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Effect of Feature Selection Using Recursive Feature Elimination on Tensile Strength Prediction Modeling of Low-Alloy Steel

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Abstract

In machine learning-based tensile strength prediction modeling of low-alloy steel, significant complexity often arises due to variations in chemical composition and heat treatment temperature. Therefore, this study applies feature selection using Recursive Feature Elimination (RFE) combined with the Random Forest algorithm to identify the most influential chemical elements and heat treatment temperature affecting the tensile strength of low-alloy steel. The RFE-Random Forest model was evaluated using different numbers of input features, and model performance was assessed using three evaluation metrics: Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and R-squared (R^2). The results indicate that the model incorporating seven input variables (C, Mn, Ni, Cr, Mo, V, and Temperature) achieved the best predictive performance, with an MAE of 20.333, an RMSE of 30.412, and an R-squared value of 0.945. External validation using unseen data demonstrated a significant improvement compared with the training stage, yielding an MAE of 13.472, an RMSE of 17.334, and an R-squared value of 0.978. These findings suggest that feature selection using RFE combined with Random Forest is a reliable approach for efficiently designing and predicting the mechanical properties of low-alloy steel.

Keywords: *Tensile strength; low-alloy steel; feature selection; Recursive Feature Elimination; Random Forest.*

1. Introduction

Low-alloy steel plays a vital role in various industries, including construction and manufacturing. One of the most critical characteristics of steel is its tensile strength, which serves as a key parameter for evaluating material quality and durability. A thorough understanding of the tensile strength of low-alloy steel can help minimize the occurrence of premature material failure [1]. According to [2], knowledge of the mechanical properties of a material is essential not only for preventing premature failure of machine and industrial components but also for ensuring user safety. The tensile strength of low-alloy steel is strongly influenced by its microstructure, chemical composition, and heat treatment temperature [3]. Therefore, understanding the relationship between chemical composition and mechanical properties is of great importance for researchers seeking to develop materials tailored to specific application requirements. However, experimental testing of chemical composition and mechanical properties is often associated with several challenges, including high costs, lengthy testing periods, and the need for specialized expertise. These limitations can hinder the analysis and development of low-alloy steel materials.

The advancement of machine learning techniques in materials science has significantly transformed the design, understanding, and optimization of material mechanical properties. In recent years, technological progress and the increasing availability of experimental data have accelerated the adoption of machine learning approaches in this field [4]. One of the most widely studied topics is the prediction of steel mechanical properties using machine learning algorithms such as Random Forest, Support Vector Machines, and Neural Networks [5], [6], [7]. These methods offer several advantages, including their ability to handle complex relationships among variables and adapt to diverse datasets. Machine learning models can effectively capture intricate and nonlinear patterns within data [8]. However, achieving accurate and robust predictive performance often requires additional techniques, such as hyperparameter optimization, data augmentation, and feature selection [9]. Recursive Feature Elimination

(RFE) is a feature selection technique used in machine learning to identify the optimal subset of relevant features from a dataset. The primary objective of RFE is to improve model performance by reducing the number of input features, thereby producing simpler and more efficient models. RFE operates through an iterative process in which a model is initially trained using all available features, followed by the removal of the least important feature at each iteration. This process continues until the desired number of features is reached or no further features can be eliminated [10].

The importance of understanding the impact of feature selection on tensile strength prediction of low-alloy steel has been highlighted in several previous studies. For example, [11] investigated the application of RFE combined with various machine learning algorithms for predicting the tensile strength of steel bars produced in an electric arc furnace. The dataset consisted of 97 features monitored during the steel manufacturing process. The results demonstrated that RFE combined with Random Forest was capable of identifying the most relevant features and achieved superior predictive performance compared with other algorithm combinations. Similarly, [12] applied Random Forest Recursive Feature Elimination (RF-RFE) for structural damage detection in construction systems. The proposed method was designed to extract the most relevant features for identifying structural damage while reducing the number of variables involved. Experimental results showed that the method produced a smaller feature subset while achieving higher identification accuracy and faster detection times. Furthermore, [13] presented a comprehensive study on the application of RFE to a large-scale steel wire dataset. Their findings revealed that RFE not only improved prediction accuracy but also significantly reduced the risk of overfitting. These studies collectively confirm the effectiveness of RFE as a feature selection tool for addressing the complexity of large and high-dimensional materials datasets.

