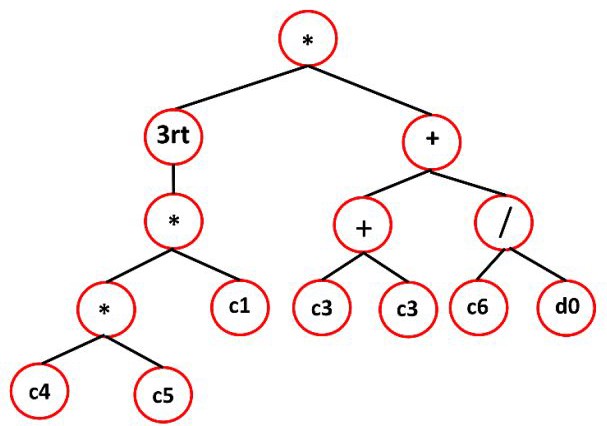
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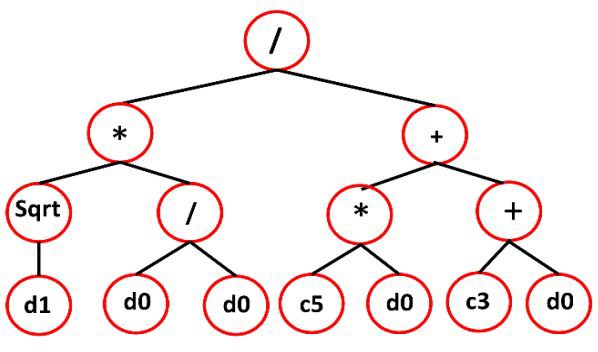
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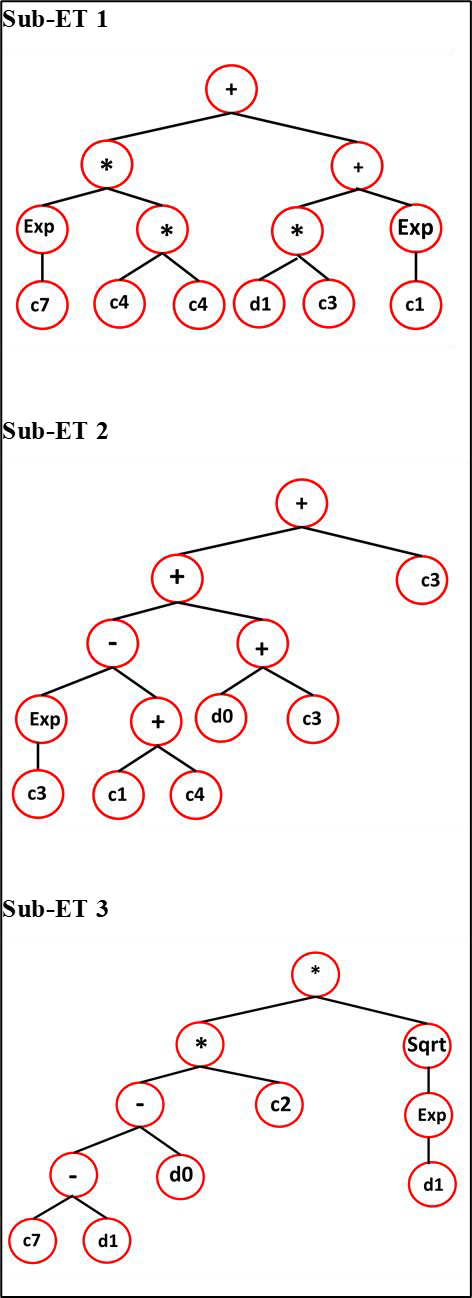
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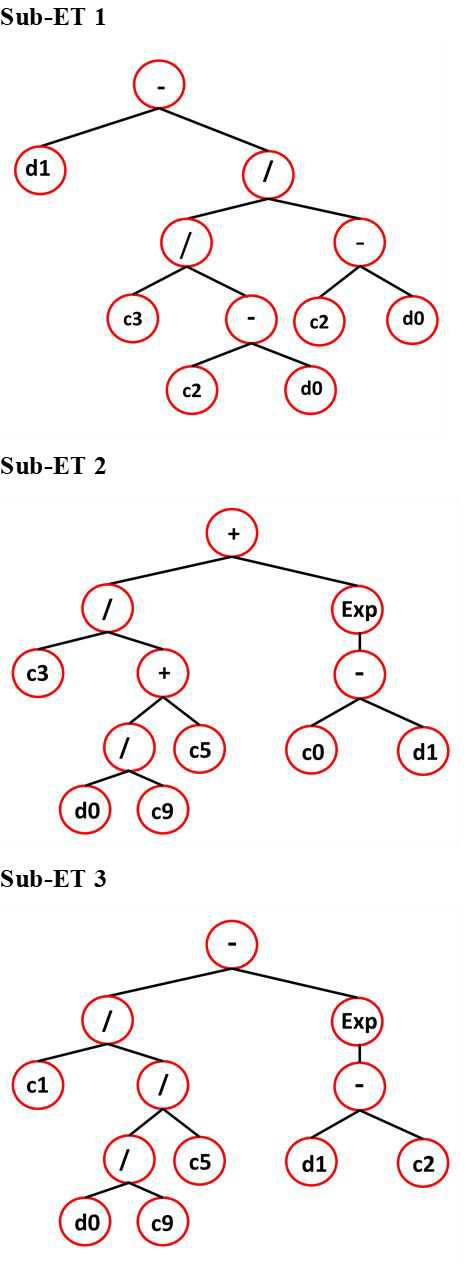
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52 (c) (d)

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1. **Fig. 2.** Illustration of GEP model in the form of expression trees (ET) for (a) thermal
2. conductivity, (b) density, (c) viscosity, and (d) specific heat

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## 3 2.3 Adaptive neuro-fuzzy inference system

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5 The adaptive neuro-fuzzy inference system (ANFIS) is an intelligent computation

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8 modeling technique. It combines the learning and logical reasoning abilities of ANNs and fuzzy

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10 logic. ANFIS provides higher prognostic capabilities and is a preferable alternative to

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12 conventional neural networks for complicated non-linear issues [25]. A typical fuzzy inference

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14

15 system (FIS) has five steps, starting with the introduction of inputs to aid in the fuzzification of

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17 fuzzy sets based on linguistic rule activation. Specialists design certain rules, which are

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19 subsequently generated from test results. The next phase is inference, which involves mapping

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21 fuzzy sets based on established criteria. The fuzzy sets are then defuzzied, yielding the final

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24 output values. Consequently, the ANFIS strategy involves data preparation, ANFIS creation,

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26 variable selection, training, validation, and output generation [28].

