Analysis of Mechanical Property Prediction of Cast Copper Alloys Based on Chemical Composition Using Machine Learning

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Abstract

Cast copper alloys are vital in industrial applications due to superior conductivity, corrosion resistance, and favorable mechanical properties. However, their ultimate tensile strength (UTS) and yield strength (YS) are highly sensitive to chemical composition variations, rendering conventional testing costly and time-consuming. To address this, this study develops a predictive model for these mechanical properties based on elemental composition using machine learning. Using a dataset of 100 cast copper alloy profiles from MakeItFrom.com, 22 chemical elements were utilized as input features with UTS and YS as target variables. The methodology involved data preprocessing, correlation analysis, hyperparameter optimization, and modeling with Decision Tree (DT) and Random Forest (RF) algorithms. Performance was evaluated via RMSE, MAE, and R^2, using 5-fold cross-validation across three data splits (60:40, 70:30, and 80:20). Results demonstrated that DT consistently outperformed RF. The optimal DT model, utilizing a 70:30 split, achieved an RMSE of 95.618, an MAE of 65.652, and an R^2 of 0.833 for UTS. For YS prediction, it yielded an RMSE of 62.614, an MAE of 40.481, and an R^2 of 0.838. Ultimately, the Decision Tree algorithm provides a highly effective, data-driven approach to accelerate and optimize material design processes.

Keywords: *Cast copper alloys; Machine learning; Decision tree; Random forest; Mechanical properties prediction*

1. Introduction

The advancement of materials technology in the modern industrial era has increased the demand for materials with superior mechanical properties, high production efficiency, and the ability to satisfy the requirements of various engineering applications. Metal alloys continue to be developed to achieve an optimal combination of properties for manufacturing, automotive, energy, electrical, and mechanical engineering industries [1]. Among these materials, Cast Copper Alloys have been widely used because of their excellent electrical and thermal conductivity, superior corrosion resistance, and adequate wear resistance for components such as bearings, bushings, gears, and valves. The mechanical properties of Cast Copper Alloys are strongly influenced by their chemical composition, in which copper (Cu) is alloyed with elements such as zinc (Zn), tin (Sn), aluminum (Al), nickel (Ni), silicon (Si), manganese (Mn), iron (Fe), phosphorus (P), and other alloying elements. Variations in chemical composition create complex and nonlinear relationships, making conventional analytical approaches insufficient for accurately predicting mechanical properties [2].

The development of Machine Learning (ML) as a branch of Artificial Intelligence has introduced a promising approach in materials informatics by enabling the prediction of material properties directly from chemical composition data without extensive laboratory testing [3]. This approach reduces the cost, time, and resources required for material development while improving prediction efficiency. Recent studies have demonstrated that machine learning combined with data exploration, hyperparameter optimization, and synthetic data generation can significantly improve the prediction accuracy of metallic material properties [4], [5]. Decision Tree (DT) and Random Forest (RF) are among the most widely used regression algorithms because of their capability to model nonlinear relationships and provide reliable prediction performance for various metallic materials. Previous studies have reported that these algorithms achieve high prediction accuracy for stainless steels and other engineering alloys when appropriate hyperparameter optimization and model validation techniques are applied [4], [5], [6].

Despite these advances, studies focusing on the prediction of the mechanical properties of Cast Copper Alloys based on chemical composition remain limited compared with those on steel and aluminum alloys [7]. Moreover, direct comparisons between Decision Tree and Random Forest for predicting the Ultimate Tensile Strength (UTS)

and Yield Strength (YS) of Cast Copper Alloys are still scarce. Since materials informatics studies commonly rely on relatively small experimental datasets, selecting an appropriate machine learning algorithm and validation strategy is essential for obtaining reliable and generalizable prediction models [5], [8]. In this study, a dataset consisting of 100 cast copper alloy specimens obtained from a validated secondary source was used, and model reliability was improved through 5-fold cross-validation during hyperparameter optimization [9], [10].

Therefore, this study aimed to analyze the prediction of the mechanical properties of Cast Copper Alloys based on their chemical composition using Machine Learning techniques. Decision Tree and Random Forest models were developed and evaluated using Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2). Unlike previous studies that mainly focused on steel- or aluminum-based alloys or employed a single prediction algorithm, this study compares the performance of Decision Tree and Random Forest using a dataset containing 22 alloying elements, different train-test split scenarios, and hyperparameter optimization of maximum depth and the number of trees. In addition, Pearson correlation analysis was conducted to investigate the influence of alloying elements on the mechanical properties of Cast Copper Alloys. The findings are expected to provide an accurate prediction model and contribute to the application of materials informatics for efficient, data-driven material design and optimization.

2. Materials and Methods

2.1 Dataset

This study employed a supervised Machine Learning approach to predict the mechanical properties of Cast Copper Alloys based on their chemical composition. The dataset consisted of 100 cast copper alloy specimens obtained from the MakeItFrom.com database [11]. Machine learning has been widely applied to predict the mechanical properties of metallic materials, including stainless steels and aluminum alloys, owing to its capability to model complex and nonlinear relationships between chemical composition and material properties [4], [5], [6].

Each specimen was represented by the midpoint value of the reported composition range for each alloying element, which was used as the input variable in the prediction model. The input variables included Cu, Be, Cr, Pb, Sn, Zn, Fe, Ni, Al, Co, Si, Mn, P, Sb, S, Ti, Mg, As, B, Nb, C, and Zr. The output variables were Ultimate Tensile Strength (UTS) and Yield Strength (YS). Descriptive statistics of the dataset, including the minimum, maximum, mean, and standard deviation of each variable, are presented in Table 1.

Table 1. Descriptive statistics of the cast copper alloy dataset

Description	Data Type	Min	Max	Mean	Standard Deviation
Cu	Input	54	99.97	79.626	12.289
Be	Input	0	2.7	0.131	0.502
Cr	Input	0	0.95	0.019	0.118
Pb	Input	0	25	2.044	3.873
Sn	Input	0	20	3.3	4.698
Zn	Input	0	39	9.368	12.117
Fe	Input	0	4	0.604	0.987
Ni	Input	0	31	2.795	6.524
Al	Input	0	11.1	0.989	2.552
Co	Input	0	2.45	0.053	0.283
Si	Input	0	4.5	0.45	1.134
Mn	Input	0	20	0.674	2.402
P	Input	0	0.75	0.207	0.33
Sb	Input	0	0.4	0.061	0.083
S	Input	0	0.375	0.025	0.061
Ti	Input	0	0.25	0.004	0.026
Mg	Input	0	0.075	0.001	0.007

As	Input	0	0.025	0.001	0.004
B	Input	0	0.1	0.002	0.012
Nb	Input	0	1	0.023	0.142
C	Input	0	0.075	0.002	0.011
Zr	Input	0	0.25	0.004	0.026
UTS	Output	170	1210	404.573	204.176
YS	Output	62	1020	210.945	156.101

Based on the descriptive statistics, copper (Cu) exhibited the highest concentration among all alloying elements, whereas the remaining alloying elements showed varying composition ranges. Such variations indicate that the dataset represents diverse cast copper alloy compositions and provides sufficient compositional diversity for machine learning analysis [12]. Furthermore, the output variables, UTS and YS, exhibited broad value ranges, indicating considerable variation in the mechanical properties of the investigated alloys and providing adequate variability for regression model development [13]. The overall research methodology adopted in this study is presented in Figure 1.

