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Prediction Modeling Of Low-Alloy Steel Based On Chemical Composition And Heat Treatment Using Artificial Neural Network

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Abstract
The utilization of machine learning methods in modern material science enables the design of more efficient and innovative materials. This research aims to develop a machine learning model using the Artificial Neural Network (ANN) algorithm to predict the mechanical properties of low-alloy steel. The dataset used consists of 15 input variables and 2 output variables, namely Yield Strength (YS) and Tensile Strength (TS). In this study, three ANN architectures were designed and their performance was compared using evaluation metrics such as Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and R-squared. During the search for the best parameters for the ANN model, variations were made in the optimizer, learning rate, and batch size. The evaluation was conducted using a cross-validation technique with k=10. The evaluation results indicate that the model with the best performance in predicting YS had an MAE of 18.197, an RMSE of 23.552, and an R-squared of 0.969. For predicting TS, the model achieved an MAE of 27, RMSE of 36.696, and R-squared of 0.907. The research results demonstrate that the ANN model can be used to predict the mechanical properties of low-alloy steel based on alloy chemical composition and heat treatment temperature with reasonably high accuracy.

Keywords:
Modeling, low alloy steel, algorithm, Artificial Neural Network (ANN), mechanical properties.

1 Introduction

Low-alloy steels are widely used in the manufacturing industry of machine structures, vehicles, and building constructions that require high strength and durability [1][2]. This is because the mechanical properties of low alloy steels are superior compared to ordinary steel, such as strength, hardness, toughness, wear resistance, and better corrosion resistance[3].The increasing and widespread use of low-alloy steels in the industrial world has prompted the steel industry to develop steel alloys that are suitable for specific applications. This aims to prevent material failure, as the mechanical properties of a material play an important role in determining the right material for modern industrial components[4]. The mechanical properties of low-alloy steels are influenced by several factors, such as chemical composition, microstructure, and heat treatment. These factors can effectively control the microstructure, grain size, and defects, which are all closely related to the material's tensile properties[5][6]. A good understanding of the factors that affect the mechanical properties of low-alloy steels can assist in developing materials that are suitable for specific needs [7]. Therefore, comprehensive testing and experimental laboratory work are necessary to understand the mechanical properties of low alloy steels, which require a long time, high costs, and adequate human resources.

Materials informatics is a new approach in material science that integrates information technology and material science to optimize the process of discovering new materials more efficiently and innovatively [8][9]. In materials informatics, experimental and simulation data are integrated with data-based methods such as big data and machine learning to generate deeper knowledge about material properties. This approach is considered a new paradigm in material science that combines the first three paradigms of experiment, theory, and simulation [10][11][12].Artificial Neural Networks (ANN) are one of the machine learning algorithms that are inspired by the human nervous system and can be used to predict the mechanical properties of materials such as low-alloy steels. ANN consists of interconnected layers of artificial neuronsand can learn by adjusting the weights within it through learning from the given data [13]. ANN is capable of discovering hidden patterns in data and can consider interactions between various factors that affect the mechanical properties of materials, such as chemical composition, microstructure, and heat treatment, which are very complex to calculate manually. This allows ANN to be used to predict the mechanical properties of low-alloy steels that have not been experimentally tested[14]. Based on previous research [13], discussed the computer-based optimization of steel chemical composition design using Taguchi Particle Swarm Optimization (TPSO) with ANN. The research results indicate that the TPSO method with ANN can predict the chemical composition of steel rods, closely approximating actual data. In another study [15], ANN with default parameters can predict the mechanical properties of steel quite well based on chemical composition. ANN is also highly effective in predicting the mechanical properties of materials even when the testing data is not part of the model training data [14][16]. Furthermore, an Artificial Neural Network (ANN) model has been developed to predict various anisotropic mechanical properties and hardening behavior of Inconel 718 alloy. The ANN model is trained using the Levenberg-Marquardt algorithm and demonstrates good accuracy with a very high correlation coefficient and significantly low average absolute error. Validation of the developed ANN model's accuracy is confirmed through f-test and paired mean t-test results [17].

Based on the advantages of ANN in predicting the mechanical properties of materials, this study aims to design a machine-learning model with ANN to predict the mechanical properties of low alloy steels based on chemical composition and heat treatment. In this study, the model is trained using low alloy steel chemical composition and heat treatment data as input, while the output of the model is Yield Strength (YS) and Tensile Strength (TS).Expected outcomes of this research include obtaining the optimal parameter settings for the ANN algorithm in predicting the mechanical properties of low-alloy steel based on input variables such as chemical composition and heat treatment temperature.

2 Research Method

This study is an experimental research using a quantitative approach. Experimental research is a type of research conducted by controlling research variables and varying one or more independent variables to observe their effect on the dependent variable [18]. The ANN model is created using the Python programming language using the TensorFlow library, then the best

parameters are searched using tuning parameters such as model architecture, optimizer, learning rate, and batch size. The model validation used is cross-validation and evaluated using Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and R-squared.This study consists of several stages as shown in Fig. 1.