Based on the aforementioned challenges and previous studies, RFE combined with Random Forest has proven to be highly effective in reducing model complexity, improving interpretability, minimizing overfitting risk, and reducing computational cost, particularly when applied to datasets with a large number of features. Therefore, this study aims to apply RFE with Random Forest for feature selection in the prediction of the tensile strength of low-alloy steel. The findings of this research are expected to provide valuable insights into improving the effectiveness and predictive accuracy of machine learning models for estimating the mechanical properties of low-alloy steel through feature selection using RFE and Random Forest.

2. Materials and Methods

In this study, a predictive model for the tensile strength of low-alloy steel was developed using the Random Forest algorithm. The model was further enhanced through a feature selection approach based on Recursive Feature Elimination (RFE). This approach was employed to identify the most influential input variables, including chemical composition and heat treatment temperature, affecting the output variable, namely tensile strength. The model was developed using Python and implemented in the Google Colab environment. The overall research procedure is presented below.

2.1 Dataset

The dataset used in this study consists of tensile test results for low-alloy steel, including mechanical properties such as Tensile Strength (TS), chemical composition percentages, and heat treatment temperature. The data were obtained from Kaggle.com [14] and comprise 915 observations with 15 input variables and 3 output variables. However, only one output variable, namely Tensile Strength (TS), was considered in this study, as presented in Table 1. The dataset was used as training data for developing a predictive model of the tensile strength of low-alloy steel. During the modeling stage, variables considered less relevant were eliminated through a feature selection process using the Recursive Feature Elimination (RFE) method.

Table 1. Statistical summary of the low-alloy steel dataset.

Variables	Data Type	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
Tensile Strength (Mpa)	Output	162	6661	496.25

2.2 Data Preprocessing

Data preprocessing consists of a series of steps performed to clean and prepare the data for optimal use in predictive modeling. The primary objective is to improve prediction accuracy and enhance data analysis. This stage includes missing data handling and data normalization. The dataset was examined to identify missing values in relevant variables, including TS, chemical composition, and heat treatment temperature. Missing values were handled using mean substitution or other appropriate imputation methods.Data normalization was subsequently applied to ensure that the variable values were distributed within a desired range. In this study, the MinMax Scaler was employed for data normalization. This technique transforms the values of variables in the dataset into a uniform scale. The MinMax Scaler method is defined by Equation (1).

$$\left[X_{sc} = \frac{X - X_{min}}{X_{max} - X_{min}}\right] \quad (1)$$

Where (X) is the original data, while (X_{sc}) is the normalized data. The purpose of data normalization is to eliminate potential bias in the data caused by differences in the scales of each variable [7].

2. 3 Recursive Feature Elimination (RFE)

RFE is a feature selection method used in machine learning. This method aims to eliminate less important features from a dataset [11]. This approach works by iteratively removing features based on their contribution to the model's performance. Figure 1 illustrates the application of RFE in selecting the most appropriate input variables for the output variable.

