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Hybrid Machine Learning Techniques and Computational Mechanics: Estimating the Dynamic Behavior of Oxide Precipitation Hardened Steel

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ABSTRACT A new generation of Oxide Dispersion Strengthened (ODS) alloys called Oxide Precipitation Hardened (OPH) alloys, has recently been developed by the authors. The excellent mechanical properties can be improved by optimizing the chemical composition in combination with heat treatment. However, the behavior of such materials requires the consideration of a large number of variables, nonlinearities, and uncertainties in the analyses, and the modeling of such alloys by analytical methods is not accurate enough. Therefore, artificial intelligence (AI) methods, such as machine learning (ML), can be beneficial to alleviate the problems associated with the complexity of these alloys. In this work, three different hybrid ML techniques have been employed to estimate the ultimate tensile strength (UTS) and elongation in these special alloys. The proposed methods include a feedforward artificial neural network (FF-ANN) trained using particle swarm optimization (PSO) and two adaptive neuro-fuzzy inference system (ANFIS) methods trained using both fuzzy C-means (FCM) clustering and subtractive clustering (SC). Since OPH alloys are mainly produced via mechanical alloying (MA) of a mixture of powder components followed by consolidation and hot rolling, a series of standard tensile tests were performed on the different variants of the OPH alloy. In this way, some critical parameters such as UTS and elongation could be extracted from the experimental results. The main contribution of the present study is to estimate these important parameters based on some material properties including Aluminum (Al), Molybdenum (Mo), Iron (Fe), Chromium (Cr), Tantalum (Ta), Yttrium (Y) and Oxygen (O), MA and the heat treatment conditions. The results show that the proposed strategies are not only able to accurately determine the complex behavior of OPH alloy with an accuracy of about 95%, but they can also help the designer to benefit from these powerful tools to design new versions of such materials without analytical calculations.

INDEX TERMS Oxide precipitation hardened (OPH) steels, tensile strength, artificial neural network (ANN), particle swarm optimization, ANFIS, Fe–Al–O, machine learning, computational mechanics.

I. INTRODUCTION

Developing new structural alloys for industrial applications requires a shared effort between the commercial sector and the push for green environment. These efforts will thrive with implementing industries utilizing a carbon emission-free, safe, and globally available energy source. One of the primary structural materials challenges is the mechanical properties, mainly focused on Ultimate Tensile Strength (UTS), elongation, and toughness [1]. As the new generation of ODS alloys, OPH alloys have been considered as a promising candidate for industrial applications, attributing to their high

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strength, corrosion resistance, and toughness [2]–[5]. Based on the importance of the oxide nanoparticles, they have been widely studied concerning their morphology, composition, crystallographic structure, and interface relationships with the matrix [6]–[8]. However, further improvement of ODS steels' mechanical properties needs appropriate composition designs, which have become a hot topic for researchers. Y_2O_3 is one of the typical oxides usually used to develop ODS as well as OPH steels. However, its strengthening effect is not ideal due to its growth at high temperatures [9]–[12]. Reactive elements, such as Cr, Ti, and Zr, could be added to the Al-free ODS steels to reduce the size of oxide dispersoids and produce stable oxide dispersoids [13]–[15]. To extend the maximum temperature capability of superalloys, such as Chrome or Iron Aluminum-based OPH alloys, the mechanical alloying (MA) of powder feedstock, followed by Hot Rolling (HR) and Heat Treatment (HT) were studied [14], [16]. This new design expresses the leading idea in the OPH steel processing: dissolve a required amount of O in the matrix during mechanical alloying and let a fine dispersion of oxides precipitate during hot consolidation. Such a microstructure evolution depends on the initial chemical components and the entire thermomechanical processing history through all processing operations, which still needs optimization [13], [17].

Nowadays, the complexity of engineering problems has been increased, and modeling and simulation methods have been appearing as essential computational tools that can explore and reveal insights into investigated processes [18]–[22]. Many theoretical methodologies have been conducted to survey the physical parameters of materials [23]–[28]. In this regard, the use of Machine Learning (ML) techniques is considered a powerful way of conquering the problems associated with conventional methods [29]–[31]. The literature study reveals that ML algorithms like artificial neural network (ANN) and Adaptive Neuro-Fuzzy Inference System (ANFIS) display superior performance in terms of high accuracy and low error content compared to conventional statistical methods [32]. ANFIS can combine the least-squares and the back-propagation gradient descent method to identify the effective parameters of Sugeno-type fuzzy inference systems. It has the benefits of both neural networks and fuzzy logic principles [30]. Fuzzy C-means clustering (FCM) is a data clustering technique in which each data point belongs to two or more clusters. FCM has a smaller number of rules, higher speed, and better results [33]. These properties make FCM-ANFIS more efficient for data simulation [34]. Moreover, the ANFIS-Subtractive Clustering (SC) method is another helpful technique reported by several authors [35].

Researchers have been attracted to AI and ML, which originated from artificial neural networks (ANNs), to find the potential relationships between inputs and outputs in complex functions and systems. This theory imitates the human neuron network structures, including data processing, intention-making, and learning [36]. However, this methodology has essential weaknesses, like landing at a local minimum using many parameters and a slow convergence rate. Therefore, many attempts have been made to solve these problems. One effective way of dealing with these issues is to conclude the hybridization of ANNs with intelligence algorithms and merging the neural network using powerful optimization techniques [23]–[28]. Particle Swarm Optimization (PSO) is the most useable optimization model for robust ANN, defined as a population-based algorithm [37]. The PSO algorithm is beneficial due to its easy implementation, fewer parameters, and high convergence speed. The role of PSO is to optimize the weights and biases of ANN to get the highest performance capacity of the hybrid intelligent systems [38]. In recent years, researchers have shown great interest in modeling various alloys' mechanical properties using ML techniques [26], [27]. Table 1 gives useful information about some very recent publications with a focus on applications of AI-based methods for studying and analyzing materials. This way, Stanev *et al.* tried to use AI for the search and discovery of quantum materials [39]. In that field of materials, the rise of new experimental and computational techniques has increased the volume and the speed with which data are collected, and AI is used to impact the exploration of new materials such as superconductors, spin liquids, and topological insulators [39]. They outlined how the use of data-driven approaches is changing the landscape of quantum materials research, with the result that artificial intelligence is already well on its way to becoming the lynchpin in the search and discovery of quantum materials [39]. Wang *et al.* surrogated the model via Artificial Intelligence Method for Accelerating Screening Materials and Performance Prediction [40]. They used deep learning models, which have been verified as an effective and efficient method for handling computer vision and neural language problems [40]. Using a deep learning surrogate model (DLS) for predicting the maximum stress value under complex working conditions reproduced the finite element analysis model results with 98.79% accuracy [40]. They outlined that deep learning has great potential with a new approach for material screening in practical engineering [40]. Guo *et al.* investigated Artificial intelligence and machine learning in the design of mechanical materials [41]. They show that the performance of an ML-based materials design approach relies on the collection or generation of a large dataset that is properly preprocessed using the domain knowledge of materials science underlying chemical and physical concepts, and a suitable selection of the applied ML model [41]. Recent breakthroughs in ML techniques have created vast opportunities for not only overcoming long-standing mechanics problems but also for developing unprecedented materials design strategies [41]. Eser *et al.* used Artificial Intelligence-Based Surface Roughness Estimation Modelling for Milling of AA6061 Alloy [42]. The cutting speed, depth of cut, and feed rate were evaluated as input parameters for their experimental design [42]. The results show that the depth of cut is the most effective parameter for surface roughness [42]. Prediction models developed using ANN and RSM were compared in terms of prediction

TABLE 1. An overview on the latest publications in the terms of applications of AI in material analysis.