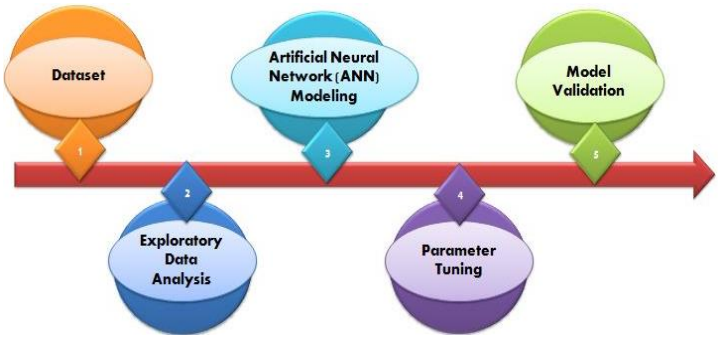


Fig. 1. Research stages.

2.1 Dataset

The dataset used in this study is the result of tensile tests on low-alloy steel, which includes chemical composition percentage, heat treatment temperature, and mechanical properties such as Yield Strength (YS) and Tensile Strength (TS). This data was obtained from Kaggle.com and consists of 915 data with 15 input variables and 2 output variables.

2.2 Exploratory Data Analysis (EDA)

This stage is very important because poor data understanding can affect the quality of prediction results. Therefore, the correlation between the data is analyzed using a correlation heatmapto understand the data [2]. Preprocessing of the data is also performed in this stage, such as: (a) data cleaning, which involves removing or correcting damaged, missing, or incomplete data;(b) data integration, which aims to replace missing data with data from other sources with the same characteristics; (c) data transformation, which is done to change the data format to suit the analysis needs, such as changing the data scale or normalizing the data.

Data normalization is one of the techniques in data preprocessing that aims to change the data scale to the same range or equivalent range between 0 to 1. In this study, data normalization is performed using the MinMaxScaler method. MinMaxScaler is the most commonly used normalization method in machine learning, which can be calculated using Eq. 1.

$$Xsc = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (1)$$

Where X is the original data, while Xsc is the normalized data. The purpose of this normalization is to eliminate bias that may exist in the data resulting from different scales in each variable [19][20].

2.3 Artificial Neural Network (ANN) Modeling

The architecture of the Artificial Neural Network (ANN) for predicting the mechanical properties of low alloy steel in this study consists of three main interconnected layers. The first layer used is the input layer, which receives input data in the form of informationabout chemical composition and heat treatment temperature. This layer consists of several neurons that correspond to the number of input variables. In the second layer, several hidden layers aim to extract information from the input before being forwarded to the output layer. These hidden layers use the Rectified Linear Unit (ReLU) activation function to avoid vanishing gradient problems and accelerate model convergence. The last layer is the output layer, which provides the predicted results of the mechanical properties of low-alloy steel, in this case, Yield Strength (YS) and Tensile Strength (TS). The illustration of the ANN architecture is shown inFig. 2.

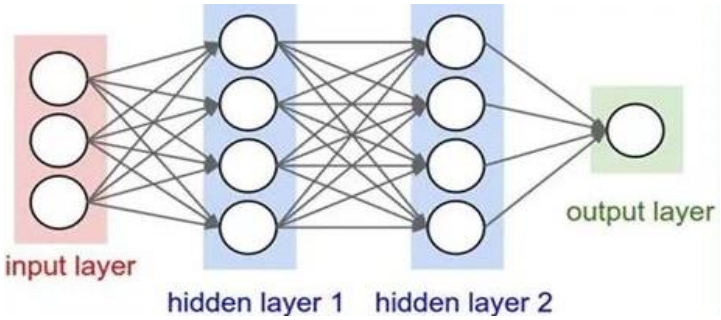


Fig. 2. Illustration of Artificial Neural Network (ANN) architecture [21].

2.4 Tuning Parameters

In this research, the Artificial Neural Network (ANN) model was tuned using hyperparameter tuning technique. The parameters that were adjusted were the number of layers, number of neurons, optimizer, learning rate, and batch size. The number of layers in ANN can affect the model's ability to learn complex patterns [16]. Therefore, variations in the number of layers were made by increasing or decreasing the number of layers in the model. The number of neurons in each layer was also analyzed by increasing or decreasing the number of neurons in each layer. Choosing the appropriate optimizer, learning rate, and batch size can optimize the model's performance[22][23].

After that, the model was evaluated to measure how well the machine learning model can predict the mechanical properties of low-alloy steel. The evaluation metric used to measure the performance of the model [24]:

1. Mean Absolute Error (MAE)

MAE measures the average absolute difference between the model's prediction and the target value. The lower the MAE value, the better the model is at making predictions. MAE can be calculated using Eq. 2.

$$MAE = \frac{i}{N}\sum|Y_i - Z_i| \quad (2)$$

Where i is the index of data in the sample, N is the total number of samples, Y_i is the actual value of the i^{th}data, and Z_i is the predicted value of the model for the i^{th} data.

2. Root Mean Square Error (RMSE)

RMSE is the square root of the average of thesquare difference between the model's prediction and the target value. RMSE provides a measure that is the same unit as the target variable and is generally more sensitive to large differences. The lower the RMSE value, the better the model is at making predictions. RMSE can be calculated using Eq. 3.

$$RMSE = \sqrt{\frac{1}{n}\sum_i^n = 1\,(f(X_i) - Y_i)^2} \quad (3)$$

Where n is the number of data used to test the model, $f(X_i)$ is the value predicted by the model for the ith data, and Y_i is the actual value for the ith data.