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28 The ANFIS design is comprised of five separate levels, as seen in **Fig. 3**. The first layer

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31 is the input layer, which accepts the input value and generates fuzzy values using membership

32

33 functions (MF). This layer contains adaptive type nodes, each with its node function. The

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35 product layer is the second layer, and it multiplies the input signal. It is made up of fixed nodes

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38 that assess the weight or firing strength. It often employs the fuzzy operator 'AND.' The nodes

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40 in the third tier are all fixed nodes. The firing strength is computed in this layer. The normalized

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42 firing strength represents the output. The fourth layer, which contains adaptive nodes, is utilized

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44 to define the output membership function. The last layer is known as the output layer. It has a

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47 single fixed node that summits all incoming signals from preceding layers [44][45]. To alter the

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49 parameters of the membership functions throughout the ANFIS training process, a hybrid

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51 learning strategy combining the least-squares estimate and the gradient descent approach is

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54 used. The node outputs are processed in the forward pass until the least-squares estimate

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56 determines the output membership function layer and the associated parameters. After the error

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58 signals have been carried backward, the backward pass uses the gradient descent approach to

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3 update the premise parameters. A fuzzy set's membership function is a mathematical extension

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5 of the indicator function. It is an extension of valuation in fuzzy logic that indicates the degree

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8 of validity. Because the ANFIS structure requires a better selection of acceptable form and

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10 number of membership functions, every ANFIS application requires a firm grasp of fuzzy logic.

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12 This has an impact on the ANFIS-based model's effectiveness and computation cost. The

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15 number of rules in the ANFIS rule-base is determined by the number of input space partitioning

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17 membership functions. In addition, the number of parameters in each membership function has

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19 an effect on training costs. Because of its smooth representation of the input space, the Gaussian

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21 form of the membership function has only two parameters and is the most commonly used in

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24 the literature [46][32]. **Fig. 4** shows the ANFIS flow chart. **Fig. 5** illustrates the fuzzy logic and

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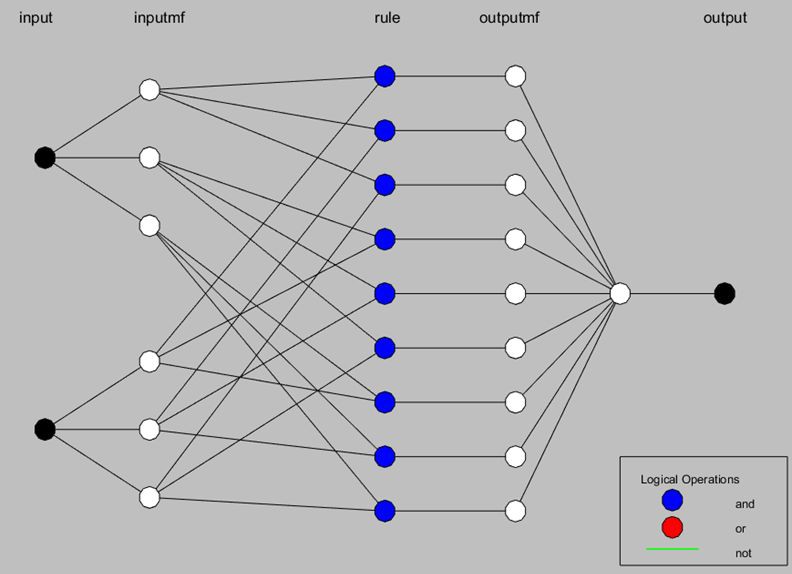
26 membership function for each output model. As illustrated in **Fig.6**, the model's output may be

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28 seen using a fuzzy inference system (FIS) designed for each output model.

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58 **Fig. 3.** ANFIS architecture

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**Select input variables**

**Start**

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**Data partition**

**Testing**

**Training**

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**MSE**

**Satisfactory?**

**No**

**Yes**

**MSE**

**Satisfactory?**

**No**

**Yes**

**Train & test**

**MF number decision**

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**MF number decision**

**Train & test**

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**Proposed model**

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**% Error**

**Prediction**

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**End**

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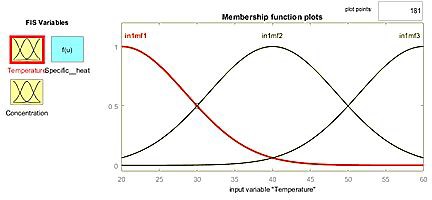
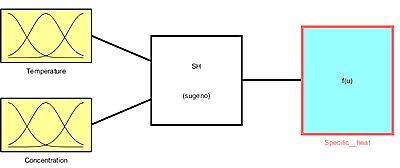
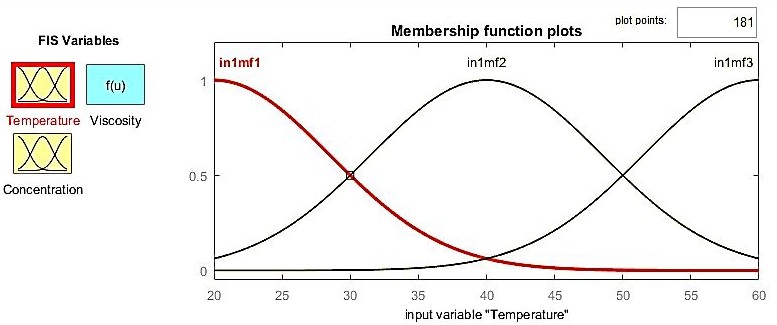
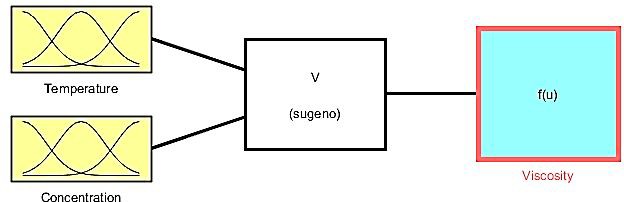
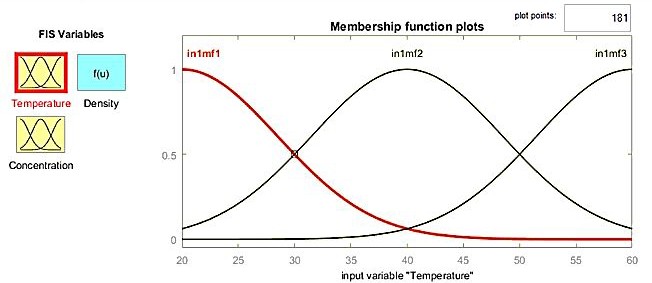
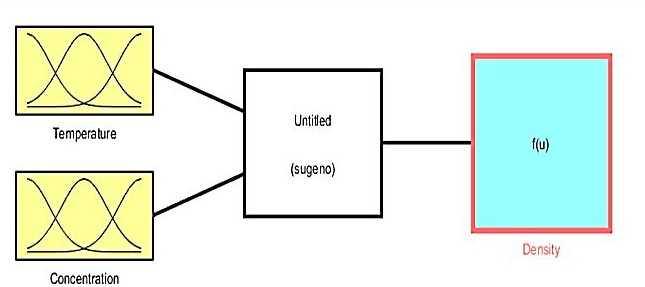
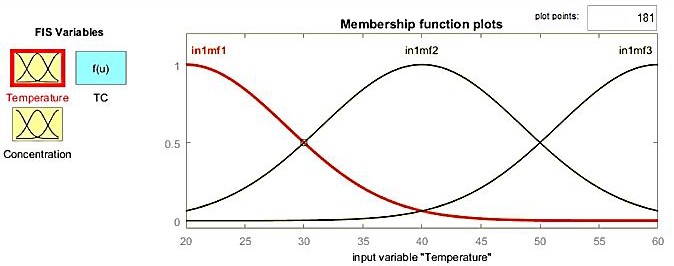
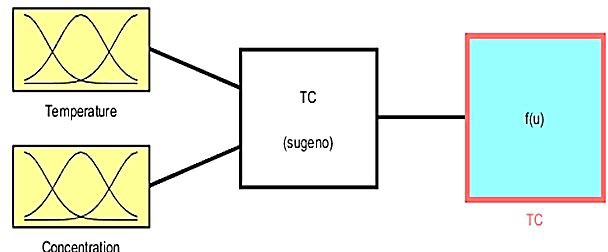
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3 **Fig. 4.** The flow chart of implemented ANFIS modeling technique