Year	Author	Technique	Application	Objectives	Differences
2021 [39]	Stanev, Valentin, Kamal Choudhary, Aaron Gilad Kusne, Johnpierre Paglione, and Ichiro Takeuchi	AI and ML	Prediction	Review use of data-driven approaches	Quantum material, verity of methods
2021 [40]	Wang, Tian, Mingqi Shao, Rong Guo, Fei Tao, Gang Zhang, Hichem Snoussi, and Xingling Tang	deep learning surrogate model	Performance Prediction	Method for Accelerating Screening Materials and Performance Prediction	FEA model base not experimental, not focused on special type of material
2021 [41]	Guo, Kai, Zhenze Yang, Chi-Hua Yu, and Markus J. Buehler	ML and DL	Design	materials design and computational methods	Used existing data base from a bunch of different materials, Data generation
2021 [42]	Eser, Aykut, Elmas Aşkar Ayyıldız, Mustafa Ayyıldız, and Fuat Kara	ANN and RSM	Estimation	Based Surface Roughness Estimation Modelling for Milling of AA6061 Alloy	Completely different Alloy, Different parameter estimation
2020 [43]	Kabaldin, Yuri, Maksim Anosov, and Dmitrii Shatagin	AI and FA	Evaluation	Evaluation of the mechanism of the destruction of metals based on approaches of artificial intelligence and fractal analysis	Different material, different parameters

accuracy R2, MEP, and RMSE [42]. The data estimated from ANN and RSM were found to be very close to the data acquired from experimental studies [42]. The value R2 of the RSM model was higher than the values of the ANN model which demonstrated the stability and sturdiness of the RSM method [42]. Kabaldin *et al.* evaluated the mechanism of the destruction of metals based on approaches of artificial intelligence and fractal analysis [43]. They showed that a relationship has been established between the fractal values of fractures of specimens tested for impact from a value and the impact strength KCV [43]. With an increase in toughness, a decrease in the fractal dimension of the sample fracture is observed [43]. Also, it has been shown that when recognizing a viscous component in fractures of steel 45 using an INS, the recognition error does not exceed 8% [43].

The appropriate features of OPH alloys make them great alloys for different applications. Since the estimation of these alloys always involves a number of uncertainties and nonlinearities, the application of an efficient model is essential for developing and studying such alloys. Accordingly, in this research, some hybrid ML-empowered methods are employed to address the complex behavior of these materials. The hybrid ML methods include two neuro-fuzzy methods based on Adaptive Neuro-Fuzzy Inference System (ANFIS) [44] and an FF-ANN to estimate the UTS and strain in OPH steels. These parameters play a crucial role in considering the properties of OPH alloys. Therefore, understanding the relationship between these critical parameters and other structural parameters can lead to great improvements in the accuracy and speed of designing OPH alloys. Moreover, since the experimental data are used to determine the behavior of the above parameters, the resulting models are more reliable and accurate than the mathematical models which do not cover many nonlinearities or complexities. The ANFIS techniques include SC and FCM to generate a fuzzy inference system. Also, a hybrid of the ANN-PSO optimization method is used to model the mechanical properties.

The rest of this paper includes four sections. Section II describes the experimental procedure and the special properties of the new OPH alloy based on metal powders. Subsequently, the proposed adaptive neuro-fuzzy inference system (ANFIS) trained by FCM clustering and SC in addition to an ANN method trained by PSO is deployed for estimating the mechanical characteristics in Section III. Following that, the results of estimating the UTS and elongation in the OPH steel are discussed in Section IV. Finally, Section V summarizes the conclusions.

II. EXPERIMENTAL PROCEDURE

The new OPH Alloy is based on metal powders using powder metallurgy [45]. The main powders (Fe and Al) and other components (Table 2) are mechanically alloyed in a vacuum low energy ball mill developed by the authors (Fig. 1). While the MA is completed, the mixture of powders is transferred to a low-alloy steel rolling container with no contact to the air, evacuated, and sealed by welding. Afterward, it is rolled in three steps (Fig. 2) under 900 °C to a final thickness of 3.2 mm. An approximately 2.5 mm thick OPH sheet covered on both sides by a 0.3 mm thick scale from the rolling container is produced in this way.

The samples are then cut using a waterjet parallel to the rolling direction (Fig. 3), followed by grinding to get a final thickness of 2 mm. Using a servo-hydraulic MTS machine (Fig. 4), all tensile tests were carried out with a strain rate of 1×10.3 s-1. Standard size specimens with a thickness of 2 mm and a geometry of 53mm height and 13mm width with the active part length of 25mm were tested. A central data logger recorded all the measurements while the elongation was measured using a video camera extensometer (Fig. 5). Three samples were tested for each state and the average values of UTS and elongation to failure (A) were statistically calculated.

As shown in Fig. 5, the DIC technique was used to measure the elongation of the samples. Speckle patterns were sprayed

TABLE 2. Material parameters.

Material No.	Milling time (h)	Rolling Temp. (°C)	Annealing	Chemical composition (wt. %)
OP1	150	925	RT,1000,1100,1200 °C-0,1,5,20 h	0.72Fe–0.15Cr-0.06Al-0.03Mo–0.01Ta – 0.02Y_2O_3
OP2	230	925	RT,1000,1100,1200 °C-0,1,5,20 h	0.72Fe–0.15Cr-0.06Al–0.03Mo–0.01Ta–0.03Y_2O_3
M1	200	900	RT	0.72Fe–0.14Cr-0.06Al–0.04Mo–0.03Y_2O_3
M2	200	900	RT	0.74Fe–0.15Cr-0.04Al–0.04Mo–0.03Y_2O_3
M3	200	900	RT	0.75Fe–0.15Cr-0.04Al–0.04Mo–0.03Y_2O_3
M4	200	900	RT	0.76Fe–0.15Cr-0.03Al–0.04Mo–0.03Y_2O_3
M5	200	900	RT	0.76Fe–0.15Cr-0.02Al–0.04Mo–0.03Y_2O_3
M6	200	900	RT	0.77Fe–0.15Cr-0.01Al–0.04Mo–0.03Y_2O_3
A5	480	960	RT,1000,1100,1200 °C-0,1,5,20 h	0.85Fe-0.11Al–0.03Y_2O_3
A6	480	960	RT,1000,1100,1200 °C-0,1,5,20 h	0.87Fe-0.11Al
OP3	230	850	RT,800,1000,1100,1200 °C-0,1,5,20 h	0.75Fe–0.15Cr-0.07Al–0.03Y_2O_3
OP4	230	865	RT,800,1000,1100,1200 °C-0,1,5,20 h	0.74Fe–0.15Cr-0.07Al–0.04Y_2O_3
OP5	230	873	RT,800,1000,1100,1200 °C-0,1,5,20 h	0.72Fe–0.14Cr-0.06Al–0.04Mo-0.03Y_2O_3
OP6	230	860	RT,800,1000,1100,1200 °C-0,1,5,20 h	0.72Fe–0.14Cr-0.06Al–0.04Mo-0.03Y_2O_3

FIGURE 1. Low energy ball mill (developed by the authors).

on two opposite surfaces of the specimen using an airbrush to achieve an optimal speckle size of 3–5 pixels. A professional operator created all the patterns trying to get a coverage factor falling within the range of 42% to 50%, which then minimizes the noise. The average speckle size and coverage factors were 4.3 pixels (mean value range: 4.1 to 4.5 pixels) and 49% (range 47% to 50%) respectively. Images were acquired under the best achievable experimental conditions by using the maximum exposure time (56 ms, due to the frame rate set to 15 Hz). Later the strain was compared to what the internal measurement system of the hydraulic machine measured to be sure about the measurements.

III. THE PROCEDURE FOR COMPUTATIONAL ANALYSIS

The proposed adaptive neuro-fuzzy inference system (ANFIS) method has been trained by FCM clustering and SC, which increases the capability of the ANFIS algorithm to analyze and model complex functions. In addition, an ANN method trained by PSO has been deployed for identifying the parameters as mentioned earlier. It should be noted that these methods can predict the behavior of dynamic parameters in different materials. Therefore, using such techniques can substantially decrease the costs and time required for designing and producing new alloys. Fig. 6 demonstrates the framework in which each of the parameters was modeled.

FIGURE 2. Hot rolling machine.

FIGURE 3. Position of cut samples direction of rolling.

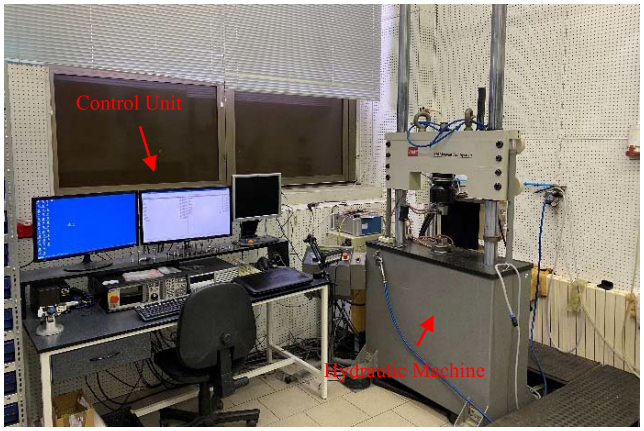

FIGURE 4. Servo-hydraulic MTS machine.

As observed in the first approach, the datasets are measured and collected for modeling purposes. Next, the aggregated data need to be prepared. After that, the prepared data are randomized and divided into two sets for training and testing.