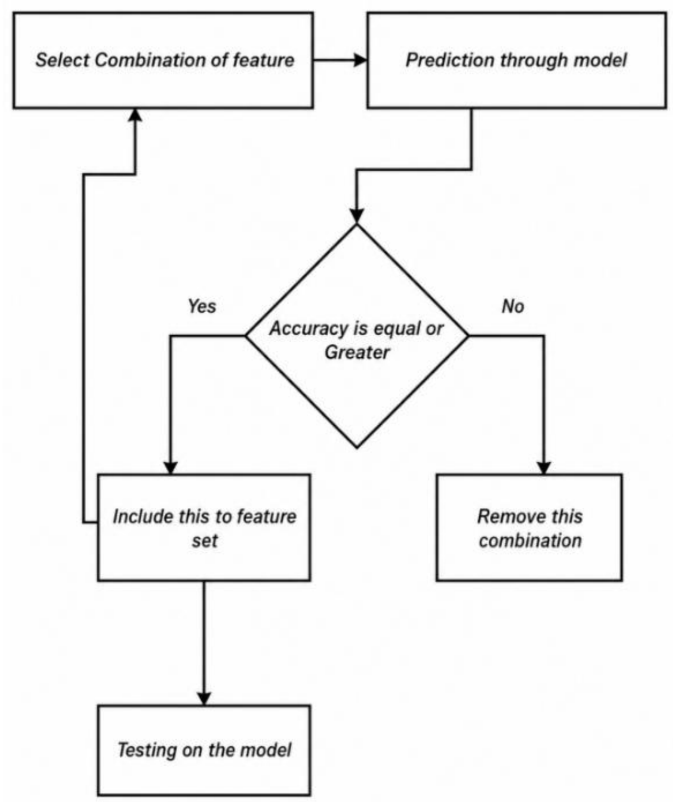

Figure 1. Illustration of RFE in determining the most influential features.

In general, the RFE algorithm works as follows: (1) initializing a machine learning model using all features available in the dataset, (2) calculating the importance of each feature in the model, (3) removing features that are not significant to the output variable, and (4) repeating steps 2 and 3 until the desired number of features is achieved [10]. In this way, the RFE algorithm can help improve the accuracy of machine learning models by eliminating less important features from the dataset.

The predictive model used in this study is Random Forest. This algorithm works by constructing multiple decision trees and combining them to obtain more stable and accurate predictions. The forest formed by Random Forest is a collection of decision trees that are typically trained using the bagging method. The basic idea of the bagging method is to combine learning models to improve overall performance. The Random Forest algorithm introduces an additional element of randomness into the model while constructing decision trees. Instead of searching for the most important feature when splitting a node, Random Forest searches for the best feature among a randomly selected subset of features [15]. This approach produces substantial diversity and generally results in a better-performing model. In this study, the Random Forest model was implemented using the default parameters provided by the scikit-learn library version 1.2.2 [16], as shown in Table 2.

Table 2. Random Forest Parameters

No	Parameter	Value
1	n_estimators	100
2	criterion	'squared_error'
3	max_depth	None
4	max_features	1.0
5	random_state	None

It is worth noting that all Random Forest models in this study were implemented using the default hyperparameters provided by the scikit-learn library, as listed in Table 2, without additional optimization. This decision was made considering that the primary focus of the study is to evaluate the effect of feature selection using RFE on model performance, rather than to optimize the model architecture itself. Future studies are encouraged to explore hyperparameter tuning strategies to further enhance prediction accuracy. The data used to train and test the model were divided into two subsets, namely training data (80%) and testing data (20%). The model performance was evaluated using three metrics: Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and R-squared.

2. 4 Model Evaluation

Model evaluation is the process of assessing the performance of a machine learning model using specific metrics or indicators. The purpose of model evaluation is to understand the extent to which the model can generalize and provide accurate predictions on previously unseen data [17]. At this stage, the Random Forest model was tested using new data according to the number of features selected based on the previous RFE process.

3. Results and Discussion

The dataset used for predicting the tensile strength of low-alloy steel was divided into two categories: 815 samples for the training phase and 100 samples for external testing. This external testing was conducted to verify that the resulting model was capable of making accurate predictions on new data.