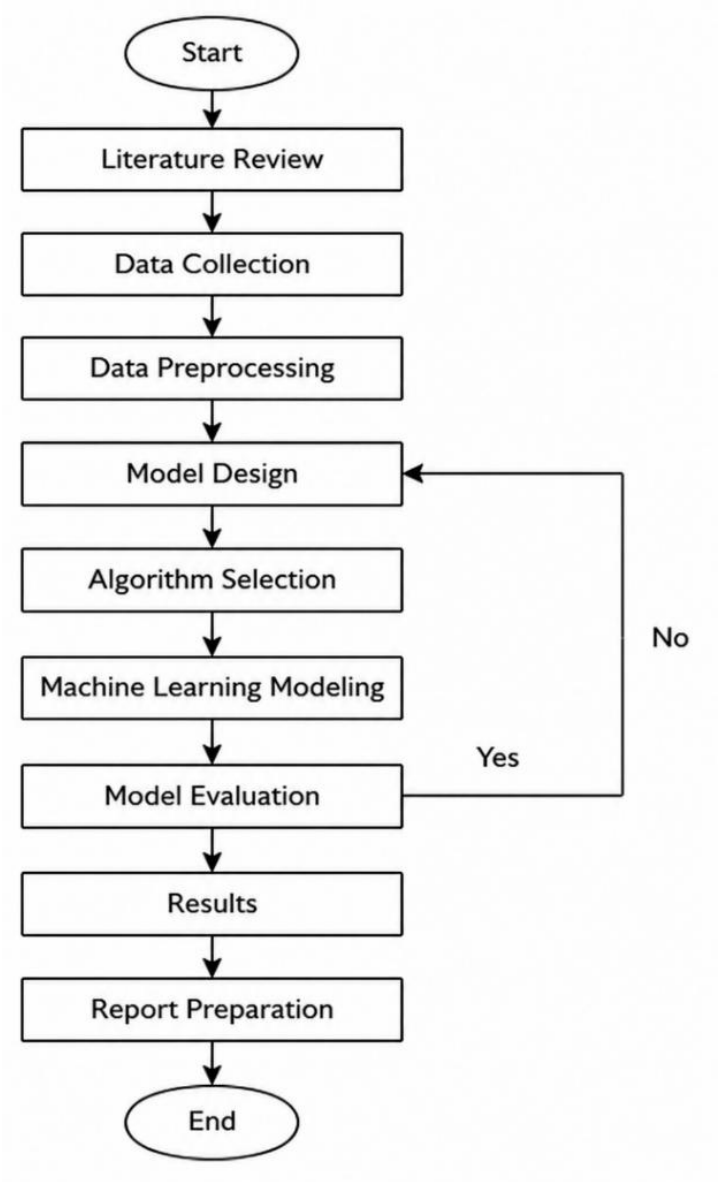


Figure 1. Research workflow

2.2 Data Preprocessing

Prior to model development, the dataset underwent several preprocessing procedures to ensure data quality and improve model performance. The first step involved examining the dataset for missing values. The analysis confirmed that all variables contained complete observations; therefore, no data imputation was required. Subsequently, outlier detection was performed using descriptive statistical analysis to identify extreme values in each variable [14]. The identified values were retained because they remained within the valid chemical composition ranges of Cast Copper Alloys reported in the original dataset and were considered to represent the actual characteristics of the materials [11]. The numerical variables were then normalized using the Min-Max normalization method to transform all variables into the same numerical range. This normalization process reduced differences in variable scales, thereby improving the stability and efficiency of the machine learning algorithms during the training process [15]. All preprocessing procedures were performed using RapidMiner Studio. The preprocessing workflow employed the Retrieve and Normalize operators prior to the model development stage. The processed dataset was subsequently used as the input for the Decision Tree and Random Forest regression models.

2.3 Model Developmen

Prediction models were developed using the Decision Tree (DT) and Random Forest (RF) regression algorithms because both methods are capable of modeling nonlinear relationships between chemical composition and the mechanical properties of materials. To develop the prediction models, the preprocessed data were first partitioned into training and testing subsets using three train-test split ratios (60:40, 70:30, and 80:20). These scenarios were evaluated to investigate the effect of different training data proportions on model performance. Hyperparameter optimization was performed to obtain the optimal configuration for each prediction model [16]. For the Decision Tree algorithm, the maximum depth parameter was varied from 1 to 12. For the Random Forest algorithm, combinations of maximum depth values ranging from 1 to 12 and the number of trees of 20, 40, 60, 80, 100, 120, 140, 160, 180, and 200 were evaluated to determine the optimal model configuration [17]. Model development was carried out using RapidMiner Studio. The modeling workflow utilized the Split Data, Decision Tree, Random Forest, and Apply Model operators to train the prediction models and generate predictions for the testing dataset.

2.4 Model Evaluation

The predictive capability of the developed models was assessed using three regression performance metrics: Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2). MAE quantifies the average magnitude of the absolute differences between predicted and observed values, whereas RMSE places greater emphasis on larger prediction errors. The coefficient of determination (R^2) indicates the proportion of variance in the observed data that can be explained by the prediction model. Lower MAE and RMSE values, together with an R^2 value closer to 1, indicate better predictive performance [18]. To improve the reliability of the evaluation results and reduce bias caused by data partitioning, 5-fold cross-validation was employed during the hyperparameter optimization process. In this approach, the dataset was randomly divided into five subsets. Four subsets were used for model training, while the remaining subset was used for validation. This process was repeated five times until each subset had served as the validation set once, and the average performance was used to determine the optimal model configuration [10]. Despite the application of cross-validation, this study has several limitations. The dataset consisted of only 100 cast copper alloy specimens, resulting in a relatively small testing dataset under the 80:20 train-test split scenario. Consequently, the evaluation results may still be influenced by sampling variability. Therefore, future studies are recommended to employ larger datasets to improve model robustness and generalization capability [19].

3. Results and Discussion

3.1 Correlation Analysis of Chemical Composition and the Mechanical Properties of Cast Copper Alloys

Pearson correlation analysis was conducted to examine the relationships between the chemical composition variables and the mechanical properties of Cast Copper Alloys. The results of the analysis were visualized in the form of a correlation heatmap, as shown in Figure 2. The correlation coefficient ranges from -1 to 1, where positive values indicate a positive relationship, negative values indicate an inverse relationship, and values close to zero indicate a weak relationship.