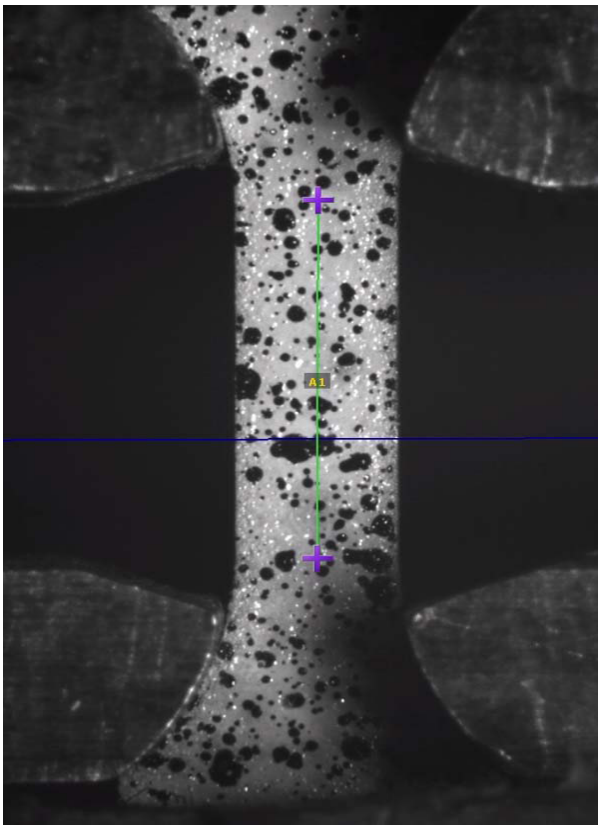

FIGURE 5. Measurements through extensometer.

In the next stage, three different scenarios are considered to complete the process of estimation. As mentioned above, there are three ML-based approaches that have been used to identify the desired characteristics of the understudied alloy.

A. ANFIS-SUB

Subtractive clustering is functional, especially when there is no indicated technique to distribute the data in the centers and the number of clusters [35]. The algorithm is typically summarized as follows:

1. A set of data points placed into a dimensional space should be considered. In this regard, the most potential data point in putting in the center of the first cluster needs to be chosen.
2. The density index D_i of the corresponding to data x_i is then calculated as in (1):

$$D_i = \sum_{j=1}^{n} \exp\left(-\frac{\|x_i - x_j\|^2}{(r_a/2)^2}\right) \tag{1}$$

r_a is defined as a number showing the radius in which all the points within its area are accounted as neighborhoods. Accordingly, the data point with the most potential density measure is opted for the first center group indicated with x_{c1} its density D_{c1}.

3. D'- the density measurement - is recomputed for each data point x_i with the use of the equation (2):

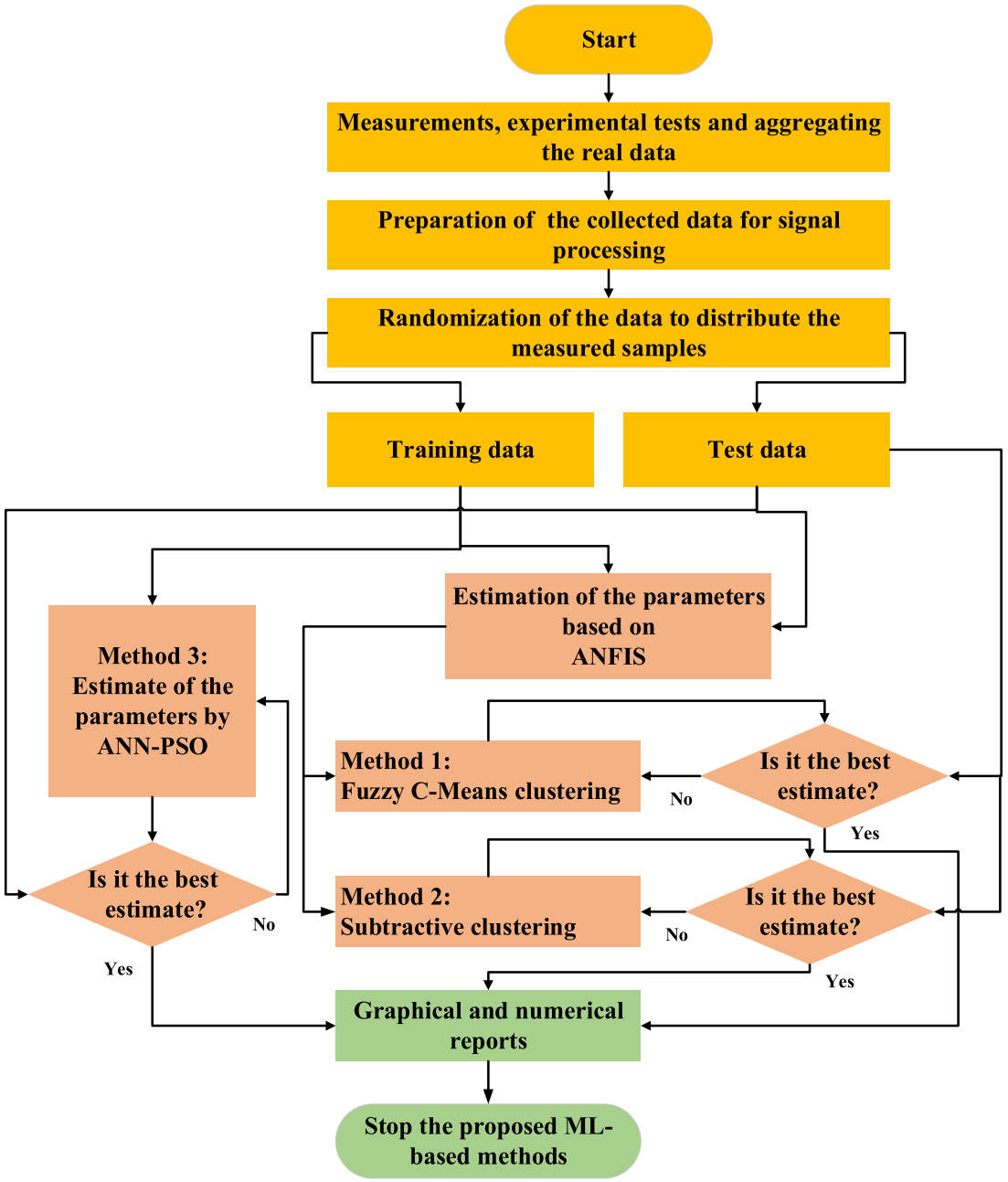

FIGURE 6. The diagram of the proposed scenarios to identify the dynamics of the UTS and elongation.

$$D_i' = Di - D_{c1} \exp\left(-\frac{\|x_i - x_j\|^2}{\left(r_a/2\right)^2}\right) \tag{2}$$

4. D_i, D' and other parameters are recalculated and the procedures until adequate cluster centers are produced.

B. ANFIS-FCM

The second approach is ANFIS-FCM. In this approach, firstly, the number of clusters is chosen based on the system's dynamic. Coefficients for each data point are then determined randomly and placed into the clusters built-in before the stage [46]. In the following step, the algorithm needs to be repeated until the best results are reached. In other words, the center of each cluster (the centroid) is calculated. In addition, the coefficients, which are used for placing the data points in the clusters, are computed again. Generally, the FCM algorithm can be described as equation (3):

$$FCM = \arg_c \min \sum_{i=1}^{n} \sum_{j-1}^{c} \left(\frac{1}{\sum_{k=1}^{c} \left(\frac{\|x_i - c_j\|}{\|x_i - c_k\|} \right)^{\frac{2}{m-1}}} \right) \times \|x_i - c_j\|^2 \tag{3}$$