3.1 Recursive Feature Elimination (RFE)

In general, there are three groups of feature selection methods, namely filter, wrapper, and embedded selector methods. Filter methods evaluate each feature independently of the classifier, rank the features based on the evaluation results, and select the most relevant ones. Wrapper methods require a machine learning algorithm and use its performance as the evaluation criterion. This method searches for the feature subset that is most suitable for the machine learning algorithm and aims to improve its performance. Embedded selector methods combine filter and wrapper approaches by incorporating feature selection into the machine learning algorithm itself. Recursive Feature Elimination (RFE) belongs to the wrapper group of feature selection methods [18]. This method requires a machine learning algorithm and uses its performance as the evaluation criterion. It searches for the feature subset that is most suitable for the machine learning algorithm and aims to improve the algorithm's performance. In this study, the machine learning algorithm used was Random Forest.

The RFE process begins by training the model using the entire feature set and then evaluating the contribution of each feature to the model's performance. The feature with the lowest contribution is eliminated. This iteration continues until the desired number of features is achieved. At this stage, the number of features was varied from 5 to 15 features. Each feature subset was evaluated using performance metrics such as MAE, RMSE, and R-squared. The feature subset selected for evaluation using new data was the model with the best evaluation metrics. The results of RFE using Random Forest are shown in Figure 2.

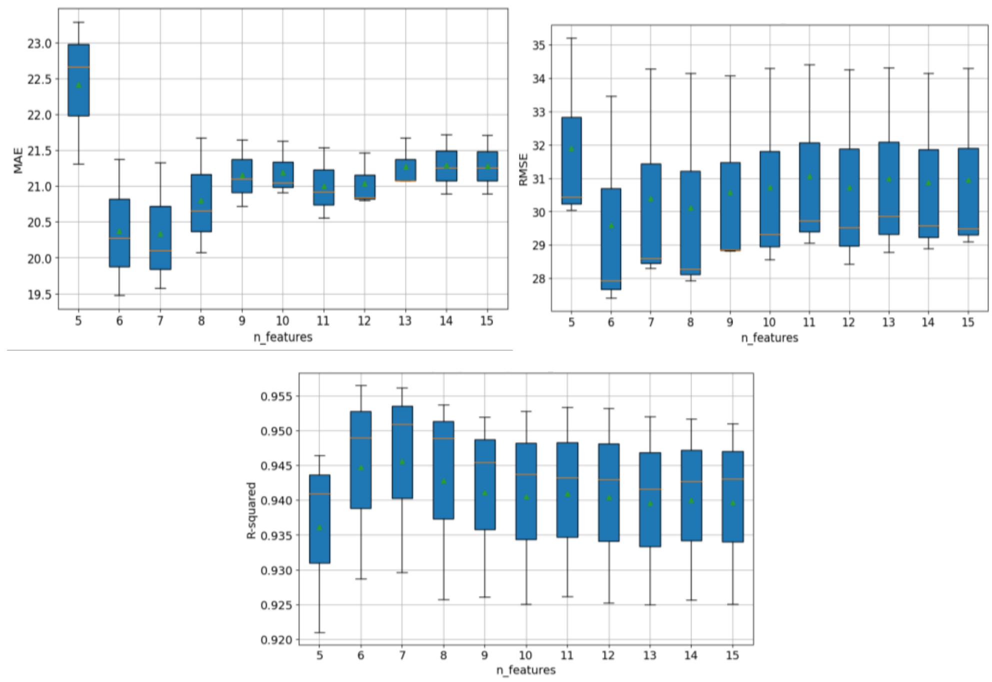

Figure 2. Comparison of RFE Results with Different Numbers of Features

Based on the RFE results shown in Figure 2, it can be observed that feature sets consisting of 6 and 7 features produced relatively better evaluation metrics compared to the other feature sets. The model with 6 input variables achieved an average MAE of 20.421, an RMSE of 29.831, and an R-squared value of 0.944. Meanwhile, the model with 7 input variables obtained an MAE of 20.333, an RMSE of 30.412, and an R-squared value of 0.945. These results indicate that the model with 7 input variables achieved slightly better evaluation metrics overall. In general, it can be observed that feature sets containing fewer than 6 features produced the poorest evaluation results. However, predictive models with more than 7 features did not consistently yield better evaluation metrics than those obtained with 6 or 7 features. The variables used in each feature subset variation are presented in Table 3.