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# 14 Fuzzy logic Membership function

15 (a)

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For

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# 27 Fuzzy logic Membership function

28 (b)

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# 39 Fuzzy logic Membership function

40 (c)

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# 53 Fuzzy logic Membership function

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55 (d)

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58 **Fig. 5.** ANFIS fuzzy logic and membership function for (a) - Thermal conductivity

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60 (b) - Density; (c) – Viscosity; (d) - Specific heat

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4 The ANFIS helped in mapping the effects of input parameters on the physio-thermal

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6 properties of hybrid nanofluids. The 3D surface diagrams depicting the effects of input

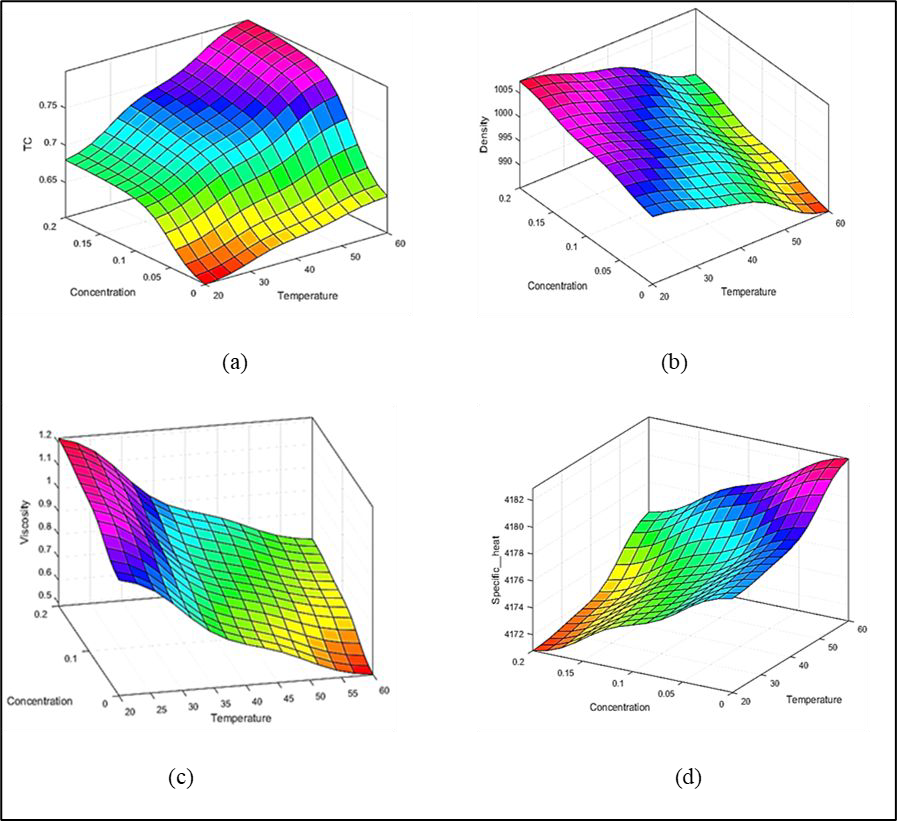
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9 parameters are shown in **Fig. 6**.

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1. **Fig. 6.** 3D surface diagrams for (a) - Thermal conductivity; (b) – Density; (c) – Viscosity; (d)
2. - Specific heat

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## 3 2.4. Statistical evaluation of prediction models

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5 The current study investigates model reliability in depth by subjecting the created model

6

7

8 to different error metrics invariant to scale transformation, as well as uncertainty estimation

9

10 measures, to assess the robustness of the ANFIS and GEP-based models. Though commonly

11

12 used model evaluation metrics were used to compare model performance to similar studies,

13

14

15 each result was supported by values obtained from a correspondingly scaled variation of the

16

17 original metric to address the metric's inherent limitations while retaining the attribute of the

18

19 conventional measure.

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## 24 2.4.1. Pearson’s coefficient of correlation (R)

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26 To assess the relationship between measured and predicted output values, the Pearson

27

28 correlation coefficient (R) and coefficient of determination were employed [47]. R is just a

29

30

31 normalized measurement of covariance, with the result always lying between 0 and 1. It is the

32

33 product of the covariances of two variables and their standard deviations. Like covariance, the

34

35 measure may only represent a linear correlation of variables and ignores several other kinds of

36

37

38 linkage or relationship. R has limitations in reporting the correlation if one or more data points

39

40 are missing. The maximum likelihood estimator is utilized in such a case. The expression used

41

42 for the estimation of R is given in Eq. (1).

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45 𝑅 =

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∑𝑛

𝑖 = 1

∑𝑛

𝑖 = 1

(𝑥𝑖 ― 𝑥 )2 ∑𝑛 ( 𝑦𝑖 ― 𝑦)2

𝑖 = 1

(𝑥𝑖 ― 𝑥)(𝑦𝑖 ― 𝑦)

(1)

## 51 2.4.2. Coefficient of determination (R2)

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53 Correlation is a comprehensive measure of the strength of a link between variables. The

54

55

56 most common application of the term correlation in the sense of a linear link between two

57

58 continuous variables is Pearson product-moment correlation. A Spearman rank correlation can

59

60 be employed to measure monotonic association for nonnormally distributed continuous data,

1

2

3 ordinal data, or data with noteworthy outliers. Both correlation coefficients are scaled from –1

4

5 to +1, with 0 indicating no linear or monotonic association and 1 indicating a greater

6

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8 relationship that eventually approaches a straight line [34][48].