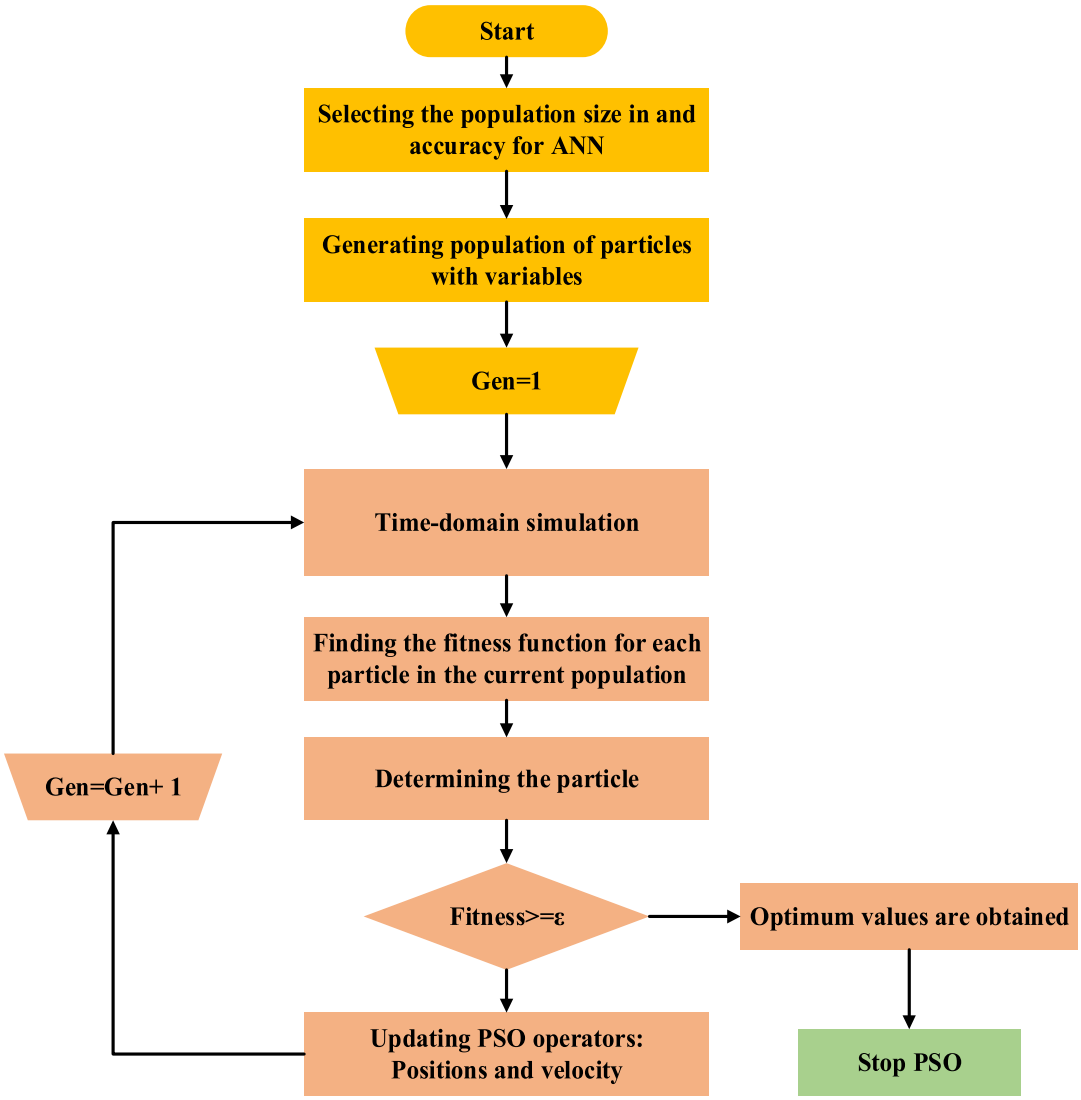

FIGURE 7. The proposed algorithm, which is a combination of PSO and ANN.

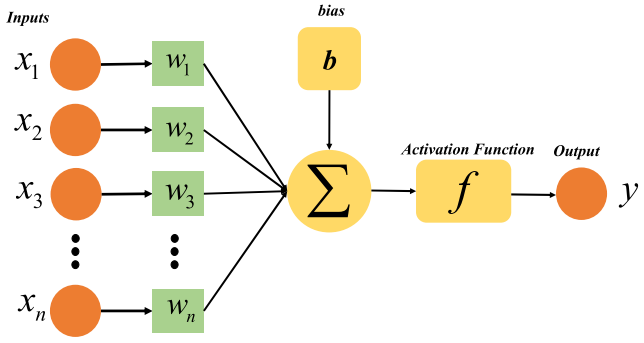

FIGURE 8. The structure of a neuron in a conventional MLP-FF-ANN.

where the fuzzy cluster level c_i is controlled by m which is a hyper-parameter while x_i shows the data point.

C. PSO-ANN

In optimization application, PSO is defined as a computing technique utilized to optimize a complex problem by an iterative method. In this algorithm, considering the required quality, the algorithm can calculate the best possible value for a candidate solution that has the potential to be the best solution [47]. The population of particles called dubbed particles plays a crucial role in this method. In other words, this algorithm tries to move these particles around a certain search-space area using some simply specific formulas over the velocity and position of the particles. In this part, we use this algorithm to train an ANN to estimate the parameters as mentioned above in the alloy. Fig. 7 illustrates a combination of the PSO algorithm and ANN as a hybrid methodology. As observed in this figure, firstly, the size of population is selected depending on the required accuracy. Next, the population of particles is generated with different kinds of variables. Now, the first generation is available to complete the initialization phase.

In the proposed technique, firstly, a cost function is considered to be minimized or maximized depending on the optimization problem. After that, a number of particles is

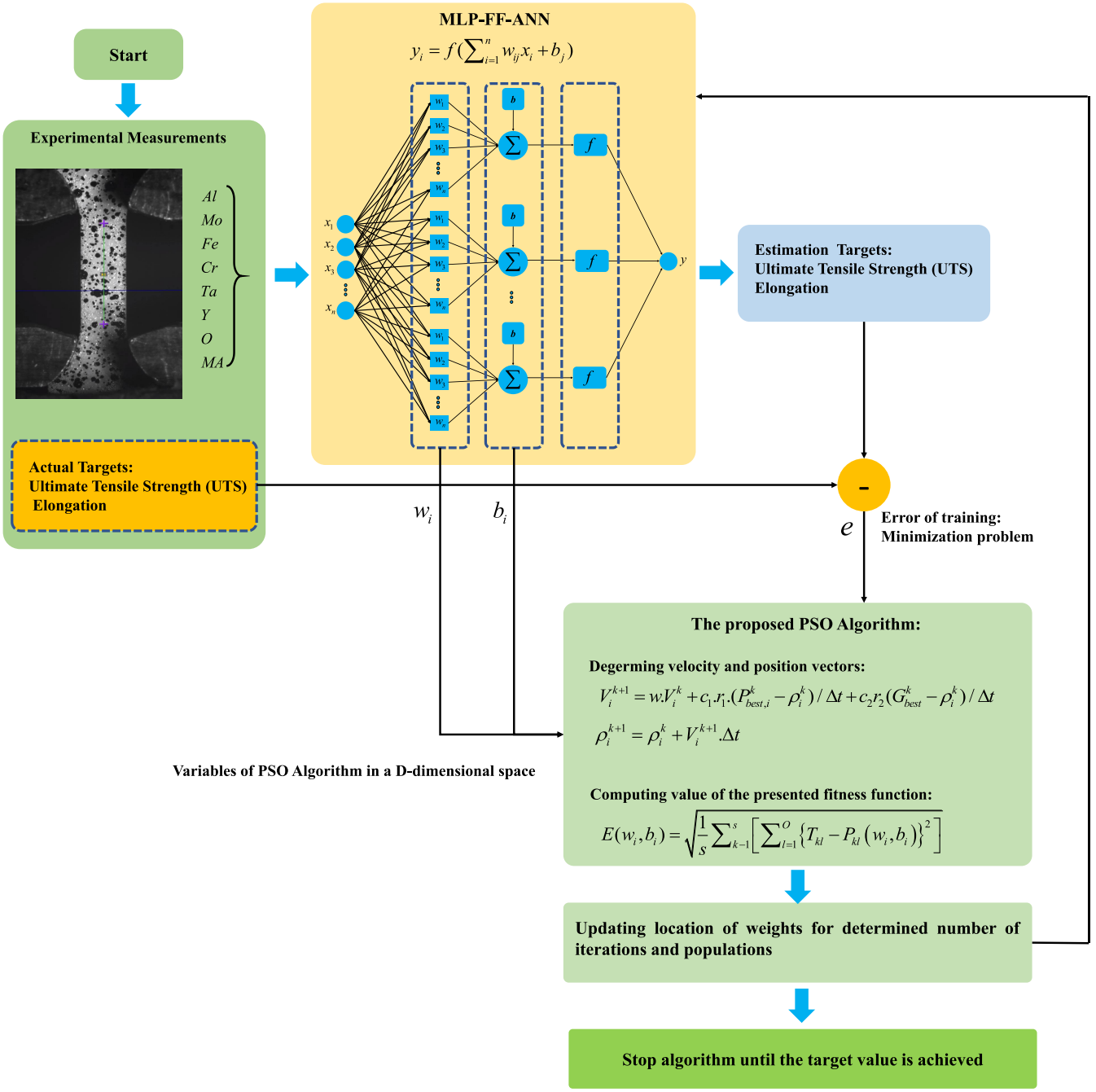

FIGURE 9. The process of training MLP-FF-ANN using PSO algorithm for estimation of UTS and Elongation.