Attributes	Cu	Be	Cr	Pb	Sn	Zn	Fe	Ni	Al	Co	Si	Mn	P	Sb	S	Ti	Mg	As	B	Nb	C	Zr	Ultimat...	Yield str...
Cu	1	0.281	0.244	-0.165	0.116	-0.776	-0.297	-0.322	-0.067	0.161	0.275	-0.388	0.161	-0.019	-0.023	0.015	-0.029	-0.126	-0.082	-0.066	-0.056	-0.146	-0.131	0.029
Be	0.281	1	0.058	-0.139	-0.183	-0.203	-0.111	0.048	-0.096	0.313	-0.067	-0.066	-0.166	-0.195	-0.109	0.533	-0.027	-0.044	-0.041	-0.043	-0.043	0.165	0.476	0.507
Cr	0.244	0.058	1	-0.083	-0.110	-0.122	-0.087	-0.067	-0.058	0.028	-0.050	-0.045	-0.100	-0.117	-0.065	0.009	-0.016	-0.026	-0.025	-0.026	-0.026	-0.022	0.000	0.084
Pb	-0.1...	-0.139	-0.083	1	0.156	-0.070	-0.201	-0.068	-0.193	-0.100	-0.191	-0.097	0.406	0.843	0.083	-0.090	-0.054	-0.075	-0.082	-0.087	-0.087	-0.074	-0.427	-0.317
Sn	0.116	-0.183	-0.110	0.156	1	-0.327	-0.312	-0.115	-0.267	-0.132	-0.269	-0.183	0.642	0.506	0.155	-0.120	0.092	-0.106	-0.006	-0.110	-0.116	-0.064	-0.407	-0.176
Zn	-0.7...	-0.203	-0.122	-0.070	-0.327	1	0.167	-0.162	-0.047	-0.146	-0.086	0.280	-0.274	-0.210	0.046	-0.132	-0.070	0.254	0.154	-0.127	-0.128	0.000	0.051	-0.135
Fe	-0.2...	-0.111	-0.087	-0.201	-0.312	0.167	1	0.127	0.711	-0.071	-0.157	0.227	-0.302	-0.326	-0.165	-0.033	-0.038	-0.073	-0.061	0.069	0.075	-0.011	0.442	0.203
Ni	-0.3...	0.048	-0.067	-0.068	-0.115	-0.162	0.127	1	0.002	0.033	-0.126	0.030	-0.217	-0.123	-0.063	0.344	0.177	-0.067	-0.048	0.482	0.468	0.364	0.328	0.286
Al	-0.0...	-0.096	-0.058	-0.193	-0.267	-0.047	0.711	0.002	1	0.141	-0.079	0.149	-0.245	-0.286	-0.152	-0.064	-0.040	-0.056	-0.050	-0.064	-0.064	-0.050	0.344	0.136
Co	0.161	0.313	0.028	-0.100	-0.132	-0.146	-0.071	0.033	0.141	1	-0.059	-0.053	-0.119	-0.140	-0.078	0.099	-0.019	-0.032	-0.030	-0.031	-0.031	-0.027	0.108	0.090
Si	0.275	-0.067	-0.050	-0.191	-0.269	-0.086	-0.157	-0.126	-0.079	-0.059	1	-0.064	-0.243	-0.262	-0.138	-0.047	-0.005	0.187	-0.054	-0.029	-0.029	-0.046	0.049	-0.026
Mn	-0.3...	-0.066	-0.045	-0.097	-0.183	0.280	0.227	0.030	0.149	-0.053	-0.064	1	-0.177	-0.207	-0.114	-0.023	-0.022	-0.041	-0.044	0.008	0.008	-0.014	0.180	0.080
P	0.161	-0.166	-0.100	0.406	0.642	-0.274	-0.302	-0.217	-0.245	-0.119	-0.243	-0.177	1	0.608	0.089	-0.108	-0.064	-0.103	-0.092	-0.099	-0.099	-0.087	-0.459	-0.290
Sb	-0.0...	-0.195	-0.117	0.843	0.506	-0.210	-0.326	-0.123	-0.286	-0.140	-0.262	-0.207	0.608	1	0.181	-0.127	-0.074	-0.073	-0.011	-0.122	-0.122	-0.059	-0.535	-0.374
S	-0.0...	-0.109	-0.065	0.083	0.155	0.046	-0.165	-0.063	-0.152	-0.078	-0.138	-0.114	0.089	0.181	1	-0.071	-0.040	-0.000	0.906	-0.041	-0.041	0.267	-0.211	-0.157
Ti	0.015	0.533	0.009	-0.090	-0.120	-0.132	-0.033	0.344	-0.064	0.099	-0.047	-0.023	-0.108	-0.127	-0.071	1	-0.017	-0.029	-0.027	-0.028	-0.028	0.819	0.443	0.293
Mg	-0.0...	-0.027	-0.016	-0.054	0.092	-0.070	-0.038	0.177	-0.040	-0.019	-0.005	-0.022	-0.064	-0.074	-0.040	-0.017	1	0.022	-0.016	0.017	-0.017	-0.014	0.215	0.387
As	-0.1...	-0.044	-0.026	-0.075	-0.106	0.254	-0.073	-0.067	-0.056	-0.032	0.187	-0.041	-0.103	-0.073	-0.000	-0.029	0.022	1	-0.026	-0.027	-0.028	-0.024	0.065	0.060
B	-0.0...	-0.041	-0.025	-0.082	-0.006	0.154	-0.061	-0.048	-0.050	-0.030	-0.054	-0.044	-0.092	-0.011	0.906	-0.027	-0.016	-0.026	1	-0.026	-0.026	0.359	-0.027	-0.036
Nb	-0.0...	-0.043	-0.026	-0.087	-0.110	-0.127	0.069	0.482	-0.064	-0.031	-0.029	0.008	-0.099	-0.122	-0.041	-0.028	0.017	-0.027	-0.026	1	0.994	-0.023	0.081	0.120
C	-0.0...	-0.043	-0.026	-0.087	-0.116	-0.128	0.075	0.468	-0.064	-0.031	-0.029	0.008	-0.099	-0.122	-0.041	-0.028	-0.017	-0.028	-0.026	0.994	1	-0.023	0.068	0.101
Zr	-0.1...	0.165	-0.022	-0.074	-0.064	0.000	-0.011	0.364	-0.050	-0.027	-0.046	-0.014	-0.087	-0.059	0.267	0.819	-0.014	-0.024	0.359	-0.023	-0.023	1	0.350	0.184
Ultimate ...	-0.1...	0.476	0.000	-0.427	-0.407	0.051	0.442	0.328	0.344	0.108	0.049	0.180	-0.459	-0.535	-0.211	0.443	0.215	0.065	-0.027	0.081	0.068	0.350	1	0.890
Yield stre...	0.029	0.507	0.084	-0.317	-0.176	-0.135	0.203	0.286	0.136	0.090	-0.026	0.080	-0.290	-0.374	-0.157	0.293	0.387	0.060	-0.036	0.120	0.101	0.184	0.890	1

Figure 2. Pearson correlation heatmap of chemical composition and mechanical properties

Based on Figure 2, most alloying elements exhibit relatively weak correlations with the mechanical properties, suggesting that these properties are governed by the combined influence of multiple alloying elements rather than by any individual element. This finding indicates that the relationship between chemical composition and the mechanical properties of Cast Copper Alloys is complex and nonlinear, making it difficult to accurately describe using a simple linear model. The Ultimate Tensile Strength (UTS) and Yield Strength (YS) variables exhibit a very strong positive correlation, with a correlation coefficient of 0.890. This value indicates that materials with higher UTS values tend to have higher YS values, demonstrating that these two parameters are closely related in describing the material's ability to withstand mechanical loading. Several alloying elements exhibit positive relationships with the mechanical properties. Nickel (Ni) has a correlation coefficient of 0.328 with UTS and 0.286 with YS, while magnesium (Mg) shows correlation coefficients of 0.215 with UTS and 0.387 with YS. In addition, zirconium (Zr) also exhibits positive correlations with UTS (0.350) and YS (0.184). These results indicate that increasing the concentrations of these alloying elements tends to be accompanied by an improvement in the mechanical strength of the material.

Conversely, several alloying elements exhibit negative correlations with the mechanical properties. Antimony (Sb) has correlation coefficients of -0.535 with UTS and -0.374 with YS, while phosphorus (P) exhibits correlation coefficients of -0.459 with UTS and -0.290 with YS. Lead (Pb) also shows negative correlations with UTS (-0.427) and YS (-0.317). These values indicate that increasing the concentrations of these elements in the dataset tends to be accompanied by a decrease in both the tensile strength and the yield strength of the material. From a metallurgical perspective, the influence of each alloying element on the mechanical properties of Cast Copper Alloys is governed by the strengthening mechanisms that occur within the material's microstructure. Nickel (Ni) is known to improve both tensile strength and yield strength through the solid solution strengthening mechanism by increasing the resistance to dislocation movement within the copper matrix. In addition, magnesium (Mg) and zirconium (Zr) contribute to grain refinement, thereby enhancing the mechanical strength of the material. In contrast, lead (Pb) tends to form soft phases that are not completely soluble in the copper matrix, which may act as stress concentration sites and reduce the material strength. At certain concentrations, antimony (Sb) and phosphorus (P) may also form intermetallic compounds or promote microsegregation, thereby reducing ductility and decreasing the mechanical strength of the material. Therefore, changes in the mechanical properties of Cast Copper Alloys are influenced not only by individual alloying elements but also by the interactions among alloying elements and the resulting microstructural changes.