3. R-squared (R^2)

R-squared (R^2) is a coefficient of determination that provides information about how well the model fits the data. R^2 is the ratio of the total variation explained by the model to the total variation present in the data. The value of R^2 ranges from 0 to 1, and the higher the R^2 value, the better the model is at explaining the variation in the data. R-squared can be calculated using Eq. 4.

$$R = \frac{\sum_i^n=1(f(X_i)-f(\bar{X}))(Y_i-\bar{Y})}{\sqrt{\sum_{i=1}^n(f(X_i)-f(\bar{X}))^2}\sqrt{\sum_{i=1}^n Y_i-\bar{Y})^2}} \quad (4)$$

Where $f(X_i)$ is the predicted value of the dependent variable (Y) based on the independent variable (X) at the i^{th} observation,

$f(X)$ is the average of all predicted values $f(X_i)$ overall observations, Y_i is the actual observation value of the dependent variable at the i^{th} observation, $\bar{Y}$is the average of all observation values Y_i over all observations, and n is the total number.

2.5 Model Validation

Cross-validation is a model evaluation technique used to measure the performance of a model by dividing the data into two parts: the training data and the test data. In cross-validation, the training data is divided into several different subsets or folds, and each subset is iterated as the test data, while the remaining subsets are used as the training data [12]. In this modeling, 10-fold cross-validation is used, where the data is divided into 10 different subsets or folds and iterated 10 timesby selecting each subset alternately as the test data and the remaining subsets as the training data. The evaluation results of the model in each iteration will be averaged to obtain a more valid evaluation metric value, Fig. 3 illustrates the use of 10-fold cross-validation.

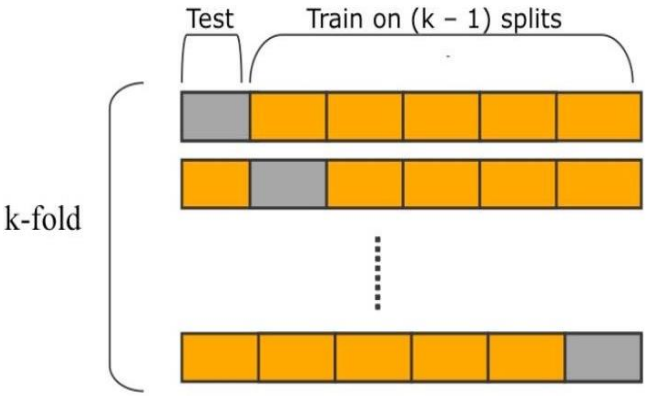


Fig. 3. Illustration of cross-validation[23].

3 Results and Discussion

3.1 Dataset

This low-alloy steel dataset consists of 15 input variables, consisting of chemical elements and heat treatment temperature, with 2 output variables, namely Yield Strength (YS) and Tensile Strength (TS), with data characteristics shown in Table 1.

Table 1. Statistics of low-alloy steel dataset

Variables	Data types	Min	Max	Mean
C	Input	0.09	0.34	0.17
Si	Input	0.18	0.52	0.31
Mn	Input	0.42	1.48	0.81
P	Input	0.006	0.03	0.01
S	Input	0.003	0.022	0.01
Ni	Input	0	0.6	0.14
Cr	Input	0	1.31	0.43
Mo	Input	0.005	1.35	0.44
Cu	Input	0	0.25	0.08
V	Input	0	0.3	0.06
Al	Input	0.002	0.05	0.01
Ni	Input	0.0025	0.015	0.01
Ceq	Input	0	0.437	0.09
Nb + Ta	Input	0	0.0017	0.00
Temperature (°C)	Input	27	650	351.60
Yield strength (MPa)	Output	27	690	328.22
Tensile strength (MPa)	Output	162	6661	496.25

3.2 Exploratory Data Analysis (EDA)

The low-alloy steel dataset consisting of chemical elements, heat treatment temperature, and mechanical properties was analyzed using a correlation heatmap to observe the correlation between chemical elements, heat treatment temperature, and the output variables, Yield Strength (YS) and Tensile Strength (TS), as shown in Fig. 4.