provided and employed throughout the problem with D dimensional space. In fact, any particle includes some variables of the problem. Therefore, the fitness function (cost) can be computed for each particle. Consequently, the position and velocity of these elements should be updated based on equations (4) and (5) as follows:

$$V_i^{k+1} = w.V_i^k + c_1.r_1.(P_{best,i}^k - \rho_i^k)/\Delta t + c_2 r_2 (G_{best}^k - \rho_i^k)/\Delta t \quad (4)$$

$$\rho_i^{k+1} = \rho_i^k + V_i^{k+1}.\Delta t \quad (5)$$

where i and k in order are defined as the number of particle and the number iteration. Also, $V_i = \{v_{i1}, v_{i2}, \ldots, v_{ij}, \ldots, v_{iD}\}$ and $\rho_i = \{\rho_{i1}, \rho_{i2}, \ldots, \rho_{ij}, \ldots, \rho_{iD}\}$ in order are defined as the velocity and position vectors. Moreover, $P_{best,i}^k = \{p_{i1}, p_{i2,} \ldots, p_{ij}, \ldots, p_{iD}\}$ and $G_{best}^k = \{g_1, g_2, \ldots, g_D\}$. Furthermore, c_1 is a cognitive parameter and c_2 is a social parameter. In this regard, w is considered to be the internal weight utilized of preservation of the previous velocity while the optimization process is performed, whilst r_1 and r_2 are considered as two random

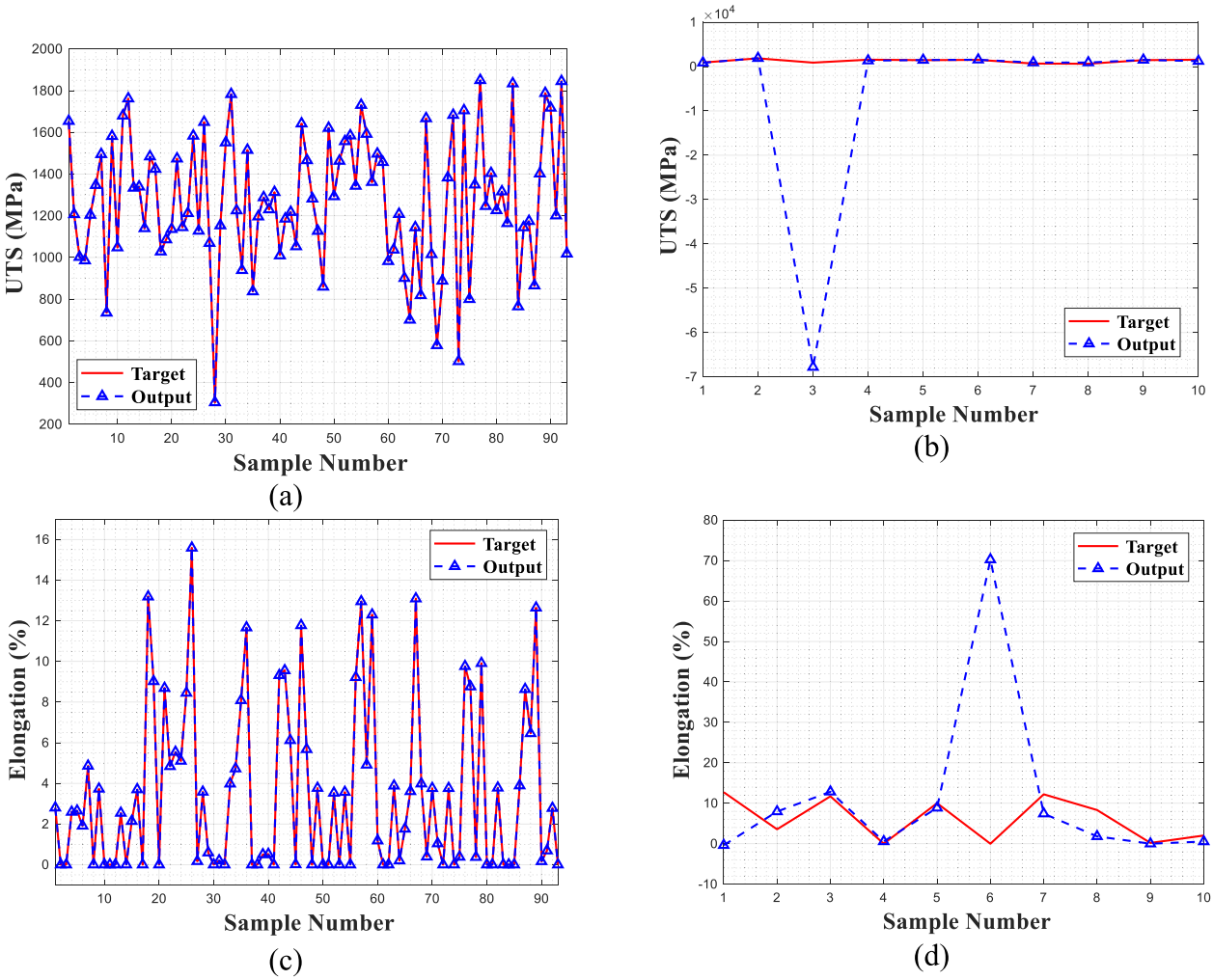

FIGURE 10. A comparison between the results of the ANFIS-SUB method and the actual measurements; (a) and (c) show the training data while (b) and (d) illustrate test results.

numbers which are uniformly distributed between 0 and 1. Δ_t is the time interval for updating velocity and position and it is typically equal to 1.

In fact, the process of training for an ANN contributes to minimizing the problems which can be performed through metaheuristic or mathematical algorithms [48]. Fig. 8 demonstrates the structure of a conventional multilayer perceptron feed-forward ANN (MLP-FF-ANN). As is shown in this figure, there are three important layers, input layer, hidden layer and output layer that can be described via equation (6):

$$y_i = f(\sum_{i=1}^{n} w_{ij} x_i + b_j) \tag{6}$$

where x_i and y_j are considered as the values in the previous and current layers respectively. This way, b_j and w_i are defined as biases and weights of the ANN. In addition, f is an activation function used for computing the value of the ANN. Training is a process in which biases and weights of the ANN are calculated in order to minimize the error between the outputs of the network and the real values (targets). That is why we face a minimization problem when it comes to training an ANN.

In the proposed method, PSO as the activation function helps the ANN to reduce the errors by calculating the optimized values, considering some structural parameters, such as biases and weights. Hence, variables of PSO are weights and biases of the network. In addition, the suitable space of the problem is related to the intervals. The fitness function (cost) of particles is calculated via equation (7):

$$E(w_i, b_i) = \sqrt{\frac{1}{s} \sum_{k-1}^{s} \left[\sum_{l=1}^{O} \{T_{kl} - P_{kl}(w_i, b_i)\}^2 \right]} \tag{7}$$

here P_{kl} is the predicted output and T_{kl} is the target output. Also, the number of neurons is defined by O. In the proposed network, the parameters of the PSO algorithm are defined as Swarm Size = 200; Max Iteration = 35; C1 = 2; C2 = 4 - C1.