9

(

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11 𝑅2 = 1 ―

∑𝑛

𝑖 = 1

∑𝑛

(𝑥𝑖 ― 𝑦𝑖)2

( 𝑦𝑖)2

(2)

12 𝑖 = 1

13

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## 17 2.4.3. Mean absolute percentage error

18

19 MAPE is a measure for predicting accuracy. It is also known as a loss function and is

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21 used to interpret relative error evaluation. A MAPE value can be any positive number between

22

23 0 and 1. The mean absolute percentage error (MAPE) is one of the most often used metrics of

24

25

26 forecast accuracy due to its scale independence and interpretability. On the other hand, MAPE

27

28 has a certain limitation of giving infinite or undefined answers for zero or close-to-zero real

29

30 numbers [49]. However, the combined usage of R2 and MAPE overcomes this difficulty by

31

32

33 presenting an overall quality of prediction. The following formula was used to compute MAPE:

34

35 𝑀𝐴𝑃𝐸 = 1∑𝑛

|𝑥𝑎𝑖 ― 𝑥𝑝𝑖| × 100

(3)

36 𝑛

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𝑖 = 1

𝑥𝑎𝑖

## 41 2.4.4. Root mean squared error

42

43 The RMSE is a predictive ability statistic that considers the magnitudes of prediction

44

45 errors for several data points. The RMSE is a scale-dependent accuracy statistic used to

46

47

48 compare the prediction errors of many models on a single dataset rather than across datasets.

49

50 The RMSE number is never negative, and a value of 0 (which is seldom reached in practice)

51

52 implies that the data is perfectly matched. A lower RMSE is better than a higher RMSE in

53

54 general. Comparing different data types would be erroneous since the metric is susceptible to

55

56

57 outliers and relies on the quantity of the numbers used. The following expression was used for

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59 the calculation of RMSE:

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4 𝑅𝑀𝑆𝐸 =

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𝑛

𝑖 = 1

(𝑥𝑝𝑖 ― 𝑥𝑎𝑖)2]

𝑛

(4)

## 8 2.4.5. Nash-Sutcliffe efficiency (NSCE) and Kling-Gupta efficiency (KGE)

9

10 The Nash–Sutcliffe efficiency is a popular statistical index since it normalizes model

11

12 performance onto an understandable scale. The NSE metric measures how well-simulated data

13

14 predict output data in a model. It is a normalized statistical number between 0 and 1 that

15

16

17 indicates the ratio of residual variance ("noise") to real data variance ("information"). The

18

19 closest NSE value denotes a perfect match between experimental and model data. The Nash–

20

21 Sutcliffe Coefficient obscures fundamental behaviors that, if recast, might assist in

22

23

24 understanding model behavior in terms of bias, unpredictability, and other aspects. The

25

26 alternative "Kling-Gupta" efficiency bounds differ from those of the NSE [50][51]. The

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28 following expressions were used for the estimation of NSCE and KGE.

}

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31

𝑁𝑆𝐶𝐸 =

1 ― {

∑𝑛

𝑖 = 1

(5)

(𝑥

― 𝑥 )2 |

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35 𝐾𝐺𝐸 = 1 ―

(𝛿 ― 1)2 + (𝛼 ― 1)2 + (𝑅 ― 1)2

36

∑𝑛

𝑖 = 1

𝑎𝑖

𝑝𝑖

(𝑥𝑎𝑖 ― 𝑥𝑝)2

(6)

37 Where, (for Eq. (1) to Eq. (6)), *‘i’* represents term under consideration*, ‘n’* represents total

38

39

40 elements*, ‘xai’* denotes the actual value*, ‘xpi’* represents predicted value*,* ′𝑥𝑎′ is mean actual values*,* 𝑥𝑝 is

41

42 mean predicted values*, ‘δ’* denotes bias error*, ‘α’* denotes error in flow variability, and correlation is

43

44 shown with *‘R’.*

45

46

47

## 48 2.5 Taylor diagrams for model comparison

49

50 Taylor diagrams effectively demonstrate better models that use several model

51

52 performance metrics as a single visual comparison portrayal [52]. They are an excellent tool

53

54

55 for displaying improved models since they utilize several model performance criteria as a single

56

57 visual comparison depiction. Taylor diagrams are utilized in this research to compare

58

59 the statistical correlation between observed and ML-based model performance in simulating

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3 the thermophysical characteristics of hybrid nanofluids. Correlation, standard deviation, and

4

5 root-mean-square error were determined for the graphical representation of the relationship

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7

8 between observed and simulated data. The Taylor diagram facilitates model comparison by

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10 showing them in a single figure. The radial distance from the origin represents the standard

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12 deviation between observed and simulated data, whereas the distance from the observed point

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15 on the x-axis represents the centered root-mean-square error (CRMSE) [53].

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## 19 3. Results and discussion

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22 The research study aims to characterize the different thermophysical characteristics of

23

24 Fe3O4 coated MWCNT hybrid nanofluids utilizing two clever AI-based approaches, GEP and

25

26 ANFIS. Thermal conductivity, viscosity, density, and specific heat of hybrid nanofluids were

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28 investigated in a laboratory-scale experiment. The measurements were taken at various

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31 temperatures and nanoparticle concentration ratios in the base fluid. The experiment data was

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33 then utilized to build prediction models [54][55]. GEP was used for model generation and

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35 prediction in the first phase, whereas in the second phase, ANFIS was used for model prediction

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37

38 under comparable conditions. Each attribute was given its model using GEP and ANFIS. Their

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40 prediction abilities are then compared using statistical markers and a Taylor diagram.

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## 45 3.1 Model prediction of thermal conductivity

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47 The developed models for thermal conductivity using ANFIS and GEP were evaluated

48

49 and found to be in good agreement with observed data, as shown in **Fig. 7**. The experimentally

50

51 determined thermal conductivity and predicted thermal conductivity are compared with trend

52

53

54 lines in **Fig.7a**. In **Fig.7b**, the performance of ANFIS and GEP projected values is shown for

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56 the complete dataset. The ANFIS and GEP models both performed excellently and were found

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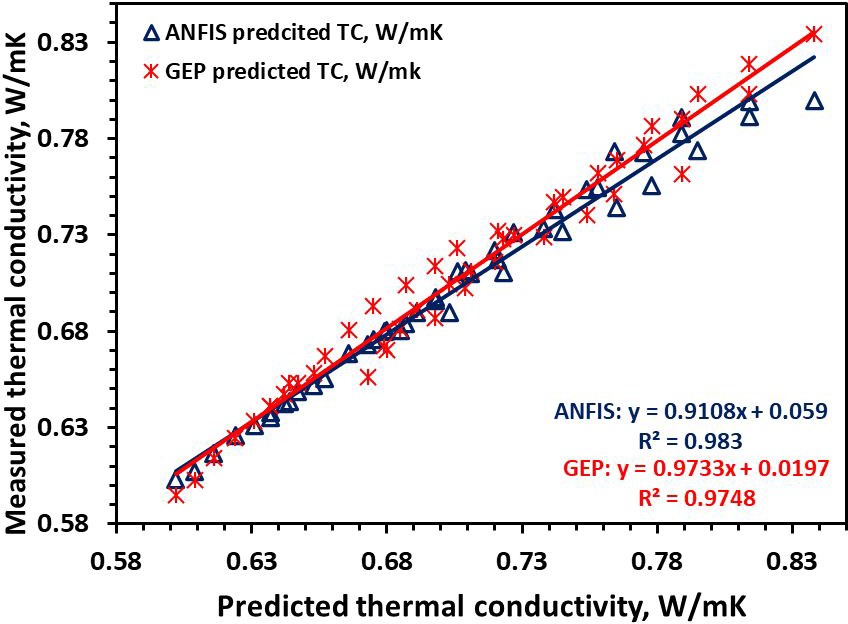
3 to be in good agreement with experimental data of thermal conductivity over a wide range of

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5 temperatures and concentration ratios.