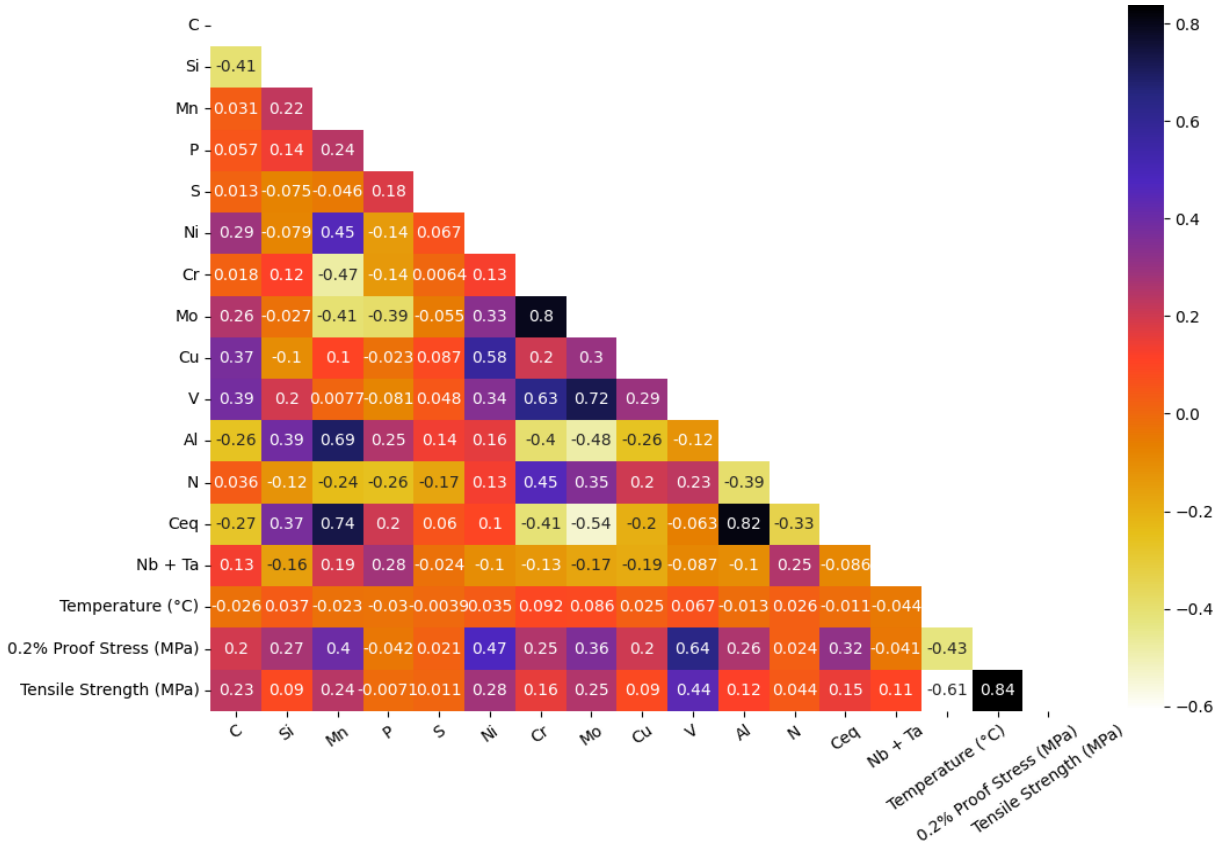


Fig. 4. Correlation heatmap of low alloy steel dataset.

Based on the correlation heatmap of the mechanical properties and chemical composition of the low-alloy steel dataset, it can be seen that the chemical element Vanadium (V) has a strong positive correlation with both Yield Strength (YS) and Tensile Strength (TS), with correlation values of 0.64 and 0.44, respectively. This indicates that an increase in the concentration of V can improve the YS and TS values. The chemical elements Nickel (Ni) and Manganese (Mn) also have a strong correlation with YS, with correlation values of 0.47 and 0.4, respectively. On the other hand, the chemical elements Nitrogen (N), Sulfur (S), and Phosphorus

(P) have very weak correlations with YS and TS. These results are consistent with previous studies [25] that found that V is one of the chemical elements that have a significant effect on the mechanical properties of low-alloy steel. Additionally, studies [26][27] also showed that a higher concentration of V can increase the tensile strength and hardness of low-alloy steel. A higher concentration of Ni and Mn can also increase the tensile strength and hardness of low-alloy steel by forming a solid alloy with the steel matrix. Nickel can improve the tensile strength of low alloy steel by increasing intergranular strength and stabilizing the microstructure of the alloy[28][29].The next step is to normalize the data, the low-alloy steel dataset consisting of chemical elements, heat treatment temperature, and mechanical properties have different value ranges. To address this issue, data normalization is performed using the Min-MaxScaler method. This method works by mapping the values of each feature to a range of 0 to 1 as seen in Fig. 5. By normalizing the data, the value ranges of each feature in the dataset will be adjusted to have a uniform value range. The Min-Max Scaler normalization method has a positive impact on machine learning modeling, as some machine learning algorithms are sensitive to differences in data scale [30]. By normalizing the data, the resulting model becomes more stable and accurate in classification or prediction. Additionally, normalization can also help prevent overfitting and speed up the model training process[31].

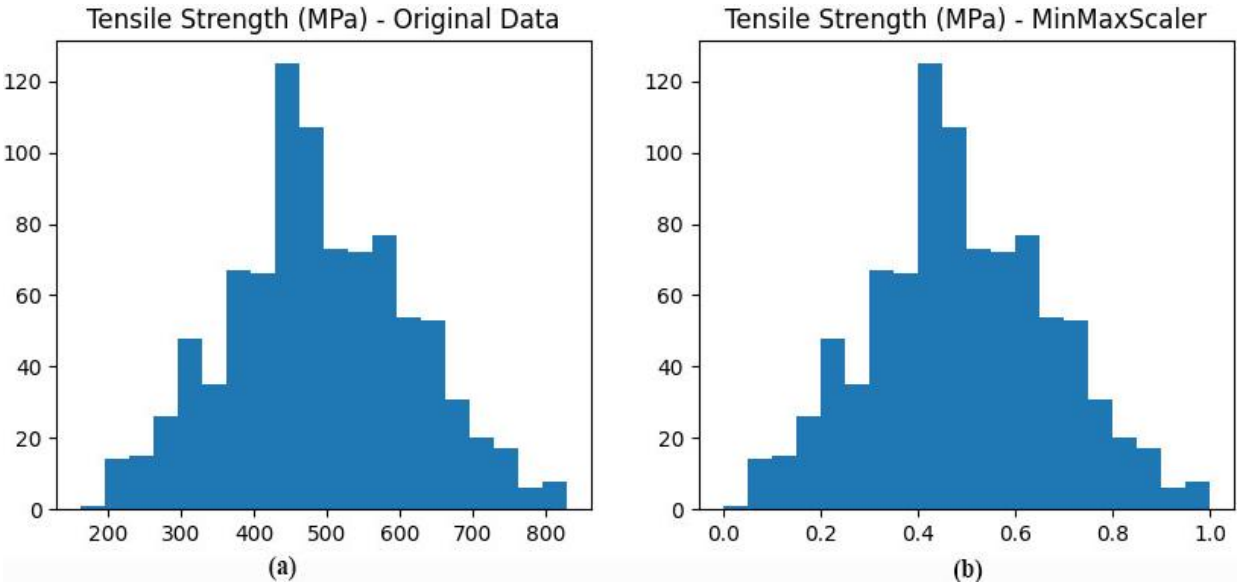


Fig. 5. Comparison of original data (a) with normalized data (b).