Table 3. Variables Used for Each Feature Subset Variation

Number of Features	Variables
5	C, Mn, Mo, V, and Temperature (°C)
6	C, Mn, Cr, Mo, V, and Temperature (°C)
7	C, Mn, Ni, Cr, Mo, V, and Temperature (°C)
8	C, Mn, Ni, Cr, Mo, V, N, and Temperature (°C)
9	C, Si, Mn, Ni, Cr, Mo, V, N, and Temperature (°C)
10	C, Si, Mn, P, Ni, Cr, Mo, V, N, and Temperature (°C)
11	C, Si, Mn, P, S, Ni, Cr, Mo, V, N, and Temperature (°C)
12	C, Si, Mn, P, S, Ni, Cr, Mo, V, N, Ceq, and Temperature (°C)

The low-alloy steel dataset was analyzed using Pearson correlation to examine the influence of alloying elements and temperature on the tensile strength of low-alloy steel. Pearson correlation is a statistical method used to measure the extent to which two variables are correlated or have a linear relationship with one another. This metric produces a correlation coefficient (r) ranging from -1 to 1. An r value close to 1 indicates a perfect positive correlation, meaning that there is a positive linear relationship between the two variables. As one variable increases, the other variable also tends to increase. An r value close to -1 indicates a perfect negative correlation, meaning that there is a negative linear relationship between the two variables. As one variable increases, the other variable tends to decrease. An r value close to 0 indicates that there is no linear relationship between the two variables [19].

Through this analysis, it is expected that the extent to which variations in alloying elements and temperature contribute to variations in the tensile strength of low-alloy steel can be revealed. This process aims to provide deeper insight into the factors affecting the mechanical properties of the material, which, in turn, can support the development of more accurate and optimized predictive models. The results of the Pearson correlation analysis are presented in Figure 3.