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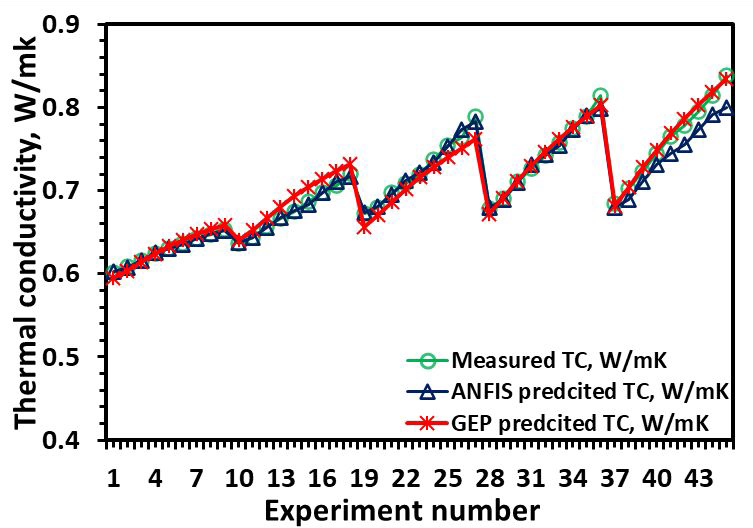
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33 (a)

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58 (b)

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3 **Fig .7.** Shows comparison with ANFIS and GEP for (a) the measured versus predicted

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5 thermal conductivities and (b) all the datapoints

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9 Statistical indicators were used to evaluate the thermal conductivity model's prediction

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11 effectiveness. In the case of ANFIS, the correlation value R was 0.9914; however, with the GEP

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13 model, it was reduced to 0.9872. R2 values for ANFIS and GEP were 0.983 and 0.9748,

14

15

16 respectively. The RMSE values for ANFIS and GEP were 0.0098 and 0.0095, respectively,

17

18 while the MAPEs were 0.74 and 1.08%, respectively. The predictive effectiveness of the

19

20 models tested using KGE for ANFIS and GEP was 0.9182 and 0.9188, respectively; similarly,

21

22

23 the NSCE for ANFIS and GEP was 0.9735 and 0.9755, respectively. **Table 1** shows the

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25 statistical indicators of model evaluation employed in this study. The Taylor diagram, shown

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27 in **Fig. 8**, is utilized to further compare the thermal conductivity models. The Taylor diagram

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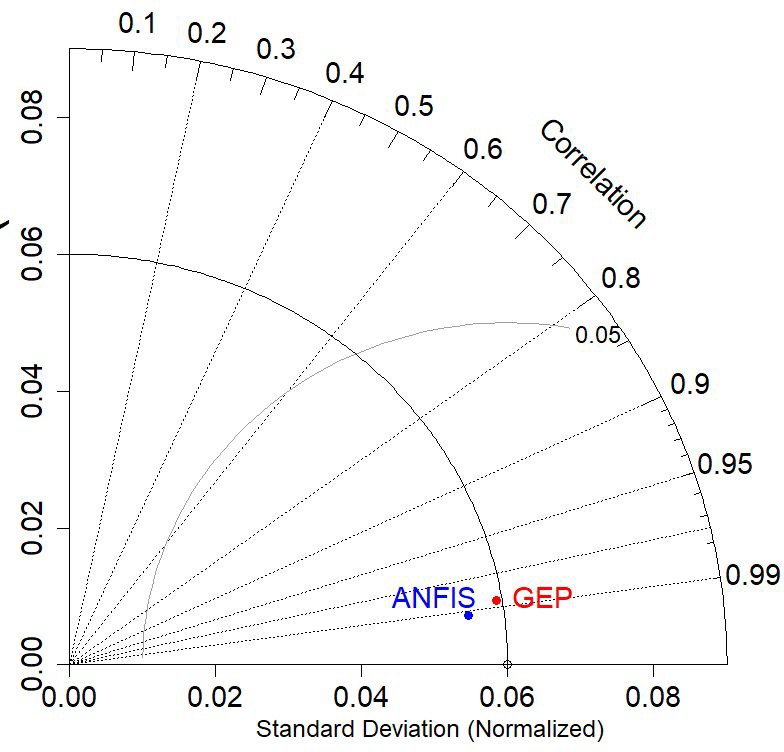
29 further proves the superiority of the ANFIS-based thermal conductivity model over the GEP

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32 model since the ANFIS model is closer to the observed values.

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3 **Fig. 8.** Taylor diagram for thermal conductivity model

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## 8 3.2. Model prediction of density

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10 The relative prediction performance of ANFIS and GEP for the density model is depicted

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12 in **Fig. 9**. Trendlines were used to compare the model projected density with observed density,

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15 as shown in **Fig. 9a**. In **Fig. 9b**, the performance of ANFIS and GEP projected values is shown

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17 for the entire density dataset. It was observed that the ANFIS and GEP models could forecast

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19 density over a wide variety of test conditions. GEP, on the other hand, outperforms ANFIS in

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22 the density model.

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24 The predictive efficacy of ANFIS and GEP-based density models is assessed using

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26 statistical indicators. In the instance of ANFIS, the correlation value R was 0.9816, but it

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28

29 improved to 0.9974 for the GEP-based density model. While the R2 for ANFIS and GEP were

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31 0.9636 and 0.9948, respectively. RMSE and MAPE were used to calculate model errors in the

32

33 present study. The RMSE for ANFIS and GEP was as low as 1.462 and 0.475, respectively

34

35 while MAPEs for ANFIS and GEP were exceedingly low, at 0.09% and 0.03%, respectively.

36

37

38 The predicted efficiencies of the density model were evaluated with KGE and NSCE. KGE was

39

40 0.8985 and 0.9965 for ANFIS and GEP based models, respectively; similarly, the NSCEs for

41

42 ANFIS and GEP were 0.98455 and 0.9985, respectively. **Table 1** shows the statistical indices

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45 obtained in this investigation. As demonstrated in **Fig.10**, all statistical indicators are depicted

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47 in a single graph using a spider plot.

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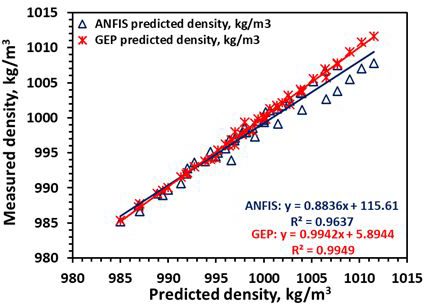
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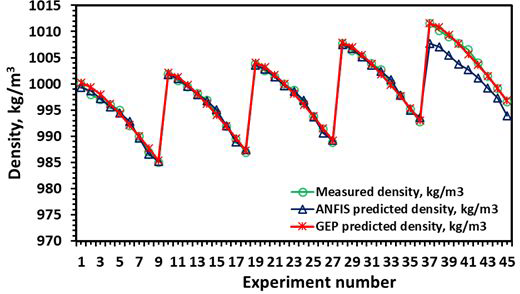
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26 **(a)**

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50 **(b)**

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53 **Fig. 9.** Shows comparison with ANFIS and GEP of (a) the measured versus predicted densities

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55 and (b) the density versus experiment number.