3.3 Artificial Neural Network (ANN) Modeling

The Artificial Neural Network (ANN) model was created using the Python programming language with the TensorFlow library. The architecture of the ANN was designed according to the number of input variables in the dataset, which are 15 chemical elements and heat treatment temperature. In this case, each neuron in the input layer receives input from one variable. Meanwhile, the output layer consists of only one neuron, which will output the prediction result of one mechanical property. In this study, the low-alloy steel dataset was tested with three different ANN architectures as shown in Table 2.

Table 2. Comparison of ANN architectures

Name	Input layer	Hidden layer	Neuron	Output layer
Architecture 1	1	2	(32*16)	1
Architecture 2	1	3	(64*32*16)	1
Architecture 3	1	4	(128*64*32*16)	1

The three models were compared, where the model that obtained the best evaluation metrics will be further parameter-tuned. The low-alloy steel dataset was divided into two parts with 80% for training and 20% for testing. The testing process was conducted in two stages, the first stage for predicting YS and the second stage for predicting TS. The testing of each ANN architecture was performed with the same parameter combination, which was using the Adam optimizer, the learning rate of 0.0001,anda batch size of 16. This modeling applied the early stopping function, which stops the training if there is no improvement in the model's performance on the validation data.

The test results showed that all three ANN model architectures were capable of providing sufficiently accurate YS predictions with R-squared values above 0.8. The best result was obtained from Architecture 2 with MAE 23.665, RMSE 38.401, and R-squared 0.915, as seen in Table 3. However, the TS prediction results were very different from the YS results, where none of the three architectures were able to obtain R-squared values above 0.8. Modeling with Architecture 3 obtained the best evaluation values with MAE 47, RMSE 74, and R-squared 0.619, as shown in Table 4. Based on these results, it can be seen that adding hidden layers and neurons does not always have a positive impact on the performance of the ANN model in predicting low-alloy steel.

Table 3. YS testing results for model architectures

Metric	Architecture 1	Architecture 2	Architecture 3
MAE	30.807	23.665	23.113
RMSE	46.314	38.401	38.663
R-squared	0.877	0.915	0.908

Table 4. TS testing results of the model architectures

Metric	Architecture 1	Architecture 2	Architecture 3
MAE	96.560	61.518	47.134
RMSE	135.292	85.111	74.868
R-squared	0.199	0.525	0.619

3.4 TuningParameter

After obtaining the best-performing model architecture, the next step is to perform tuning parameters to determine the optimal value for each hyperparameter in the model. This process is done by trying various combinations of hyperparameter values and seeing which one gives the best performance on validation or testing data. The goal of tuning parameters is to produce a model that has the best performance. The hyperparameters that are varied are the optimizer, learning rate and batch size.

3.4.1 Optimizer Search

The search process for the optimal optimizer is done by testing various optimizer variations such as Adam, RMSprop, SGD, Adadelta, and Adamax using a combination of architecture 3 for YS and architecture 2 for TS, a learning rate of 0.0001, and a batch size of 16. The test results show that the RMSprop optimizer produces the best performance in predicting both mechanical properties. YS obtains an MAE value of 19.529, RMSE 32.795, and R-squared 0.931, while TS obtains an MAE value of 42.512, RMSE 57.285, and R-squared 0.777. The optimizer search results can be seen in Table 5 for YS and Table 6 for TS.

Table 5. YS testing results for various optimizers

Metric	Adam	RMSprop	SGD	Adadelta	Adamax
MAE	23.141	19.529	61.409	151.427	24.711
RMSE	38.282	32.795	78.519	191.182	39.082
R-squared	0.915	0.931	0.630	0.263	0.908

Table 6. Testing results of various optimizers for TS

Metric	Adam	RMSprop	SGD	Adadelta	Adamax
MAE	47.134	42.512	148.934	191.615	50.403
RMSE	74.868	57.285	189.800	249.311	76.460
R-squared	0.619	0.777	0.144	-3.071	0.617

3.4.2 Learning Rate Search

After obtaining the most optimal optimizer, a search for the best learning rate was performed with variations of 0.01, 0.001, and 0.0001 using the RMSprop optimizer and a batch size of 16. The search results for YS prediction showed that the best performance was achieved with a learning rate of 0.0001, with MAE of 19.529, RMSE of 32.795, and R-squared of 0.931. Meanwhile, the best performance for TS was achieved with a learning rate of 0.001, with MAE of 35.586, RMSE of 49.104, and R-squared of 0.868. The results of the best learning rate search can be seen in Table 7 for YS and Table 8 for TS.

