

Data-Driven Quantification of Temperature-Induced Mechanical Property Variations in 5Cr–0.5Mo Steel Using Artificial Neural Networks

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Abstract

This study presents the quantitative estimation of the effect of temperature on the mechanical properties of 5Cr–0.5Mo steels using an artificial neural network (ANN) model. The developed ANN model predicts yield strength (YS, MPa), ultimate tensile strength (UTS, MPa), elongation (El, %), and reduction in area (RA, %) at different service temperatures. Predictions were validated against experimental data at critical temperatures of 450 °C and 700 °C and found to show high accuracy. Predicted results show minimal errors of 3.84%, 2.3%, 2.2%, and 0.42% for YS, UTS, El, and RA, respectively at 450 °C, and 3.7%, 0.45%, 1.88%, and 0.19%, respectively at 700 °C. Furthermore, ten-fold cross-validation confirmed the generalization capability of the developed model, yielding high coefficients of determination and correlation coefficients together with low normalized prediction errors across all output variables. Despite the absence of explicit metallurgical descriptors, the ANN model successfully quantified the influence of temperature from 25 to 700 °C, demonstrating its effectiveness as a predictive tool for high-temperature Cr–Mo steels. Furthermore, a user-friendly graphical interface was developed to facilitate rapid property estimation, demonstrating the potential of the framework as a supportive tool for the preliminary assessment of high-temperature Cr–Mo steels.

Keywords: 5Cr–0.5Mo steel; neural networks; quantitative estimation; temperature; mechanical properties

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1. Introduction

The growing global demand for energy has intensified the need for reliable materials capable of operating under severe service conditions encountered in thermal power plants, petrochemical facilities, and other high-temperature industrial systems [1]. Components used in such environments are frequently exposed to elevated temperatures and stress for prolonged periods, necessitating the use of heat-resistant steels with excellent mechanical stability and structural integrity [2]. Among these materials, 5Cr–0.5Mo steel has been extensively employed in critical components such as superheaters, steam headers, pressure vessels, and piping systems owing to its favorable combination of strength, creep resistance, oxidation resistance, and cost-effectiveness [3,4]. The mechanical performance of 5Cr–0.5Mo steel is strongly influenced by service temperature. As temperature increases, significant variations in yield strength (YS), ultimate tensile strength (UTS),

elongation (El), and reduction in area (RA) may occur due to thermally activated deformation mechanisms [5], microstructural evolution [6], and changes in dislocation mobility [7]. Accurate quantification of these temperature-dependent property variations is therefore essential for component design, life assessment, safety evaluation, and maintenance planning in high-temperature applications [8,9]. Traditionally, such information is obtained through extensive experimental testing conducted over a wide range of temperatures. However, these experiments are often costly, time-consuming, and labor-intensive, particularly when multiple temperatures and material conditions must be evaluated.

Recent advances in data-driven materials science have demonstrated the potential of machine learning techniques to accelerate materials characterization, property prediction, and alloy development. Among various machine learning approaches, artificial neural networks (ANNs) have gained considerable attention because of their ability to learn complex and highly nonlinear relationships between input and output variables without requiring explicit physical equations. ANNs have been successfully applied to predict mechanical properties [10], phase evolution [11], corrosion behavior [12], creep performance [13], and processing–structure–property relationships [14,15] in a wide range of engineering materials.

Despite these advances, relatively limited attention has been devoted to the quantitative prediction of temperature-dependent mechanical properties in heat-resistant Cr–Mo steels using machine learning approaches. Developing reliable predictive models capable of accurately capturing the influence of temperature would significantly reduce experimental effort while providing rapid estimates of material performance under service conditions. Such models could also facilitate engineering decision-making and support the development of digital tools for materials selection and structural integrity assessment.

In the present study, an optimized ANN model was developed to quantitatively predict the effect of temperature on the mechanical properties of 5Cr–0.5Mo steel. The model was trained using experimental data obtained from the National Institute for Materials Science (NIMS), Japan [16], and was employed to predict YS, UTS, EL, and RA over a wide temperature range. The predictive capability of the model was validated against independent experimental data, and a user-friendly graphical interface was developed to facilitate practical implementation. The proposed framework provides an efficient and accurate tool for assessing temperature-dependent mechanical behavior and demonstrates the potential of machine learning for supporting the design and operation of high-temperature engineering systems.

2. Materials and Methods

A dataset comprising 99 samples of 5Cr–0.5Mo steel, including information on chemical composition, austenite grain size, nonmetallic inclusions, testing temperature, and corresponding mechanical properties, was compiled from NIMS, Japan [16]. According to the original source [16], the steel was manufactured as ingots using a basic electric arc furnace. Tensile testing was performed at various temperatures using dog-bone-shaped specimens with a gauge diameter of 10 mm and a gauge length of 50 mm. Room-temperature and elevated-temperature tensile tests were conducted in accordance with JIS G 0567 [17] using an extensometer at a strain rate of 10^{-3} s^{-1} . Further details regarding the alloy chemistry and the influence of individual alloying elements on the mechanical behavior of 5Cr–0.5Mo steel have been reported in our previous study [10]. The complete dataset was randomly divided into training and testing subsets. Of the 99 available datasets, 81 (approximately 80%) were used for network training, while the remaining 18 datasets (approximately 20%) were reserved for evaluating the predictive performance of the developed ANN model.