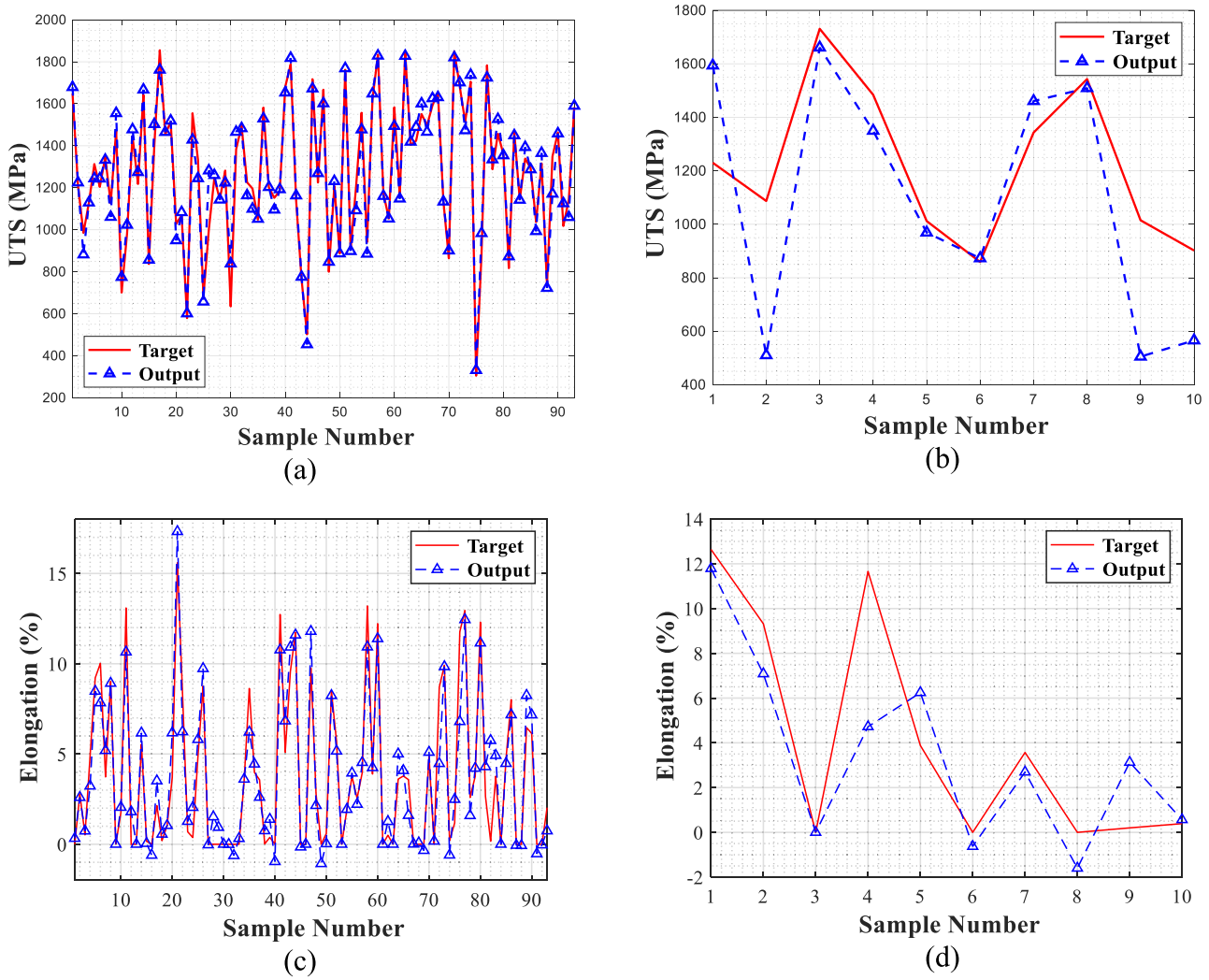

FIGURE 11. The response of the ANFIS-FCM method compared to the actual measurements; figures (a) and (c) show the training data and figures (b), and (d) illustrate test results.

This procedure is illustrated in Fig. 9. According to this figure and the above explanations, the following stages can be summarized to demonstrate the mechanism of this method:

1. After determining the number of neurons of ANN in its hidden layer, a network with initial biases and weights are built.

2. Since D is defined as the total number of the problem, each of the biases and weights is considered as a particle in a specific location in D-dimensional space of the problem.

3. Then output values of the particles in each iteration can be estimated, leading to computing value of the presented fitness function brought in Equation (7).

4. Finally, the location of weights and biases which are defined particles are updated via the PSO algorithm for an indicated number of iterations and populations and until achieving the target value.

The proposed hybrid ML-based methods have been implemented by MATLAB R2020A through a processor Intel(R) Core (TM) i7-9700 CPU @3 GHz with 16 GB (RAM).

IV. RESULTS AND DISCUSSION

A. MODELING RESULTS

In this section, the results of the estimation of the UTS and elongation in the OPH steel are discussed. The most important advantage of the utilization of the present method is to estimate these complex parameters with three ML methods without using mathematical analysis. In this approach, the material is considered to be a black-box model. Fig. 10 depicts a comparison between the output of the ANFIS-SUB model and the actual measurements.

This figure is extremely helpful as it shows the nonlinear and complex behavior of the UTS and elongation in the OPH steel. In fact, this nonlinear dynamic behavior is the reason that analytical methods cannot model or identify such materials for design purposes with the highest rate of accuracy as well as providing a reliable estimator for the prediction of UTS and elongation. Moreover, even if mathematical models can consider all uncertainties or nonlinearities, we face some complex equations that cannot be solved. That is why

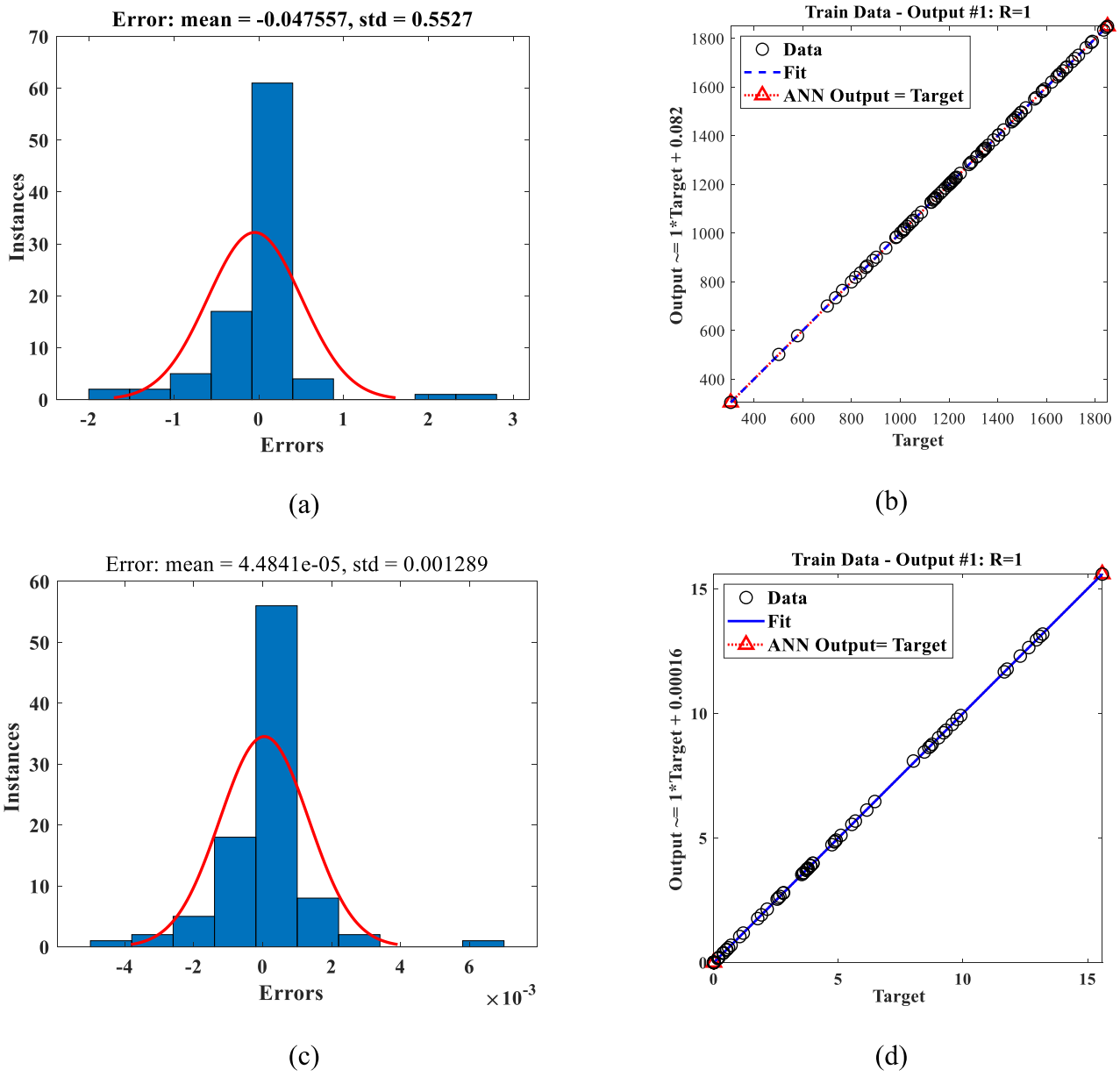

FIGURE 12. Standard deviation and error regression for SUB-ANFIS model.

the proposed method can compensate for the weaknesses of analytical strategies. However, the most challenging issue in order to apply such techniques is to have a reliable measurement. In the present work, as mentioned in section 2, we try to utilize an appropriate dataset in which the accuracy of the proposed methods is not affected.