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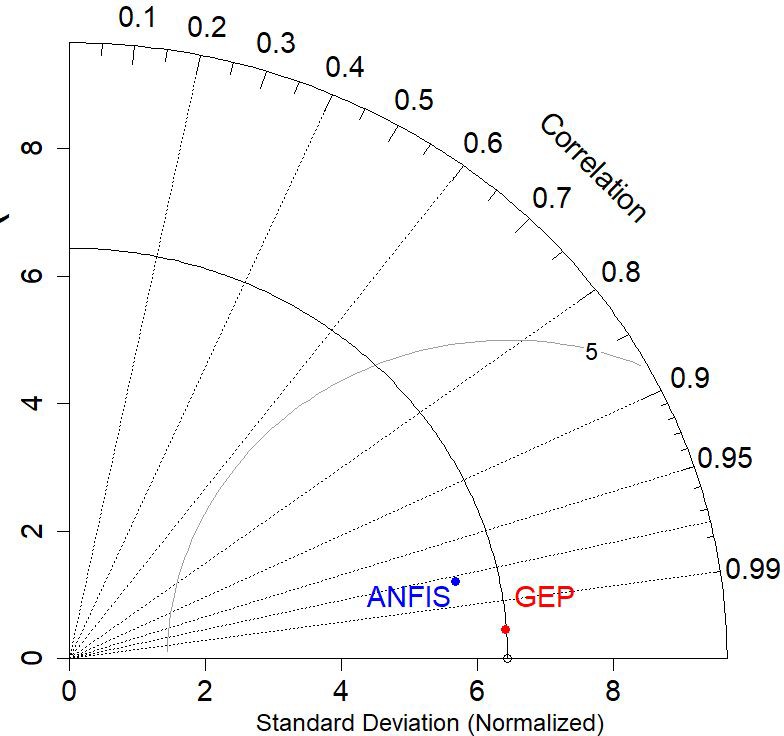
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28 **Fig. 10.** Taylor diagram for density model

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## 33 3.3 Model prediction of viscosity

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35 The viscosity data of Fe3O4 Coated MWCNT hybrid nanofluids were employed to

36

37 develop predictive models with ANFIS and GEP. **Fig. 11** compares and displays the predicted

38

39

40 outcomes of both models. A comparison graph comparing the observed and expected viscosity

41

42 is provided in **Fig. 11a**. The performance of ANFIS and GEP projected values for the entire

43

44 viscosity dataset is shown in **Fig. 11b**. The ANFIS and GEP models were validated using

45

46 measured viscosities and demonstrated excellent prediction performance over the whole range

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49 of test conditions. In contrast, the GEP-based viscosity model outperformed the ANFIS-based

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51 viscosity model.

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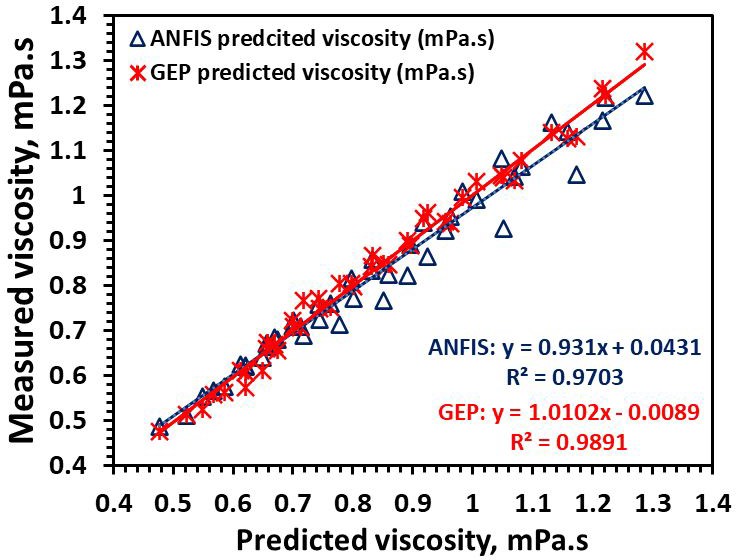
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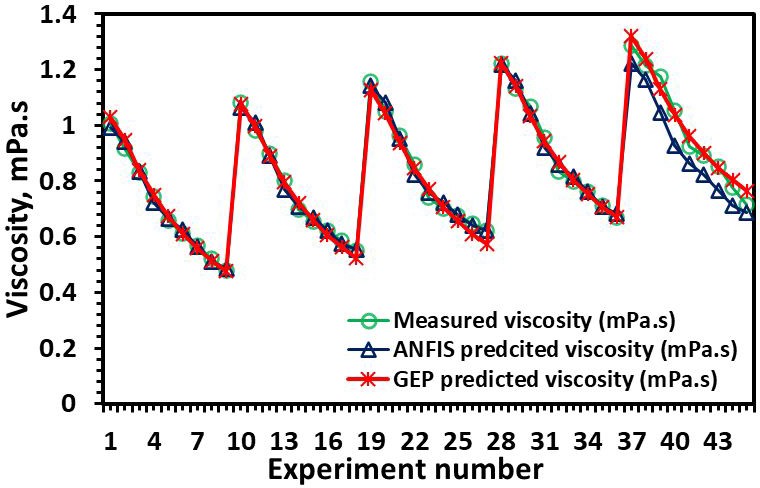
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47 **(b)**

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49 **Fig. 11.** Shows comparison with ANFIS and GEP of (a) the measured versus predicted

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51 viscosity model (b) the viscosity versus experiment number.

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54 The prediction performance of ANFIS and GEP-based viscosity models were evaluated

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57 using statistical markers. R2 values for ANFIS and GEP were 0.9702 and 0.9891, respectively.