The heatmap also reveals very high correlations among several input variables. For example, niobium (Nb) exhibits a very strong positive correlation with carbon (C), with a correlation coefficient of 0.994, while lead (Pb) shows a correlation coefficient of 0.843 with phosphorus (P). On the other hand, copper (Cu) exhibits a relatively strong negative correlation with zinc (Zn), with a correlation coefficient of -0.776, indicating a tendency for the Cu content to decrease as the Zn content increases in several cast copper alloy compositions included in the dataset.

Overall, the correlation analysis suggests that the mechanical properties of Cast Copper Alloys are governed by complex, nonlinear interactions among multiple alloying elements rather than by simple linear relationships between individual elements and the target properties. This condition supports the use of the Decision Tree and Random Forest algorithms in this study because both algorithms are capable of modeling nonlinear relationships and capturing complex interactions among variables, thereby providing more accurate predictions of mechanical properties than conventional analytical methods. These findings are also consistent with several previous studies reporting that machine learning approaches are effective in modeling the complex relationship between chemical composition and the mechanical properties of metallic materials [4], [5], [6].

3.2 Hyperparameter Optimization

The hyperparameter values for the Decision Tree and Random Forest algorithms were determined using a trial-and-error approach by evaluating various parameter combinations. For the Decision Tree algorithm, the parameter evaluated was the maximum depth, with values ranging from 1 to 12. Meanwhile, the Random Forest algorithm was evaluated using combinations of maximum depth (1-12) and number of trees (20, 40, 60, 80, 100, 120, 140, 160, 180, and 200). The predictive performance of each hyperparameter configuration was assessed using Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). The optimal parameters were selected based on the lowest RMSE and MAE values and the highest R^2 value, as these indicate a model with higher prediction accuracy and lower prediction error. The hyperparameter settings evaluated in this study are summarized in Table 2.

Table 2**.** Hyperparameter settings for model optimization

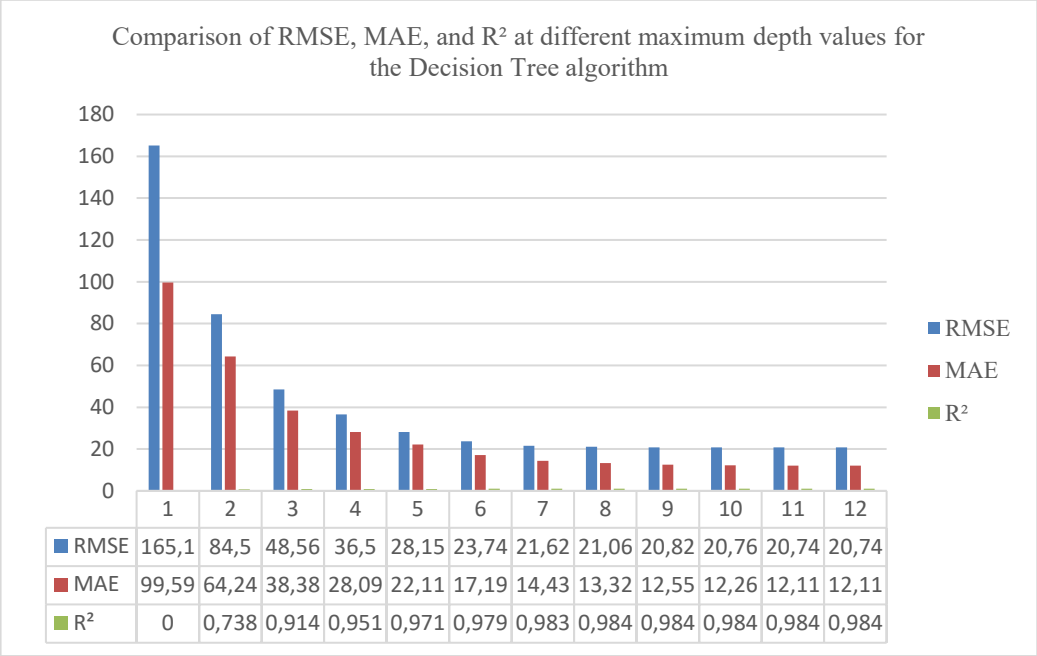
No	Algorithm	Parameter	Parameter Setting
1	Decision Tree	Maximum Depth	1,2,3,4,5,6,7,8,9,10,11,12
		Ratio	60:40, 70:30, 80:20
2	Random Forest	Number of trees	20,40,60,80,100,120,140,160,180,200
		Maximum Depth	1,2,3,4,5,6,7,8,9,10,11,12
		Ratio	60:40, 70:30, 80:20

The hyperparameter optimization results were obtained by selecting the parameter combination that produced the lowest RMSE and MAE values, along with the highest coefficient of determination (R^2). The optimization results for each algorithm are presented as follows.

a. Decision Tree (DT)

Figure 3 illustrates the effect of varying the maximum depth parameter on the performance of the Decision Tree algorithm, as evaluated using RMSE, MAE, and R^2. At a maximum depth of 1, the model produced relatively high prediction errors, indicating an underfitting condition caused by insufficient model complexity. As the tree depth increased, the RMSE and MAE values decreased substantially, while the R^2 value increased, indicating improved predictive performance. A maximum depth of 11 produced the highest predictive performance, with an RMSE of 20.737, an MAE of 12.111, and an R^2 of 0.984. This result indicates that the selected tree depth provides sufficient

model complexity to effectively represent the nonlinear relationships between alloy composition and the mechanical properties of Cast Copper Alloys while maintaining high prediction accuracy.