Table 7. Results of YS testing against learning rate

Metric	Lr = 0.01	Lr = 0.001	Lr = 0.0001
MAE	23.903	31.195	19.529
RMSE	39.188	42.449	32.795
R-squared	0.907	0.891	0.931

Table 8. TS testing results for various learning rates

Metric	Lr = 0.01	Lr = 0.001	Lr = 0.0001
MAE	55.923	35.586	42.512
RMSE	69.013	49.104	57.285
R-squared	0.687	0.868	0.777

3.4.3 Batch Size Search

A batch size search was performed by testing the model with each of the best parameter combinations obtained earlier, and then the batch size value was varied from 16, 18, 32, and 64. The model parameters for YS prediction are Architecture 3, optimizer Adam, learning rate 0.0001, while the TS parameter combination is Architecture 2, optimizer RMSprop, learning rate 0.001. The best batch size search results for YS prediction were obtained with the best model performance at a batch size of 32 with MAE 19.027, RMSE 26.686, and R-squared 0.957, while the TS prediction model obtained the best performance with a batch size of 16 with MAE 35.586, RMSE 49.104, and R-squared 0.868. The results of the best batch size search can be seen in Table 9 for YS and Table 10 for TS.

Table 9. Results of YS testing against batch size

Metric	8	16	32	64
MAE	20.715	22.362	19.027	23.388
RMSE	35.666	37.462	26.686	37.885
R-squared	0.923	0.931	0.957	0.913

Table 10. Results of TS testing on batch size

Metric	8	16	32	64
MAE	33.861	35.586	56.256	54.216
RMSE	51.902	49.104	75.267	78.664
R-squared	0.852	0.868	0.690	0.662

Based on the previous hyperparameter results, varying the optimizer, learning rate, and batch size had a positive impact on the performance of the ANN model in predicting the mechanical properties of low-alloy steel. By tuning these parameters, two model combinations were obtained: Architecture 3, RMSprop optimizer, learning rate of 0.0001, batch size of 32 for YS prediction model, and Architecture 2, RMSprop optimizer, learning rate of 0.001, batch size of 16 for TS prediction model. The evaluation metrics of the testing of these two models can be seen in Fig. 6.

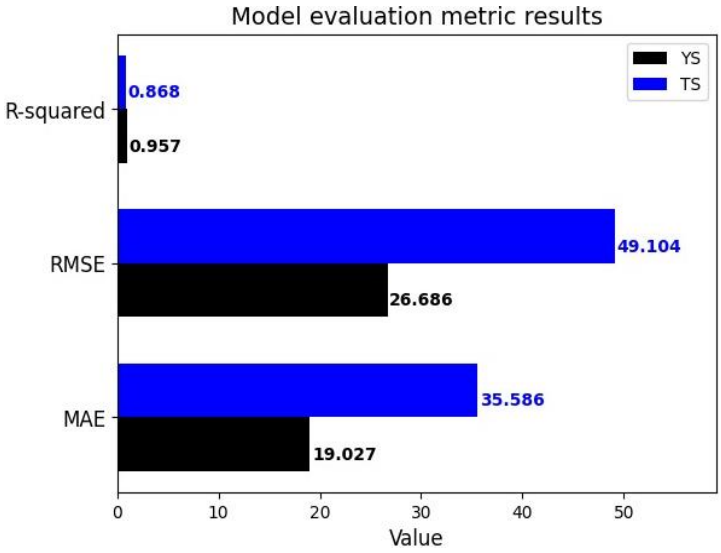


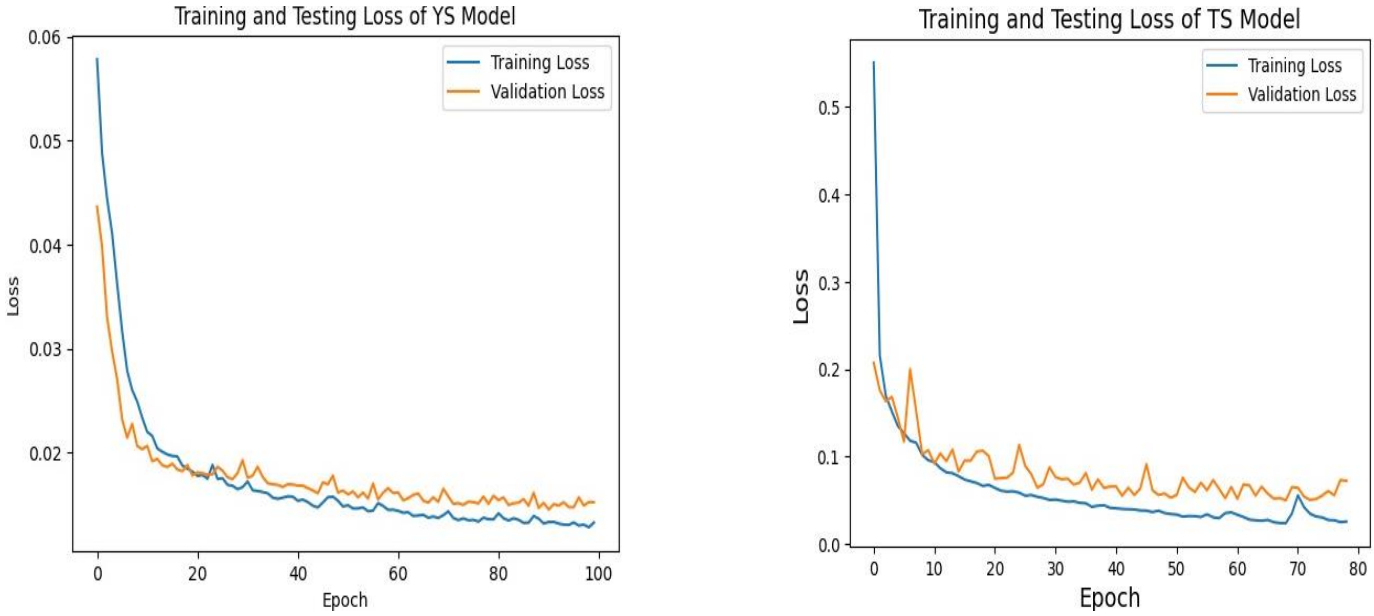
Fig. 6. Model evaluation metrics.