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59 The correlation coefficient R for ANFIS was 0.9850, whereas it was 0.9945 for GEP. The errors

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3 in the models were calculated using RMSE and MAPE. The RMSE values for ANFIS and GEP

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5 were as low as 0.0396 and 0.0221, respectively. ANFIS and GEP MAPEs were 2.93 and 2.16%,

6

7

8 respectively. The prediction efficiencies for ANFIS and GEP KGE were 0.9402 and 0.9835,

9

10 respectively, while the NSCEs for ANFIS and GEP were 0.9645 and 0.9895. The statistical

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12 indices acquired in the current study are shown in **Table 1.** The viscosity models created with

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15 ANFIS and GEP were compared using Taylor diagrams (**Fig .12**). In terms of prediction, both

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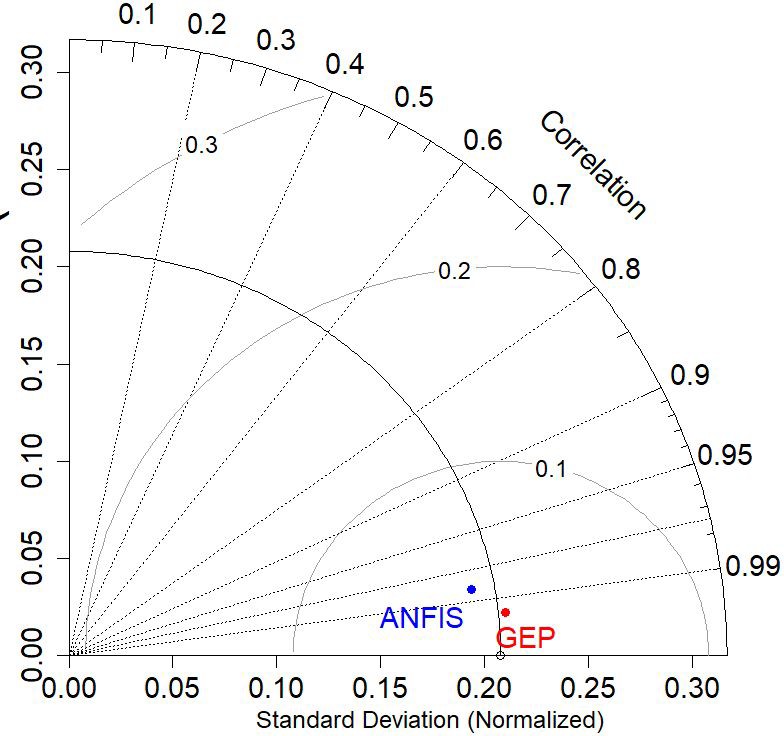
17 models were very efficient and accurate. In terms of statistical indices and the Taylor diagram,

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19 the GEP model outperformed the ANFIS model.

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46 **Fig. 12.** Taylor diagram for viscosity model

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## 51 3.4. Model prediction of specific heat

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53 The observed specific heat data of Fe3O4 coated MWCNT hybrid nanofluids were used

54

55 to build prediction models utilizing ANFIS and GEP. In **Fig. 13**, the expected results of both

56

57

58 models are contrasted and shown by comparing graphs. **Fig. 13a** depicts a graph comparing

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60 observed and predicted specific heat data. **Fig. 13b** depicts the performance of ANFIS and GEP

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3 projected values throughout the whole dataset. The ANFIS and GEP models performed

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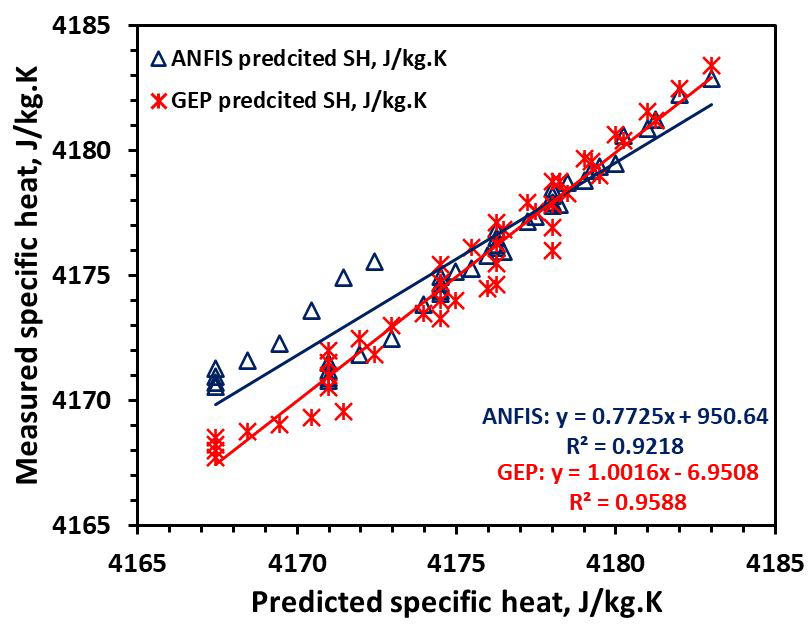
5 admirably over the whole range of test conditions. On the other hand, the GEP-based particular

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8 heat model outperformed the ANFIS-based specific heat model.

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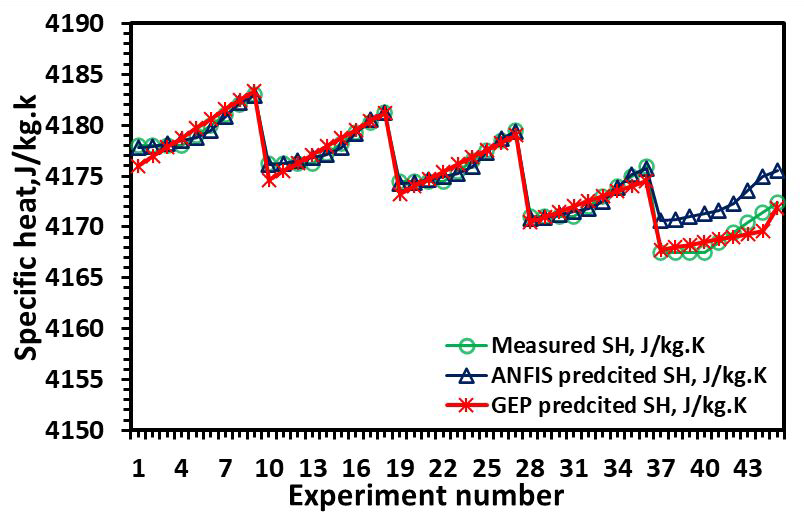
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32 **(a)**

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56 **(b)**

57 **Fig .13.** Shows comparison with ANFIS and GEP of (a) the measured versus predicted

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59 specific heat model and (b) the specific heat versus experiment number.

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3 The predictive capability of a specific heat model built using two AI-based intelligence

4

5 algorithms, ANFIS and GEP, was evaluated using statistical criteria. The correlation coefficient

6

7

8 R for ANFIS was 0.9601, while the GEP-based model increased to 0.9825. ANFIS and GEP

9

10 had R2 values of 0.9218 and 0.9654, respectively. The RMSE values for ANFIS and GEP were

11

12 1.495 and 0.7929, respectively, with MAPEs of 0.02% and 0.01%. KGE for ANFIS and GEP

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15 were 0.8015 and 0.9695, respectively. The NSCE values for ANFIS and GEP were 0.8748 and

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17 0.9566, respectively. The statistical indices acquired in this study are shown in **Table 1**. The

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19 Taylor diagram was also used to compare the individual heat models (**Fig .14**). The GEP-based

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21 specific heat model outperforms the ANFIS model, as evidenced by the Taylor diagram, which

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24 demonstrates that the GEP model is closer to the baseline value. In **Fig.15**, all statistical