Prior to model development, all input and output variables were normalized within the range of 0.1–0.9 to improve numerical stability and facilitate efficient network training. The normalization procedure was carried out using Equation (1):

$$x_n = 0.1 + \left[\frac{x - x_{min}}{x_{max} - x_{min}} \right] \times 0.8 \quad (1)$$

where x_n denotes the normalized value, (x) is the original values and x_{min} and x_{max} represent the minimum and maximum values of the corresponding variable, respectively. Following completion of the training process and identification of the optimum ANN architecture, the normalized outputs were transformed back to their original scale using Equation (2):

$$x = \left[\frac{(x_{min} - 0.1) \times (x_{max} - x_{min})}{0.8} \right] + x_{min} \quad (2)$$

where (x) represents the denormalized value corresponding to the network prediction.

The ANN model employed in this study consisted of three fundamental layers: an input layer, two hidden layers, and an output layer. The input variables included chemical composition, austenite grain size (AGS), non-metallic inclusions (NMIs), and testing temperature, whereas the output variables comprised YS, UTS, El, and RA. To establish the optimal ANN architecture, the training dataset was used to systematically evaluate different network parameters, including the number of hidden layers, the number of neurons within each hidden layer, learning rate, momentum coefficient, and training iterations. Both single- and double-hidden-layer network architectures were investigated. The number of neurons in each hidden layer was varied from 2 to 15, and the performance of each configuration was assessed using the mean squared error (MSE).

Among the investigated configurations, a double-hidden-layer architecture with seventeen neurons in each hidden layer exhibited the best performance, yielding an MSE of approximately 0.00149. Subsequent optimization of the training parameters further reduced the prediction error. The optimum momentum coefficient and learning rate were found to be 0.60 and 0.50, respectively, resulting in a minimum MSE of 0.000698. The optimum numbers of training iterations were determined to be 6000. The optimized ANN architecture was subsequently adopted as the final predictive model for the quantitative assessment of temperature-dependent mechanical properties of 5Cr–0.5Mo steel. The ANN training algorithm was developed using the C programming language, while a user-friendly GUI was implemented using Java. A detailed description of ANN modeling methodologies and their applications in materials science can be found elsewhere [18].

3. Results and Discussion

3.1. Quantitative Estimation

At the first stage, a random composition (wt.%) of 5Cr–0.5Mo steel was taken and named steel A with a composition of 0.09C + 0.31Si + 0.54Mn + 0.007P + 0.01S + 0.08Ni + 4.91Cr + 0.52Mo + 0.13Cu + 0.005Al + 0.01N. The austenite grain size was 5.5 microns with 0.1 wt.% non-metallic inclusions (NMIs). The impact of different service temperatures with increments of 50 °C was virtually studied. The predicted values were then compared with experimental results. Figure 1 illustrates the predictions of mechanical properties with increasing temperature at intervals of 50 °C, up to 700 °C. The mechanical properties were found to be temperature-dependent. Results show (Figure 1a) that steel retains its YS almost up to about 300 °C and it tends to drop gradually with increasing temperature. UTS seems to have decreased slowly at the beginning (Figure 1b) up to about 250 °C and it remains unchanged in the temperature range of 250 to 400 °C. It decreases rapidly at higher temperatures. When it comes to El and RA, there are marginal decreases up to about 400 °C and significant increases with further increases in temperature (Figure 1c,d).