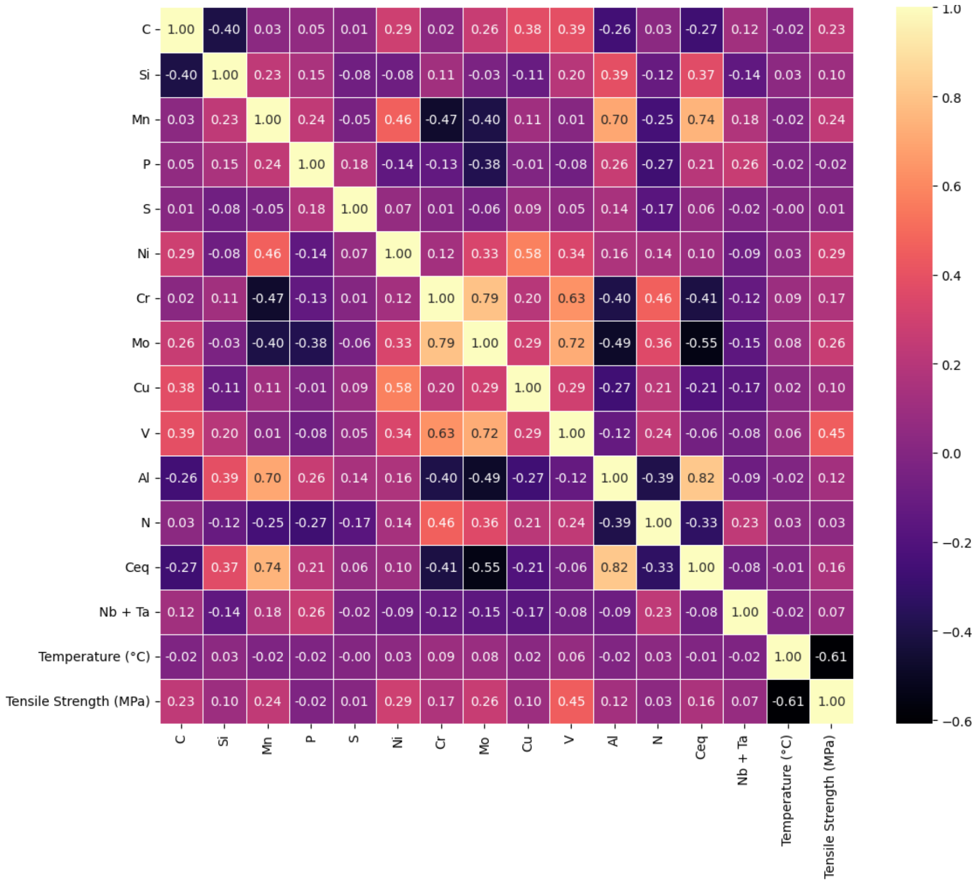

Figure 3. Relationship Between Chemical Elements, Temperature, and the Tensile Strength of Low-Alloy Steel.

Based on the Pearson correlation results, it can be observed that almost all chemical elements exhibit a positive correlation with the tensile strength of low-alloy steel, except for phosphorus (P). In contrast, temperature showed a different trend, exhibiting a relatively strong negative correlation of approximately -0.61 with tensile strength. These results indicate that the addition of alloying elements can enhance the tensile strength of low-alloy steel, whereas higher temperatures tend to reduce its tensile strength.

Based on the Pearson correlation results, six input variables were identified as having relatively strong correlations with tensile strength: Carbon (C), Manganese (Mn), Nickel (Ni), Molybdenum (Mo), Vanadium (V), and Temperature. Although Chromium (Cr) did not rank among the top six variables in the Pearson correlation analysis, it was nonetheless included in the best-performing model selected by RFE. This can be attributed to the fundamental difference between Pearson correlation and RFE as feature evaluation methods. Pearson correlation measures the linear relationship between each individual feature and the target variable independently, whereas RFE evaluates the collective contribution of features within the context of the Random Forest model, capturing multivariate interactions that may not be reflected in pairwise correlation coefficients. In the case of Cr, its contribution may be more prominent when considered in combination with other alloying elements. From a metallurgical perspective, Cr is known to improve the hardenability of low-alloy steel by promoting the formation of martensite and bainite during heat treatment, thereby indirectly contributing to higher tensile strength. This justifies its inclusion in the final feature subset selected by RFE. Therefore, the use of these features in the predictive model can be justified by their strong correlations with tensile strength, providing valuable contributions to the prediction of low-alloy steel performance. Figure 4 illustrates the influence of tensile strength under different temperatures and vanadium (V) contents.

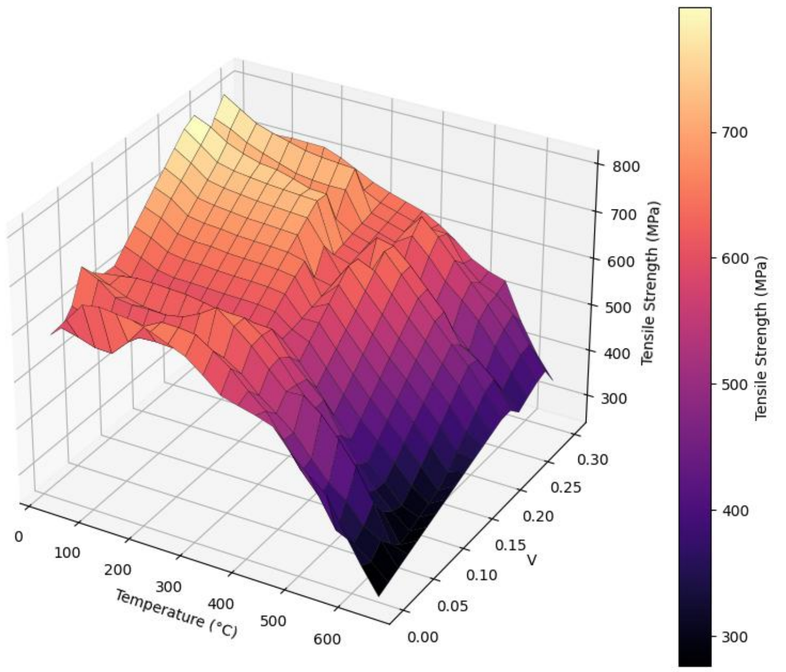

Figure 4. Influence of Temperature and Vanadium (V) Content on the Tensile Strength of Low-Alloy Steel