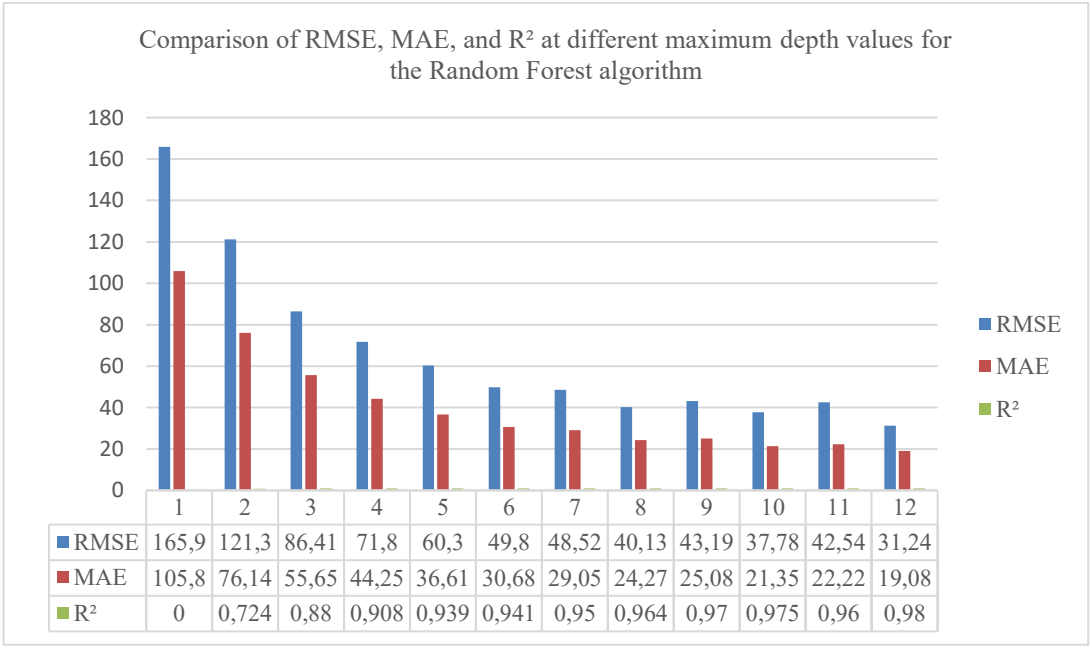


	1	2	3	4	5	6	7	8	9	10	11	12
RMSE	165,1	84,5	48,56	36,5	28,15	23,74	21,62	21,06	20,82	20,76	20,74	20,74
MAE	99,59	64,24	38,38	28,09	22,11	17,19	14,43	13,32	12,55	12,26	12,11	12,11
R²	0	0,738	0,914	0,951	0,971	0,979	0,983	0,984	0,984	0,984	0,984	0,984

Figure 3. Comparison of RMSE, MAE, and R² at different maximum depth values for the Decision Tree algorithm

b. Random Forest (RF)

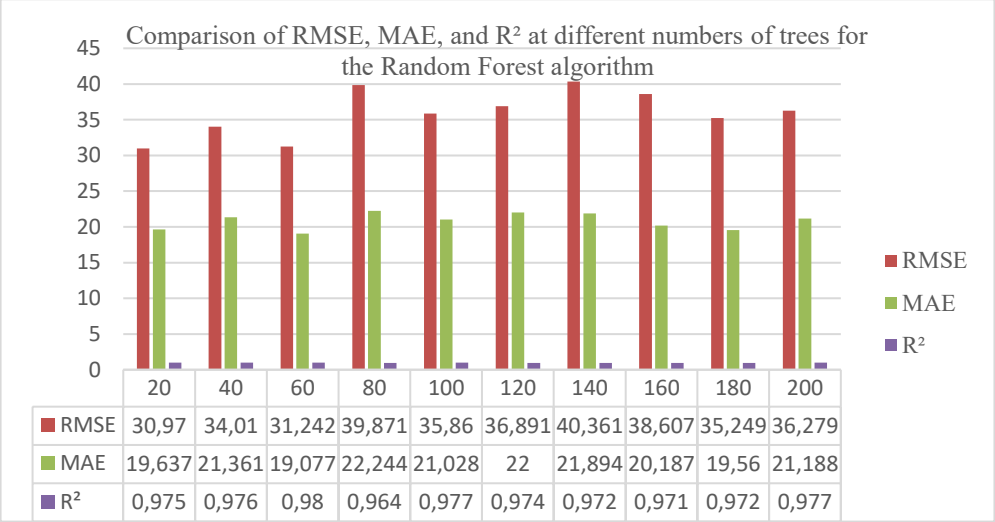
Figure 4 shows the predictive performance of the Random Forest algorithm under different combinations of maximum depth and number of trees, evaluated using RMSE, MAE, and R². The best performance for Yield Strength (YS) prediction was achieved with an 80:20 train-test split ratio, a maximum depth of 12, and 60 trees. This parameter combination produced an RMSE of 31.242, an MAE of 19.077, and an R² value of 0.980. Beyond this maximum depth, increasing the model complexity no longer resulted in significant performance improvements. Therefore, a maximum depth of 12 and 60 trees were selected as the optimal parameters for the Random Forest algorithm and were used in the subsequent model evaluation stage.



	1	2	3	4	5	6	7	8	9	10	11	12
RMSE	165,9	121,3	86,41	71,8	60,3	49,8	48,52	40,13	43,19	37,78	42,54	31,24
MAE	105,8	76,14	55,65	44,25	36,61	30,68	29,05	24,27	25,08	21,35	22,22	19,08
R²	0	0,724	0,88	0,908	0,939	0,941	0,95	0,964	0,97	0,975	0,96	0,98

Figure 4. Comparison of RMSE, MAE, and R² at different maximum depth values for the Random Forest algorithm

Figure 5 presents the effect of varying the number of trees on the performance of the Random Forest algorithm. The prediction performance improved as the number of trees increased from 20 to 60. The optimal performance was obtained using 60 trees, resulting in an RMSE of 31.242, an MAE of 19.077, and an R^2 value of 0.980. Increasing the number of trees beyond this value did not produce significant improvements in predictive performance, indicating that 60 trees provided an appropriate balance between prediction accuracy and computational efficiency.



	20	40	60	80	100	120	140	160	180	200
RMSE	30,97	34,01	31,242	39,871	35,86	36,891	40,361	38,607	35,249	36,279
MAE	19,637	21,361	19,077	22,244	21,028	22	21,894	20,187	19,56	21,188
R^2	0,975	0,976	0,98	0,964	0,977	0,974	0,972	0,971	0,972	0,977

Figure 5. Comparison of RMSE, MAE, and R^2 at different numbers of trees for the Random Forest algorithm

The optimization results identified a maximum depth of 11 as the optimal hyperparameter for the Decision Tree algorithm. For the Random Forest algorithm, the best performance was achieved with a maximum depth of 12 and 60 trees. These optimized hyperparameter settings were subsequently applied during the model validation phase.

3.3 Model Performance Evaluation

The optimized Decision Tree and Random Forest models were validated using 5-fold cross-validation to examine their predictive stability and generalization performance. Model performance was assessed across three train-test split ratios (60:40, 70:30, and 80:20) using Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). Furthermore, scatter plots of predicted versus actual values were analyzed to assess the agreement between model predictions and experimental observations. The prediction results for Ultimate Tensile Strength (UTS) and Yield Strength (YS) are presented in Figures 6 and 7.

a. Ultimate Tensile Strength (UTS)

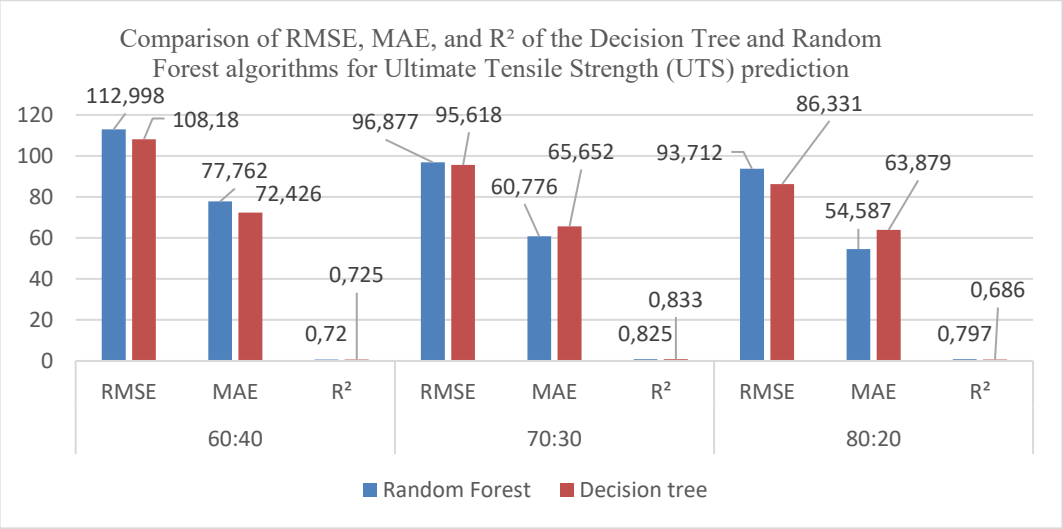


Figure 6. Comparison of RMSE, MAE, and R^2 of the Decision Tree and Random Forest algorithms for Ultimate Tensile Strength (UTS) prediction