Additionally, the performance of both combinations of ANN models was evaluated by looking at the loss values generated by the models during training and testing, as shown in Fig.7. The training and testing graphs tend to decrease similarly as the number of epochs increases, indicating that the models can generalize well on the testing data.

The results of this study indicate that the machine learning model using Artificial Neural Network (ANN) for predicting the mechanical properties of low alloy steel based on chemical composition and heat treatment has better performance in predicting YS compared to TS. The predicted results of the model testing data can be seen in Fig. 8.

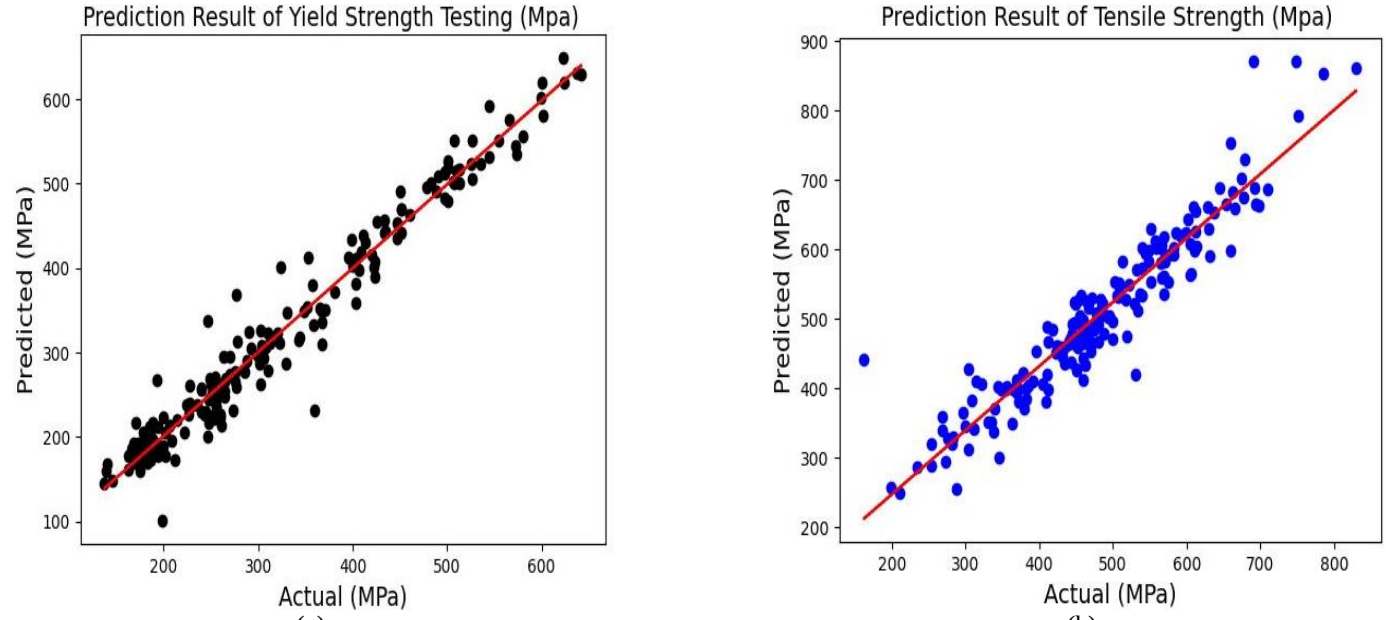
3.5 Model Validation

After obtaining the ANN model, the next step is to validate the model using cross-validation. In this modeling, a 10-fold cross-validation is utilized, where the data is divided into 10 different subsets or folds. The process involves iterating 10 times, selecting each subset in turn as the test data and the remaining subsets as the training data. This provides a good balance between variance and bias in estimating model performance. If the value of K is too small, the model's performance estimation tends to have high variance. A K value of 10 is sufficiently large to provide stable estimates while still being efficient in data utilization [32]. Moreover, a K value of 10 helps mitigate the risk of overfitting as the model is evaluated on various data subsets, making it more likely to detect more common patterns [12]. The prediction results of the ANN model using 10-fold cross-validation can be seen in Fig.9. The evaluation metrics of the model using 10-fold cross-validation indicate that the ANN model achieved a Mean Absolute Error (MAE) of 18.197, Root Mean Square Error (RMSE) of 23, and R-squared of 0.969 for predicting YS. Additionally, for TS prediction, the evaluation resulted in an MAE of 27, RMSE of 36.696, and R-squared of 0.907, as shown in Fig.10. These results demonstrate that the utilized ANN model exhibits stable performance and can be relied upon for predictions on larger and diverse datasets.