Based on Figure 4, it can be observed that an increase in temperature leads to a reduction in the tensile strength of low-alloy steel, whereas an increase in vanadium (V) content enhances its tensile strength. These findings are consistent with previous research [20], which reported that the addition of vanadium can improve the tensile strength of low-alloy steel. Vanadium forms carbides that are dispersed throughout the steel microstructure, thereby enhancing the overall hardness and tensile strength. In addition, vanadium can facilitate the formation of martensite or bainite during heat treatment, which further improves the tensile strength and hardness of the steel. Vanadium also forms carbide compounds with carbon in steel. Vanadium carbides tend to remain stable at elevated temperatures, contributing to improved wear resistance and strength under high-temperature conditions. Figure 5 illustrates the influence of carbon (C) and vanadium (V) contents on the tensile strength of low-alloy steel.

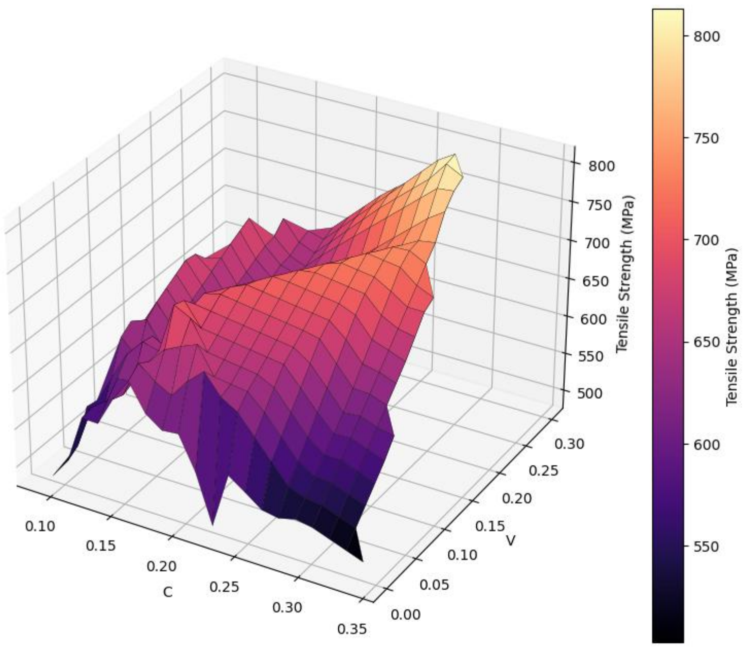

Figure 5. Influence of Carbon (C) and Vanadium (V) Contents on the Tensile Strength of Low-Alloy Steel

Based on Figure 5, it can be observed that a carbon content of 0.25% and a vanadium content of 0.3% resulted in the highest tensile strength, exceeding 750 MPa. This phenomenon can be explained by the fact that increasing the carbon content in low-alloy steel enhances its ability to form martensite during rapid cooling after heat treatment [21], [22]. Martensite typically exhibits high hardness and tensile strength.

Carbon in low-alloy steel can also influence the phase transformations that occur during heat treatment, such as the formation of carbide compounds with other metallic elements present in the steel. These phase transformations occur at specific temperatures, and the carbon content can affect the temperatures at which these transformations take place.

3.2 Model Evaluation

Model evaluation using new data is an important stage in assessing the extent to which a machine learning model can generalize and provide accurate predictions on data that were not observed during the training process. In this study, the new data consisted of samples that were not included in the model training set. Evaluating the model with new data helps determine whether the model can generalize effectively under various conditions [17].