Figure 6 compares the prediction performance of the Decision Tree and Random Forest algorithms for Ultimate Tensile Strength (UTS) under three train-test split scenarios using the 5-fold cross-validation method. The predictive capability of the models was evaluated using three regression metrics: Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). For the 60:40 split ratio, the Decision Tree algorithm achieved an RMSE of 108.180, an MAE of 72.426, and an R^2 of 0.725, whereas the Random Forest algorithm obtained an RMSE of 112.998, an MAE of 77.762, and an R^2 of 0.720. For the 70:30 split ratio, the Decision Tree algorithm achieved an RMSE of 95.618, an MAE of 65.652, and an R^2 of 0.833, while the Random Forest algorithm obtained an RMSE of 96.877, an MAE of 60.776, and an R^2 of 0.825. For the 80:20 split ratio, the Decision Tree algorithm achieved an RMSE of 86.331, an MAE of 63.879, and an R^2 of 0.686, whereas the Random Forest algorithm obtained an RMSE of 93.712, an MAE of 54.587, and an R^2 of 0.797.

The evaluation results indicate that the Decision Tree algorithm consistently produced lower RMSE values than the Random Forest algorithm across all train-test split scenarios, demonstrating better predictive accuracy for Ultimate Tensile Strength (UTS). Although the Random Forest algorithm achieved lower MAE values under the 70:30 and 80:20 split ratios, the Decision Tree algorithm provided a better overall performance balance by maintaining lower prediction errors while achieving competitive R^2 values. Furthermore, the 70:30 train-test split ratio yielded the highest R^2 values for both algorithms, namely 0.833 for Decision Tree and 0.825 for Random Forest, indicating superior model generalization compared with the other data split scenarios. Therefore, the Decision Tree model with the 70:30 train-test split ratio was selected as the best model for Ultimate Tensile Strength (UTS) prediction in this study.

b. Yield Strength (YS)

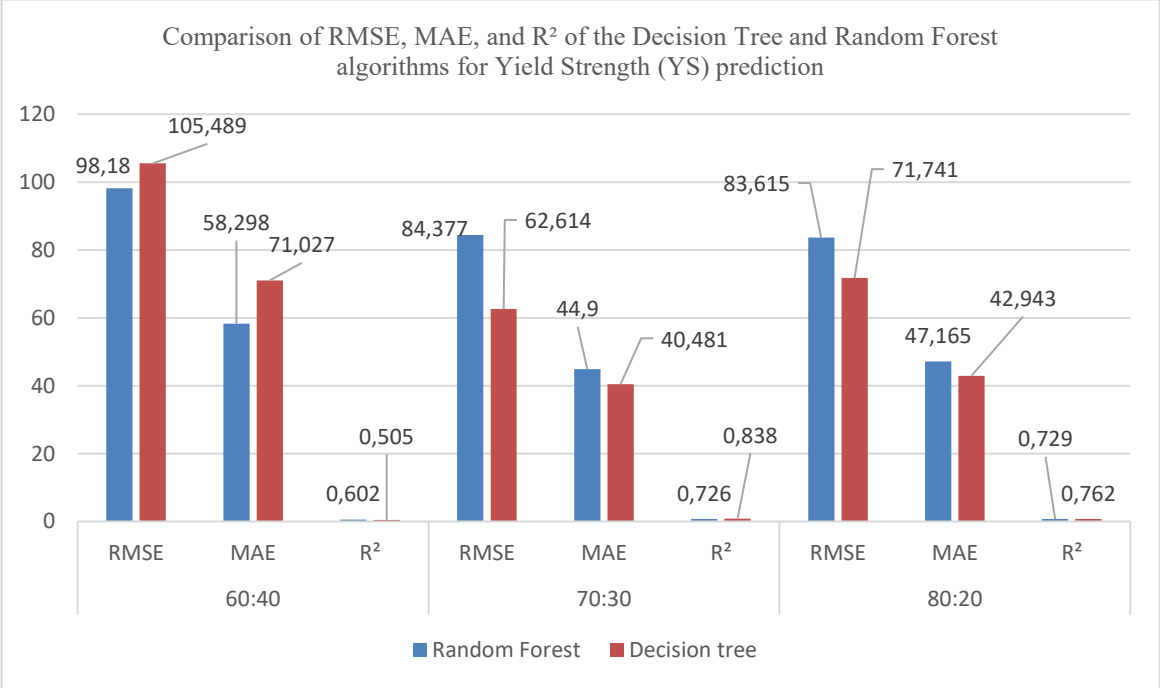


Figure 7. Comparison of RMSE, MAE, and R^2 of the Decision Tree and Random Forest algorithms for Yield Strength (YS) prediction.

Figure 7 presents the prediction performance of the Decision Tree and Random Forest algorithms for Yield Strength (YS) under three train-test split scenarios using the 5-fold cross-validation method. The evaluation was performed using Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the coefficient of determination (R^2). For the 60:40 split ratio, the Decision Tree algorithm achieved an RMSE of 105.489, an MAE of 71.027, and an R^2 of 0.505, whereas the Random Forest algorithm obtained an RMSE of 98.180, an MAE of 58.298, and an R^2 of 0.602. For the 70:30 split ratio, the Decision Tree algorithm achieved an RMSE of 62.614, an MAE of 40.481, and an R^2 of 0.838, while the Random Forest algorithm obtained an RMSE of 84.377, an MAE of 44.900, and an R^2 of 0.726. For the 80:20 split ratio, the Decision Tree algorithm achieved an RMSE of 71.741, an MAE of 42.943, and an R^2 of 0.762, whereas the Random Forest algorithm obtained an RMSE of 83.615, an MAE of 47.165, and an R^2 of 0.729.

The evaluation results indicate that the Decision Tree algorithm outperformed the Random Forest algorithm in predicting Yield Strength (YS), particularly under the 70:30 and 80:20 train-test split scenarios. This is demonstrated by its lower RMSE and MAE values together with higher R^2 values than those obtained by the Random Forest algorithm. Although the Random Forest algorithm showed better performance under the 60:40 split ratio, increasing the amount of training data in the 70:30 and 80:20 scenarios enabled the Decision Tree algorithm to construct a tree structure that more effectively represented the relationship between chemical composition and Yield Strength, resulting in more accurate predictions. Based on the overall evaluation results, the Decision Tree model with the 70:30 train-test split ratio achieved the best performance, with an RMSE of 62.614, an MAE of 40.481, and an R^2 of 0.838. Therefore, this configuration was selected as the best model for Yield Strength (YS) prediction in this study.

c. Comparison Between Predicted and Actual Values for UTS Prediction

To further evaluate model reliability, a comparison between predicted and actual UTS values was performed using the selected test scenarios. Figures 8 and 9 present the comparison between experimental values and predicted values obtained from Random Forest and Decision Tree algorithms.