According to Fig. 10, the ANFIS-SUB method can successfully estimate all three studied parameters' values. In this regard, Figs 10a and 10c depict to the training data for UTS and elongation, respectively, whereas Figs. 10b and 10d represent their related test results.

Since UTS and elongation can assist the process of the design, reaching this level of accuracy will help the designers to see the effects of changing any structural parameters on the properties of these alloys. Disregarding the excellent results, the figure shows how such methods highlight the capability of AI-based models to predict the complex behavior of different materials which can be used as a holistic approach for other materials. This can be accomplished when it comes to materials that cannot be modeled by simple equations.

In this section, two error criteria have been used as follows:

As with the ANFIS-SUB method, the results of the ANFIS-FCM model are demonstrated to evaluate the method's performance. In this respect, Fig. 11 shows

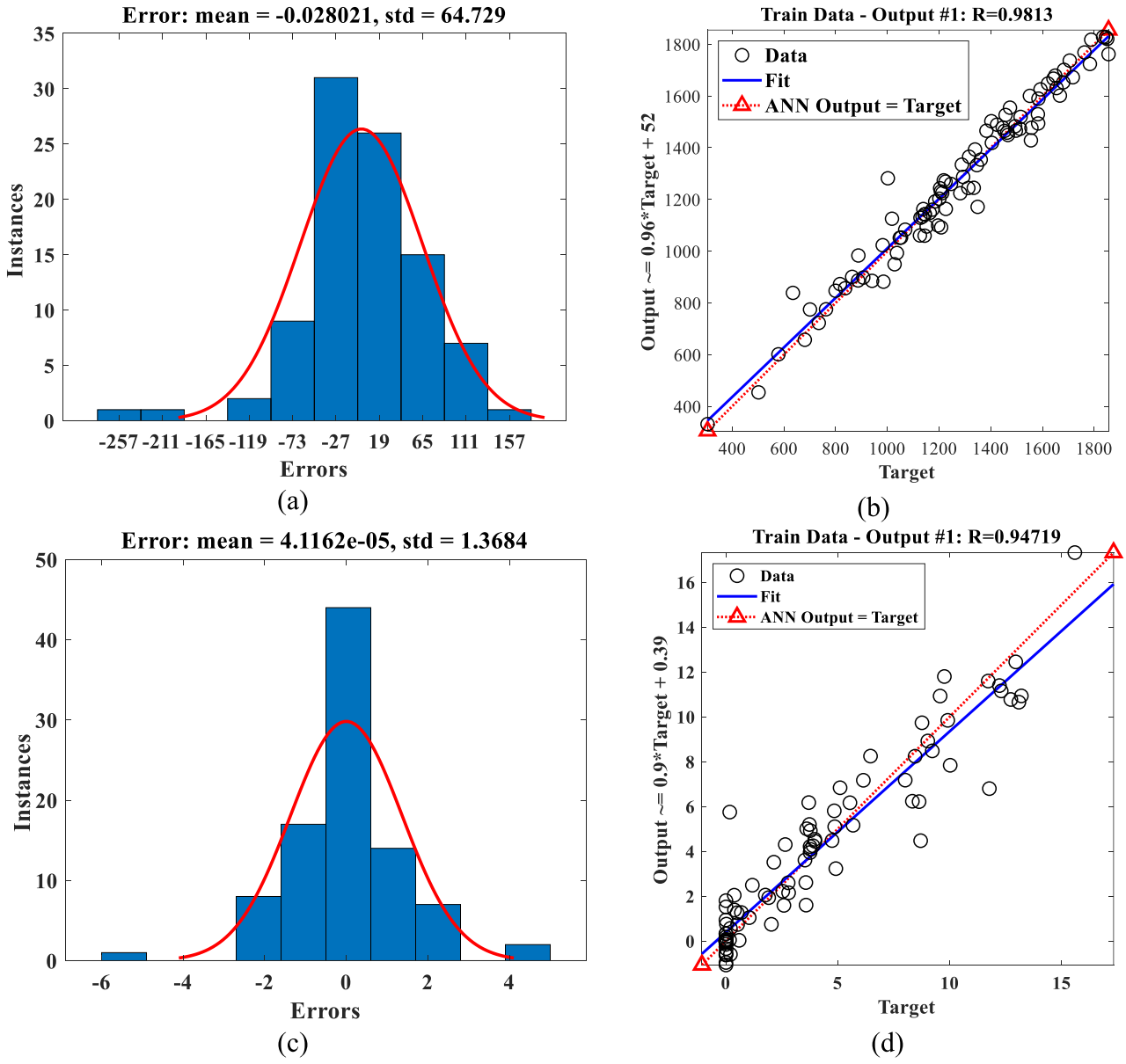

FIGURE 13. Standard deviation and error regression for FCM-ANFIS model.

the output of the ANFIS-FCM model compared to the actual measurements. As can be seen, although the introduced hybrid method based on ANFIS-FCM is suitable for identifying the parameters, the accuracy of the ANFIS-SUB model seems better. Accordingly, Figs 11a and 11c compare training data for UTS and elongation respectively, whereas Figs 11b and 11d demonstrate test data.

Moreover, Figs. 12 and 13 demonstrate the error regression graph and the Standard Deviation (SD) for ANFIS-SUB and FCM respectively. Based on these figures, the performance of the proposed hybrid methods equipped by the ANFIS model can be evaluated appropriately. Accordingly, in Fig. 12a, 12c, the SD of three parameters show desirable values about 0.55 and 0.0012 for UTS and elongation respectively. Moreover, in Figs. 12b and 12d, representing error regression graphs, there are almost no dramatic differences between the estimated data points at a specific time and the actual data points, proving the appropriate performance of the ANFIS-SUB model. However, a different scenario should be said(?) for ANFIS-FCM. According to Fig. 13, the ANFIS-FCM method does not have an appropriate performance in all the graphs in Fig 13.

After initializing the network, the simulation with the time domain is started. The fitness function for each of the generated particles is then found while in the first stage, their corresponding is determined. Consequently, the fitness function should be evaluated, in which if it is the best solution, the process ends; if not, it needs to be repeated. Fig. 14 illustrates the