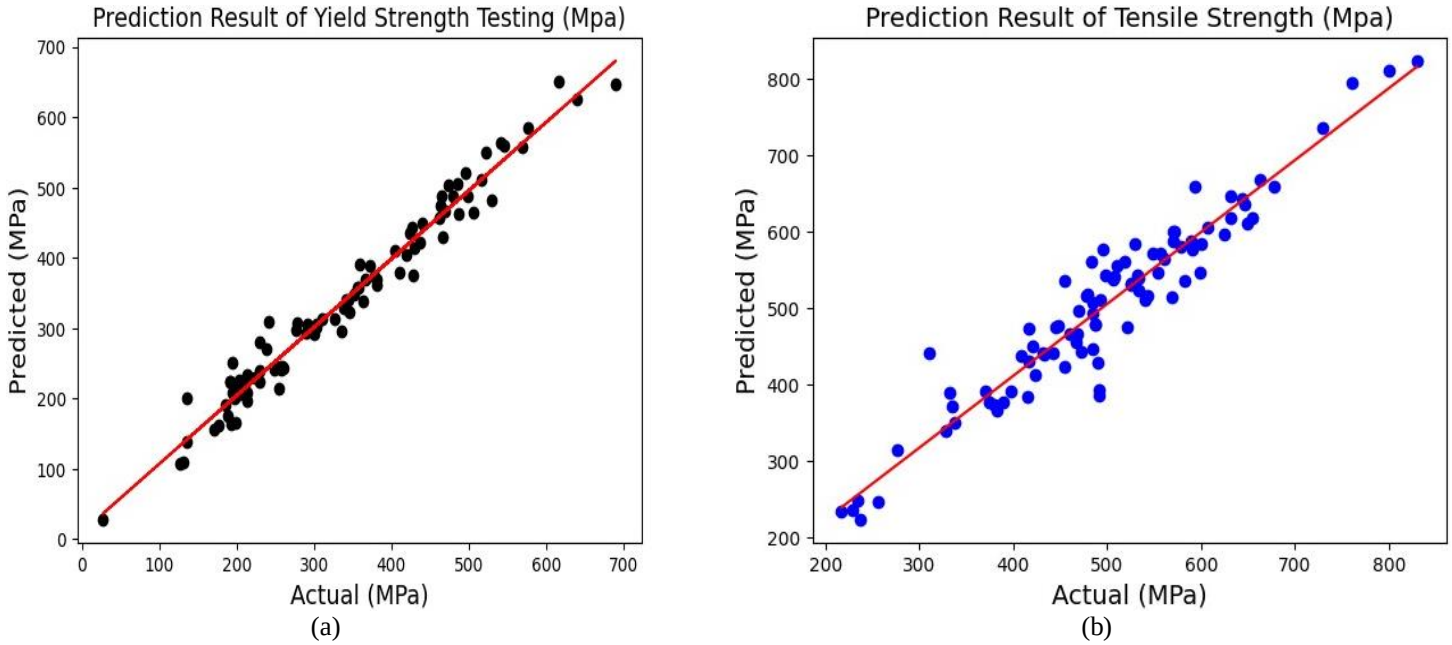
(a) (b)

Fig. 7. Model loss for YS prediction (a) and TS prediction (b).



(a) (b)

Fig. 8. Results of YS prediction (a) and TS prediction (b).



(a) (b)

Fig. 9. Results of YS prediction (a) and TS prediction (b).

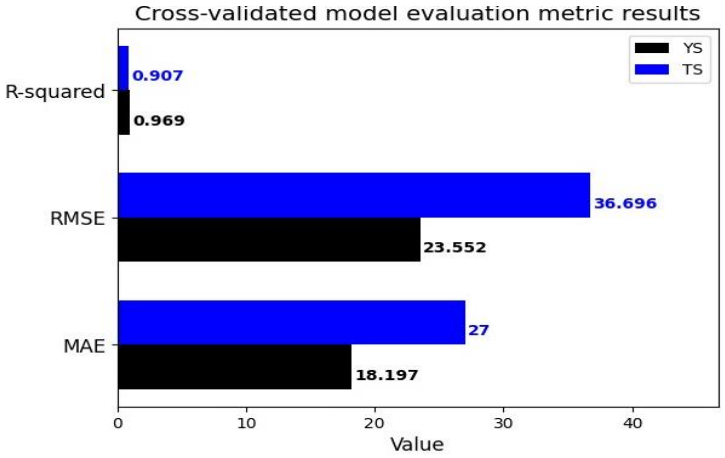


Fig. 10. Model evaluation metrics with cross-validation.

4 Conclusion

Based on the results of the prediction modeling of low-alloy steel mechanical properties using Artificial Neural Network (ANN), it can be concluded that modeling with ANN provides good results. Chemical elements such as Vanadium (V), Nickel (Ni), and Manganese (Mn) have a strong positive correlation with Yield strength (YS) and Tensile strength (TS). Increasing the number of hidden layers and neurons in the ANN architecture does not directly improve the performance of the model in predicting low-alloy steel mechanical properties. Tuning the hyperparameterscan determine the best parameters for the ANN modeling and improve the model performance. The evaluation results of the model with the observation of the loss value, the training and testing loss graphs tend to decrease as the number of epochs increases, indicating that the model can generalize well on the testing data. The results of model validation with cross-validation using k=10 showed that the designed ANN model has stable and reliable performance in predicting a larger and more diverse dataset. The ANN modeling obtained from this study showed that the ANN model has better performance in predicting YS compared to TS.

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