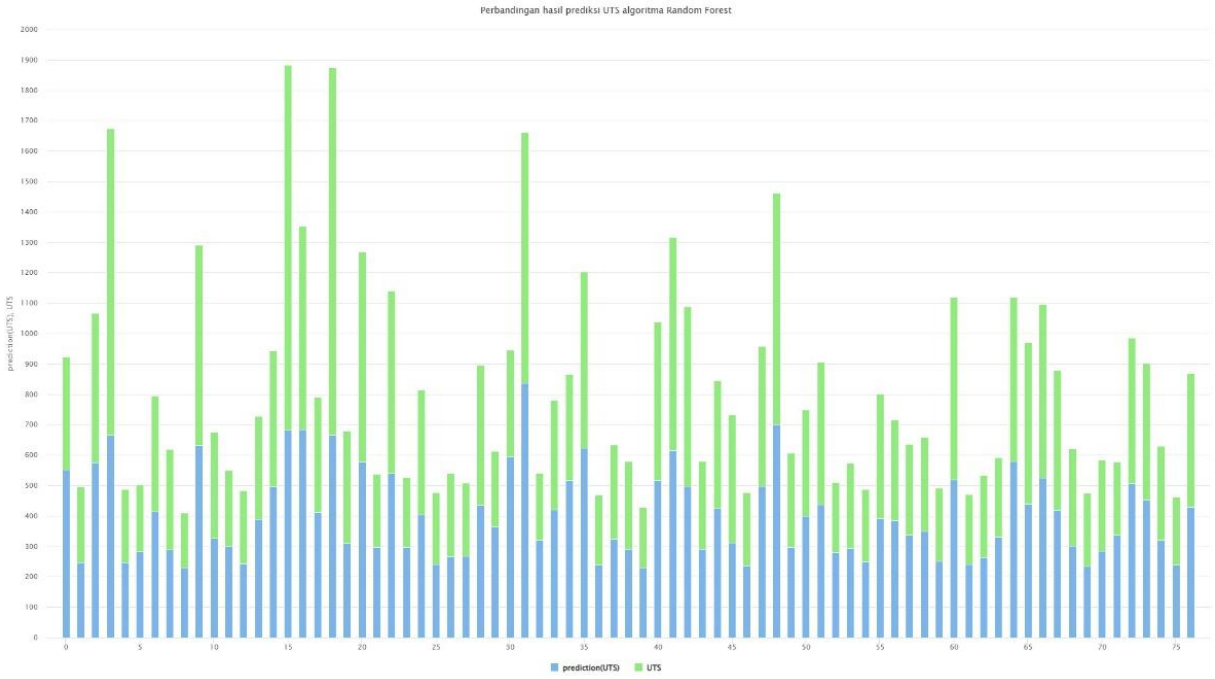


Figure 8. Comparison between predicted and actual Ultimate Tensile Strength values using Random Forest at 70:30 split ratio

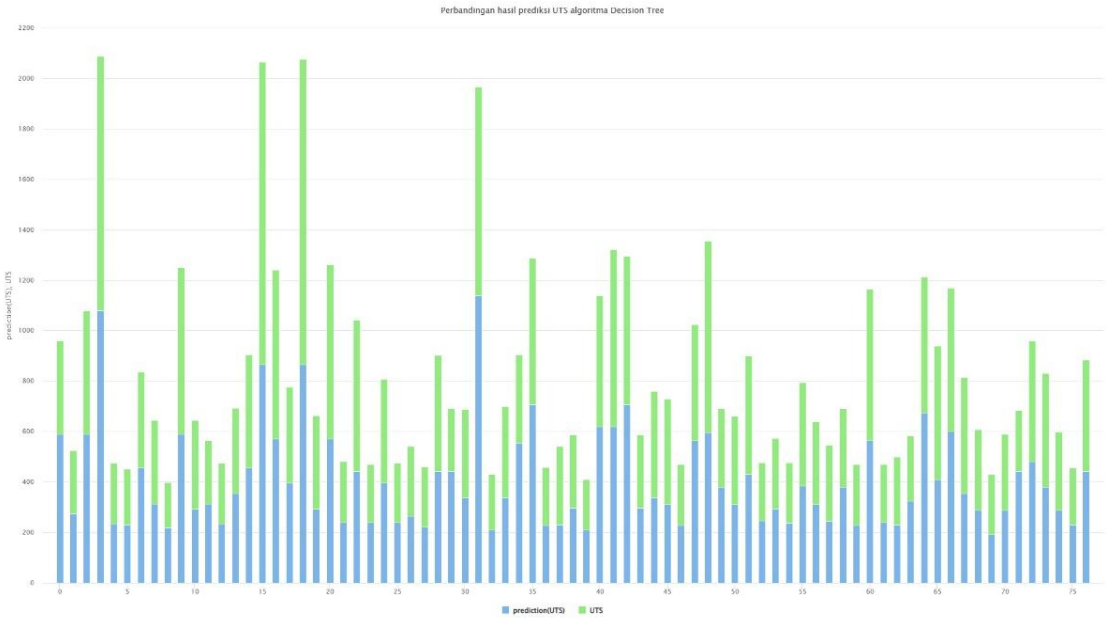


Figure 9. Comparison between predicted and actual Ultimate Tensile Strength values using Decision Tree at 70:30 split ratio

Based on Figures 8 and 9, both algorithms were able to capture the overall trend of the experimental UTS values, demonstrating their capability to model the relationship between chemical composition and the mechanical properties of Cast Copper Alloys. Nevertheless, discrepancies between the predicted and observed values were evident, particularly for specimens with higher UTS values. These deviations suggest that the complex nonlinear interactions among multiple alloying elements remain challenging for the prediction models to fully represent. The Decision Tree model showed closer agreement with the experimental values compared with Random Forest. This observation is consistent with the 5-Fold Cross-Validation results, where Decision Tree achieved lower RMSE values and higher R^2 values for UTS prediction. Therefore, Decision Tree demonstrated better capability in modeling the relationship between chemical composition and UTS for the investigated dataset.

d. Comparison Between Predicted and Actual Values for YS Prediction

The comparison between predicted and actual Yield Strength values was also performed to evaluate the predictive capability of both models. Figures 10 and 11 present the prediction results obtained from Random Forest and Decision Tree algorithms.

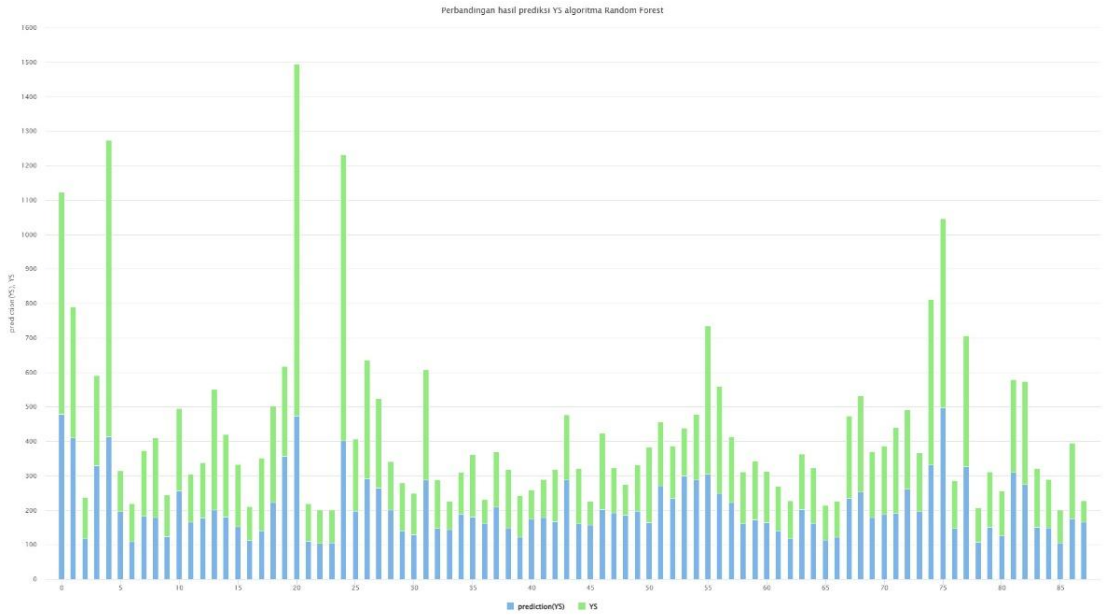


Figure 10. Comparison between predicted and actual Yield Strength values using Random Forest at 80:20 split ratio