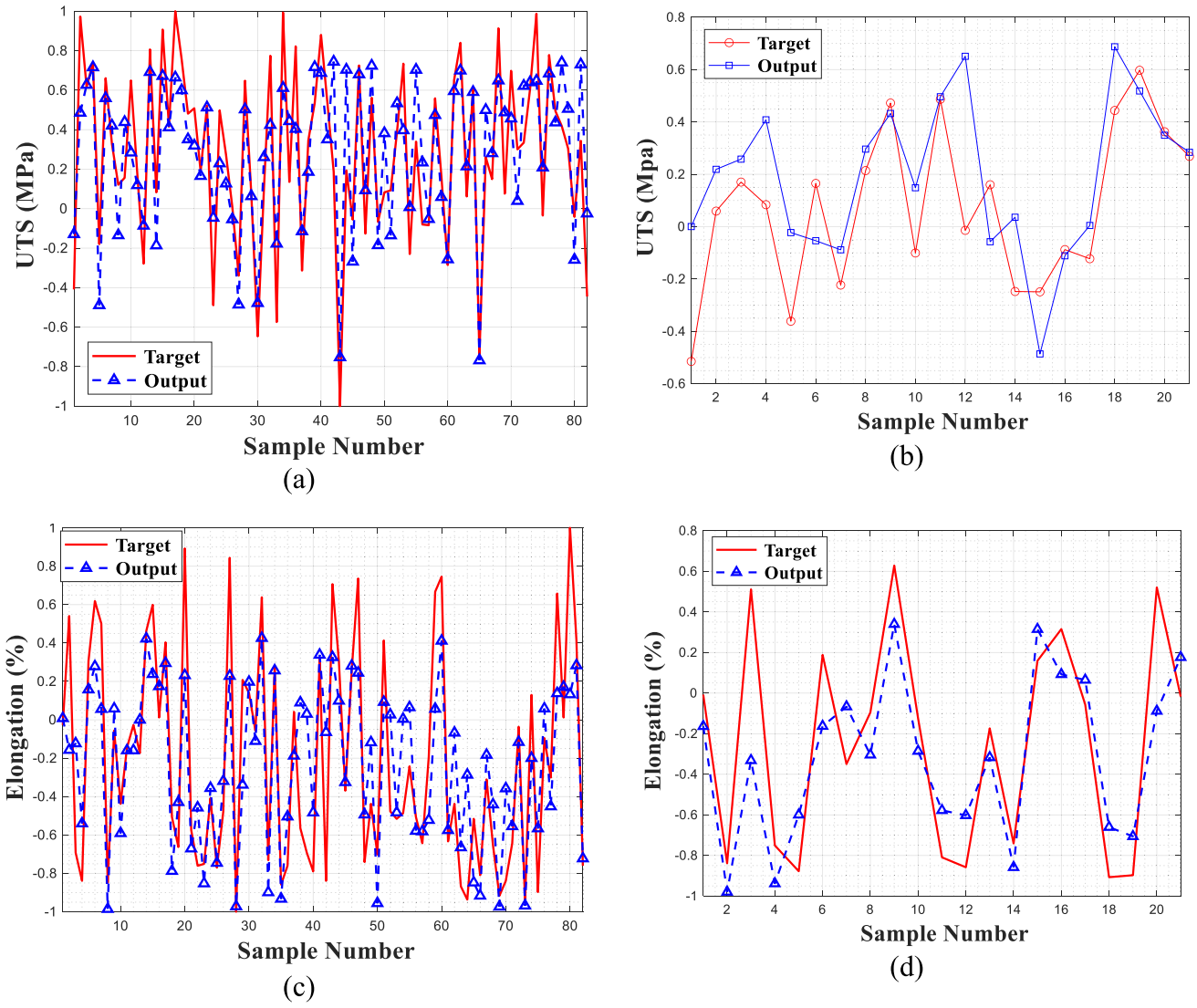

FIGURE 14. The output of the PSO-ANN model compared to actual measurements.

comparison between the output of the ANN-PSO approach and real data points. As can be seen, this method has an average performance compared to ANFIS. The first criterion is Mean Squared Deviation (MSD) -also called Mean Squared Error (MSE)- which is an estimating technique to measure the average of the squared errors. In this method, the average squared difference between the real output and the estimated output of the model.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(\widehat{y}_i - y_i)^2 \tag{8}$$

where N is defined as the number of data points, $\widehat{y}_i$ is the model's output, and y_i is the real value for the data point i.

Root Mean Square Deviation (RMSD) or the Root Mean Square Error (RMSE) is a kind of statistical method that is nearly the same as the standard deviation of the mean (SD), in which instead of $N - 1$ data points, N ones are used in RMSE:

$$RMSE = \sqrt{\left[\frac{1}{N}\sum_{i=1}^{N}(\widehat{y}_i - y)^2\right]} \tag{9}$$

Table 3 gives information about the actual values and estimated values for three parameters. As can be seen, the ANFIS method trained by the subtractive clustering method has the best fitness for identifying the parameters, while another ANFIS model optimized by the FCM algorithm shows the worst results. Moreover, the proposed ANN method trained by the PSO algorithm has an acceptable response for modeling the parameters.

One of the most significant contributions of this work compared to our recent research [20] is the methodologies that have been used. In fact, in [20] a conventional ANN trained by Levenberg–Marquardt backpropagation algorithm is used while in the present work, a hybrid ML method, which

TABLE 3. Comparison between the measured data and the estimated data for both training and testing methods.

Estimation Targets		ANFIS-SUB (MSE)	ANFIS-SUB (RMSE)	ANFIS FCM (MSE)	ANFIS FCM (RMSE)	ANN PSO (MSE)	ANN PSO (RMSE)
Training	UTS (MPa)	0.013	0.11401	0.0453	0.21283	0.0605	0.24596
	Elongation (%)	0.0356	0.1886	0.01506	0.12271	0.0223	0.14933
Test	UTS (MPa)	0.0209	0.14456	0.0921	0.30347	0.0481	0.21931
	Elongation (%)	0.1336	0.36551	0.0966	0.31080	0.0939	0.30643

TABLE 4. Comparison of the results of the proposed method and some similar methods for estimation of UTS.

	MSE	RMSE
ANFIS-SUB	0.0209	0.14456
ANFIS-FCM	0.0921	0.30347
ANN-PSO	0.0481	0.21931
Linear Regression Model [49]	Not reported	41.2
RF Model [49]	Not reported	40.4
FFBPNN [50]	Not reported	3.99
ANFIS [51]	Not reported	0.88
ANN [51]	Not reported	0.92
FIS [51]	Not reported	0.8

is trained via particle swarm optimization (PSO) is used. In this research, as for any optimization problem, minimization of the network cost is taken into consideration. This has been achieved by minimizing some form of error function between the desired and the actual network outputs, during the training phase. However, the conventional algorithms like Levenberg–Marquardt backpropagation are sensitive to the choices of the initial weights and tend to get trapped in local minima. On the other hand, evolutionary algorithms like the proposed method have proved their usefulness in introducing randomness into the optimization procedure, since they work on a global search strategy and induce a globally minimum solution for the network weights. In this regard, the utilization of an ANN trained by PSO for analyzing the behavior of the alloys leads to achieving the local-best and global-best particle positions as possible solutions to the setting of the network weights. In summary, the application of PSO for training the ANN is one of the important contributions of the presented manuscript.

Another important contribution of the present work is about the target of modeling. Although both papers used ANFIS for analyzing the alloys, the aims are completely different to each other. For example, in [20], the simulation of the hardness of OPH steels was studied, while in this work we use the ANFIS methods or the ANN-PSO method for analyzing ultimate tensile strength (UTS), and elongation. UTS and elongation are two main parameters that highlighted alloys for formability and strength. Higher UTS value usually backs with lower elongation while higher elongation increases the plasticity of the alloy. So, it is quite important to balance and optimize these two values to achieve the best performance of the final alloy. In fact, this work aims to estimate the nonlinear behavior of UTS and elongation.

The reliability and accuracy of ML-based techniques for estimating the nonlinear behavior of OPH alloys indicate that for future work a multi-objective method based on deep learning or reinforcement learning can be considered in order to increase the level of precision. It is also worth mentioning that, regardless of the satisfaction and reliability of the derived results from all the applied techniques, all ML methods should be utilized with caution as sometimes the appropriate data for a mining operation is not available, leading to effects on the simulation and prediction.

Table 4 compares the results of the proposed method with some similar papers, representing the applicability and accuracy of the introduced method in the estimation of UTS. It should be noted that measurement accuracy and input signals can significantly affect the outputs of all data-driven models.

V. CONCLUSION

In this paper, some hybrid ML techniques have been employed and evaluated for the estimation of the dynamic behavior of OPH steels. OPH alloys are types of material

TABLE 5. Glossaries.

ODS	Oxide Dispersion Strengthened
OPH	Oxide Precipitation Hardened
AI	Artificial Intelligence
ML	Machine Learning
UTS	Ultimate Tensile Strength
FF-ANN	Feedforward Artificial Neural Network
PSO	Particle Swarm Optimization
ANFIS	Adaptive Neuro-Fuzzy Inference System
FCM	Fuzzy C-Means
SC	Subtractive Clustering
MA	Mechanical Alloying
Al	Aluminum
Mo	Molybdenum
Fe	Iron
Cr	Chromium
Ta	Tantalum
Y	Yttrium
O	Oxygen
Ti	Titanium
Zr	Zirconium
HR	Hot Rolling
HT	Heat Treatment
RMSD	Root Mean Square Deviation
RMSE	Root Mean Square Error
SD	Standard Deviation of the mean
DL	Deep Learning
DLSM	Deep Learning Surrogate Model

that are typically prepared by mechanical alloying from a mixture of powder components consolidated by hot rolling followed by heat treatment. The proposed ML approaches were applied as estimators to estimate the ultimate tensile strength (UTS) and elongation based on actual measurements of the different chemical compositions of the studied alloy, such as Al, Mo, Fe, Cr, Ta, Y, and O), heat treatment conditions, and mechanical alloying conditions. The proposed methods consist of a feedforward artificial neural network (FF-ANN) trained by particle swarm optimization (PSO) and two adaptive neuro-fuzzy inference system (ANFIS) methods trained using both fuzzy C-means (FCM) clustering and subtractive clustering (SC).

The results showed that the proposed strategies can model and identify the complex behavior of OPH Steels with an approximate accuracy of 95% and can help the designer to address and predict these steels with all nonlinearities and uncertainties without using analytical calculations. In addition, the proposed methods provide designers with a tool for finding which chemical composition might have more impact on UTS or elongation in such steels.

In the future, we will work on more accurate ML-based techniques to study different materials and adapt the proposed method accordingly. There are a number of parameters for each material that can significantly affect the accuracy and reliability of the estimate. Moreover, some new DL -methods such as reinforcement learning and transfer learning can be considered to improve the applicability of the proposed method.

APPENDIX

See Table 5.

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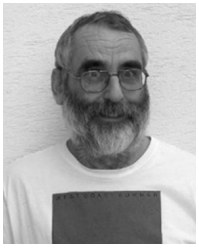

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