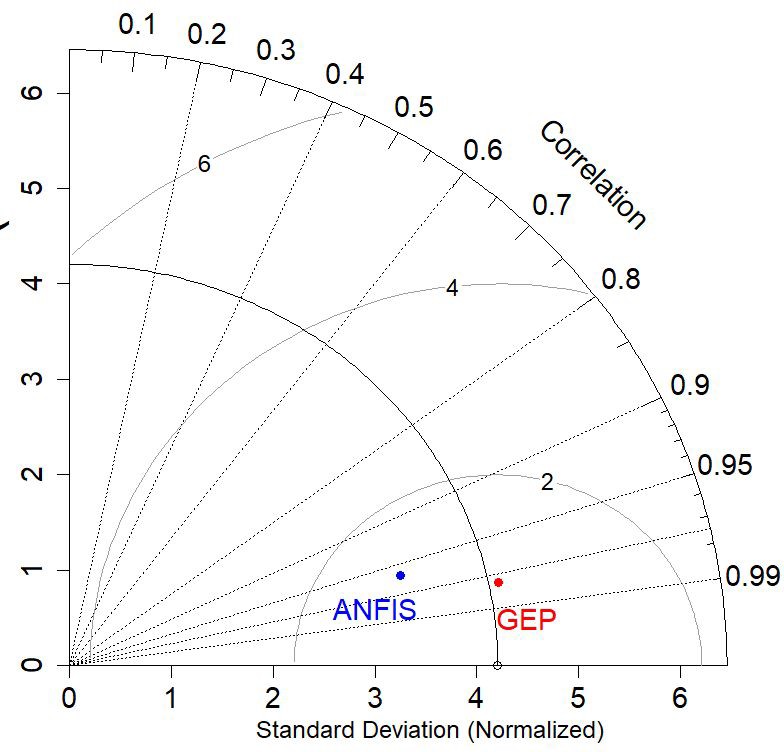
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26 indicators are shown in a single graph using a spider plot.

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55 **Fig. 14.** Taylor diagram for specific heat model

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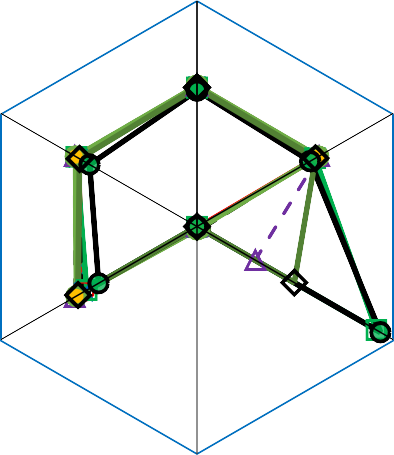
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**Thermal conductivity ANFIS Density ANFIS**

**Viscosity ANFIS**

**Specific heat ANFIS**

**Thermal conductivity GEP Density GEP**

**Viscosity GEP**

**Specific heat GEP**

**R**

**NSCE**

**1.6**

**1.4**

**1.2**

**1**

**0.8**

**0.6**

**0.4**

**0.2**

**0**

**R2**

**KGE**

**RMSE**

**MAPE**

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30 **Fig. 15.** Spider plot of various statistical indices

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34 **Table 1.** Statistical indices for ANFIS and GEP models

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## 36 Parameter R R2 RMSE MAPE KGE NSCE

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Thermal conductivity** | ANFIS | 0.9914 | 0.983 | 0.0098 | 0.74% | 0.9182 | 0.9735 |
|  | GEP | 0.9872 | 0.9748 | 0.0095 | 1.08% | 0.9188 | 0.9755 |
| **Density** | ANFIS | 0.9816 | 0.9636 | 1.462 | 0.09% | 0.8985 | 0.9845 |
|  | GEP | 0.9974 | 0.9948 | 0.4753 | 0.03% | 0.9965 | 0.9958 |
| **Viscosity** | ANFIS | 0.985 | 0.9702 | 0.0396 | 2.93% | 0.9402 | 0.9645 |
|  | GEP | 0.9945 | 0.9891 | 0.0221 | 2.16% | 0.9832 | 0.9895 |
| **Specific heat** | ANFIS | 0.9601 | 0.9218 | 1.495 | 0.02% | 0.8015 | 0.8748 |
|  | GEP | 0.9825 | 0.9654 | 0.7929 | 0.01% | 0.9695 | 0.9566 |

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## 51 4. Conclusions and future perspective

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53 The feasibility of AI-based GEP and Neuro-fuzzy techniques in modeling thermophysical

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55 characteristics of Fe3O4 coated MWCNT hybrid nanofluid was explored in this work.

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58 Laboratory analyses of the thermophysical characteristics of hybrid nanofluids provided the

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60 data for the prognostic model. Thermal conductivity, viscosity, density, and specific heat were

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3 determined in 5 ℃ increments throughout a 20 oC to 60 oC nanofluid temperature range and at

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5 various nanofluid concentrations (0%, 0.05%, 0.10%, 0.20%, and 0.30%). The model was

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8 trained using 70% of the datasets, with the remaining 15% utilized for testing and validation.

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10 Thermal conductivity, density, viscosity, and specific heat of Fe3O4 coated MWCNT hybrid

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12 nanofluid were effectively predicted using both GEP, and ANFIS approaches. The following

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15 are the main outcomes of the study:

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17  The prediction of thermophysical properties by GEP outperformed those of ANFIS. The

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19 GEP technique provides for an easier model development formulation and a higher

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22 degree of consistency between simulated and experimental data.

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24  The ANFIS and GEP models both fared well on statistical regression indices. The R for

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26 ANFIS was more than 0.9601 and greater than 0.9825 for GEP. In all situations, the R2

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29 value for ANFIS was greater than 0.9218, whereas it was greater than 0.9654 for GEP.

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31  The mean absolute percentage error (MAPE) for the ANFIS and GEP models was less

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33 than 2.93% and 2.16%, respectively. The root mean squared error (RMSE) for the

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36 ANFIS and GEP models was less than 1.495 and 0.9729, respectively.

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38  Taylor diagrams were used to compare the ANFIS and GEP-based prognostic models.

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40 These graphics demonstrate the GEP's superiority over ANFIS. For comparison, all

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42 statistical markers were displayed using a spider diagram.

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45 The proposed GEP and ANFIS-based prognostic models are efficient for forecasting the

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47 thermophysical properties of hybrid nanofluids based on temperature and nanoparticle

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49 concentrations, resulting in a cost-effective, time-saving, and dependable approach. Finally,

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52 based on the results of this study, it is crucial to emphasize that AI techniques are incredibly

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54 robust and effective tools for dealing with complicated processes, especially when mapping the

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56 properties of hybrid nanofluids. An intelligent generalization of mathematical equations to

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59 previously unknown data is possible. The author proposes that the current study be expanded

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3 to cover various additional types of AI approaches. This may assist in the development of a

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5 database that will aid in the selection of an appropriate AI technique.

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## 10 Declaration of interests

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12 The authors declare that they have no known competing financial interests or personal

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14 relationships that could have appeared to influence the work reported in this paper.

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