This evaluation ensures that the model can be applied effectively in real-world situations. Evaluation metrics such as MAE, RMSE, and R-squared were used to measure how well the model predicted the target values on the new data. These metrics provide an indication of how closely the model predictions match the actual values. The evaluation results were then used to assess the overall performance of the model. At this stage, the Random Forest model with seven input variables, namely C, Mn, Ni, Cr, Mo, V, and Temperature (°C), was tested using 100 new samples. The new dataset was adjusted to match the selected input features. The results of the external testing using the new data are presented in Figure 6. The external testing produced excellent results, as indicated by the relatively low MAE value of 13.472, an RMSE of 17.334, and an R-squared value of 0.978. These results represent a significant improvement compared with the model performance obtained during the previous training stage. This finding indicates that the model is capable of accurately predicting the tensile strength of low-alloy steel across diverse data variations.

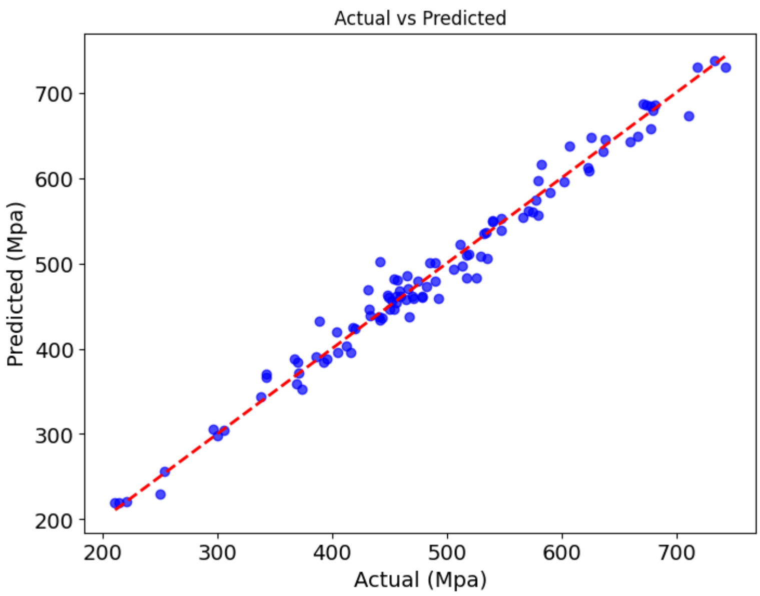

Figure 6. Comparison of model prediction results

4. Conclusion

Based on the feature selection results obtained using Recursive Feature Elimination (RFE) for predicting the tensile strength of low-alloy steel with Random Forest, it can be concluded that this approach is effective in identifying the input variables that have the greatest influence on the output variable. In this study, the low-alloy steel tensile test dataset initially consisted of 15 input variables and 1 output variable. However, after applying the RFE feature selection process with feature subsets ranging from 5 to 15 variables, the most optimal tensile strength prediction performance was achieved using 7 input variables. These seven variables were Carbon (C), Manganese (Mn), Nickel (Ni), Chromium (Cr), Molybdenum (Mo), Vanadium (V), and Temperature. The resulting model achieved excellent evaluation metrics for predicting the tensile strength of low-alloy steel. Furthermore, external testing using new data demonstrated that the Random Forest model with seven input variables was able to predict unseen data with a satisfactory level of accuracy. Overall, the findings of this study indicate that feature selection using RFE in combination with Random Forest can be considered a reliable approach for efficiently designing and predicting the mechanical properties of low-alloy steel.

Authors' Contributions

LPU: Conceptualization, Methodology, Software, Investigation, Writing (Original Draft). SA: Data Curation, Formal Analysis, Visualization. MEP: Validation, Investigation, Resources. FA: Supervision, Methodology, Writing (Review and Editing). SSS: Supervision, Project Administration, Writing (Review and Editing). All authors have read and approved the final manuscript.

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