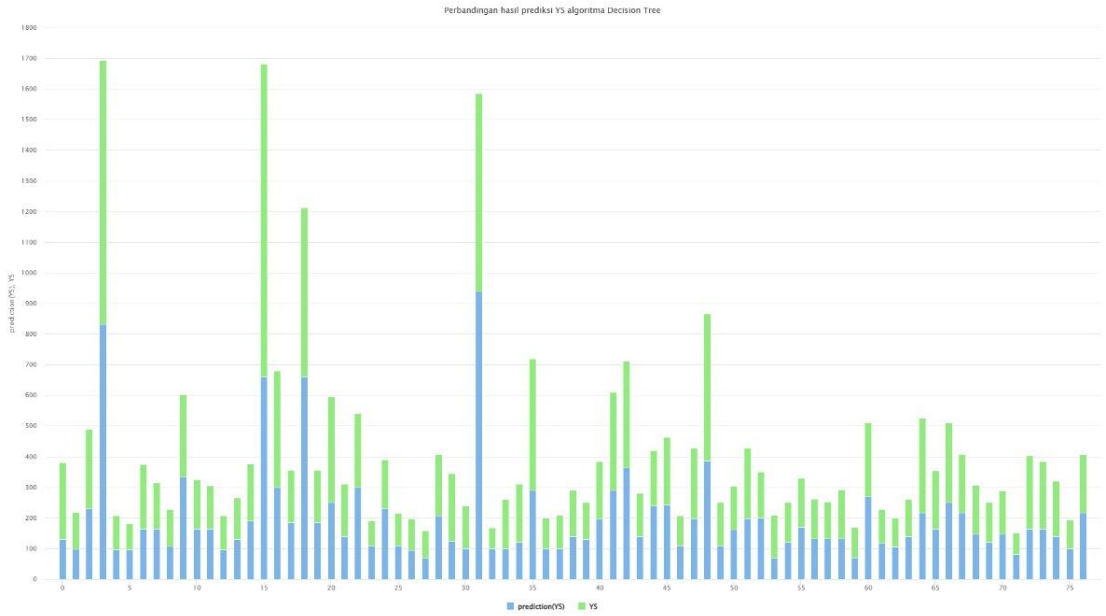


Figure 11. Comparison between predicted and actual Yield Strength values using Decision Tree at 70:30 split ratio

Figures 10 and 11 show that both Decision Tree and Random Forest were able to represent the general trend of the actual Yield Strength values. Nevertheless, some differences between predicted and actual values were observed, especially for samples with higher Yield Strength values. These deviations indicate that variations in chemical composition and interactions among alloying elements still create challenges in accurately predicting mechanical properties. The Decision Tree model showed better agreement with actual values compared with Random Forest. This result agrees with the 5-Fold Cross-Validation evaluation, where Decision Tree achieved lower prediction errors and higher R^2 values, particularly for the 70:30 and 80:20 split scenarios. Therefore, Decision Tree was considered the most suitable model for predicting Yield Strength based on the chemical composition of Cast Copper Alloys used in this study.

3.4 Comparison with Previous Studies

The summary of the best model performance is presented in Table 3.

Table 3. Summary of the best model performance

Prediction Target	Algorithm	Data Split Ratio	Best Hyperparameters	RMSE	MAE	R^2
Ultimate Tensile Strength (UTS)	Decision Tree	70:30	Maximum depth = 11	95.618	65.652	0.833
Ultimate Tensile Strength (UTS)	Random Forest	70:30	Maximum depth = 12, Number of Trees = 60	96.877	60.776	0.825
Yield Strength (YS)	Decision Tree	70:30	Maximum depth = 11	62.614	40.481	0.838
Yield Strength (YS)	Random Forest	80:20	Maximum depth = 12, Number of Trees = 60	83.615	47.165	0.729

Based on Table 3, the Decision Tree algorithm provided the best predictive performance for both Ultimate Tensile Strength (UTS) and Yield Strength (YS) compared with the Random Forest algorithm. The optimal configuration was obtained using a maximum depth of 11 with a 70:30 train-test split ratio. For the Random Forest algorithm, the best performance was achieved using a maximum depth of 12 and 60 trees; however, its overall performance remained lower than that of the Decision Tree algorithm for the investigated dataset. These results indicate that the Decision Tree algorithm was more suitable for predicting the mechanical properties of Cast Copper Alloys based on chemical composition in this study.

The results obtained in this study differ from those reported by Saputra et al. [6], who found that Random Forest achieved better prediction performance than Decision Tree for mechanical property prediction. The difference is likely related to the characteristics of the datasets used, including dataset size, feature distribution, and complexity of the relationship between input variables and target properties. In the present study, the dataset consisted of 100 Cast Copper Alloy specimens with nonlinear relationships between chemical composition and mechanical properties. Under these conditions, Decision Tree was able to establish specific splitting rules to capture patterns within the dataset effectively.

In contrast, the Random Forest algorithm employs bootstrap sampling and integrates multiple decision trees through an ensemble learning approach, which generally offers better performance when applied to larger and more diverse datasets. Therefore, the predictive performance of Machine Learning algorithms is strongly influenced by dataset characteristics, hyperparameter optimization, and the validation strategy employed [20]. These findings support previous studies indicating that appropriate dataset preparation, hyperparameter optimization, and evaluation strategies significantly influence the predictive capability of machine learning models for metallic material properties [4], [5], [6].

4. Conclusion

Pearson correlation analysis revealed that the relationship between chemical composition and the mechanical properties of Cast Copper Alloys is governed by complex interactions among multiple alloying elements. The results indicate that no individual alloying element alone determines the mechanical properties, emphasizing the nonlinear nature of the relationship between alloy composition and material performance. The Machine Learning modeling results demonstrated that the Decision Tree algorithm achieved better predictive performance than Random Forest for predicting the mechanical properties of Cast Copper Alloys. Based on the 5-Fold Cross-Validation evaluation, Decision Tree provided better generalization capability, with the optimal performance obtained at a 70:30 train-test split ratio for both Ultimate Tensile Strength (UTS) and Yield Strength (YS) predictions. The optimal Decision Tree model employed a maximum depth of 11, resulting in an RMSE of 95.618, an MAE of 65.652, and an R^2 of 0.833 for UTS prediction, as well as an RMSE of 62.614, an MAE of 40.481, and an R^2 of 0.838 for YS prediction. These findings indicate that Decision Tree is an effective machine learning approach for predicting mechanical properties of Cast Copper Alloys based on chemical composition, particularly for relatively small datasets with complex nonlinear relationships. Future studies should consider expanding the dataset size and investigating advanced Machine Learning algorithms, such as XGBoost, LightGBM, and Gradient Boosting, to further improve model generalization and prediction accuracy.

Authors' Contributions

IYA: Conceptualization, Methodology, Data Curation, Software, Formal Analysis, Investigation, Visualization, Writing (Original Draft). DL: Conceptualization, Methodology, Supervision, Validation, Writing (Review and Editing). JH: Validation, Resources, Investigation, Writing (Review and Editing). All authors have read and approved the final manuscript.

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