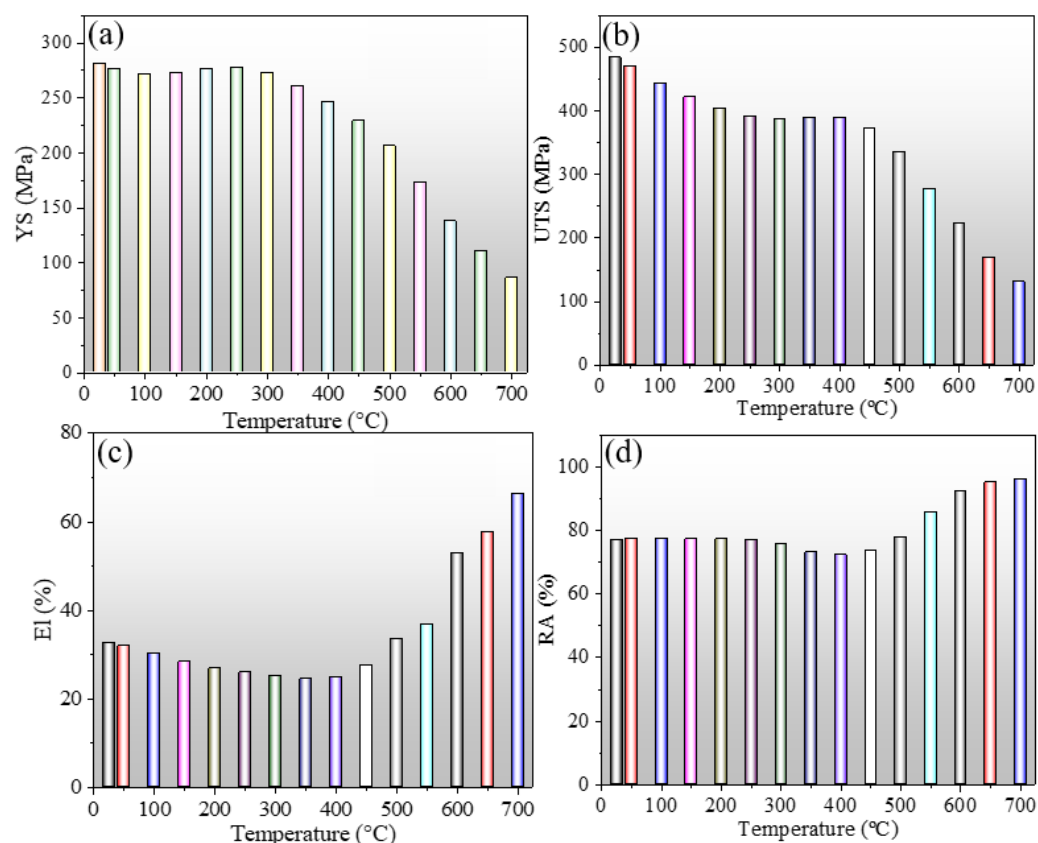


Figure 1. A graphical representation of the effect of an increase in temperature in intervals of 50 °C on (a) YS, (b) UTS, (c) El, (d) RA.

This variation in properties can be attributed to the process of precipitate formation and dissolution [19]. The M_2C phase dissolves at 400 °C and is replaced by $M_{23}C_6$ carbides which form at grain boundaries or within grains [20]. The order of carbide formation is ϵ -carbide $\rightarrow$ cementite $\rightarrow M_2C \rightarrow M_7C_3 \rightarrow M_{23}C_6 \rightarrow M_6C$ [21]. Exposure temperature and time can change the shape and composition of these carbides [4]. Many Mo atoms form these $M_{23}C_6$ carbides, which subsequently dissolve in the ferrite matrix when the temperature exceeds 400 °C [22]. This intricate cycle of carbide formation and dissolution results in an increase in El and RA as the temperature rises from approximately 450 °C.

The predicted results were further analyzed for possible percentage errors using ideal network synaptic weights, which shows that the percentage errors were very small. The model predicted YS, UTS, El, and RA at 450 °C, with minimal errors of 3.845%, 2.299%, 2.223%, and 0.424%, respectively. For the properties predicted at 700 °C, it shows improved efficiency of the model, i.e., the %errors were decreased significantly to 3.676%, 0.449%, 1.878%, and 0.191% for YS, UTS, El, and RA, respectively. It demonstrates a strong predictive ability without reliance on metallurgical or physics-based input data. The calculation details are presented in Table 1.

Table 1. Quantitative effect of temperature on YS (MPa), UTS (MPa), El (%), and RA (%) of steel A.

Temperature (°C)	YS (MPa)	Diff.	UTS (MPa)	Diff.	El (%)	Diff.	RA (%)	Diff.
25	281.46	-	483.46	-	32.60	-	77.01	-
50	276.32	−5.14	469.65	−13.81	31.97	−0.63	77.21	0.20
100	271.59	−4.73	443.75	−25.90	30.24	−1.73	77.36	0.15

150	272.85	1.26	421.27	−22.48	28.29	−1.95	77.26	−0.11
200	276.15	3.30	403.03	−18.24	26.81	−1.48	77.19	−0.07
250	277.13	0.98	390.74	−12.29	25.97	−0.84	77.08	−0.11
300	272.45	−4.68	386.66	−4.08	25.26	−0.71	75.82	−1.26
350	260.90	−11.55	389.85	3.14	24.40	−0.86	73.11	−2.71
400	246.07	−14.83	388.77	−1.08	24.87	0.47	72.22	−0.89
450	228.85	−17.22	373.22	−15.55	27.60	2.73	73.69	1.47
500	205.88	−22.97	335.43	−37.79	33.41	5.81	77.94	4.25
550	173.36	−32.52	277.00	−58.43	36.76	3.35	85.64	7.70
600	137.55	−35.81	221.93	−55.07	52.99	16.23	92.39	6.75
650	110.07	−27.48	169.34	−52.59	57.77	4.78	95.10	2.71
700	85.73	−24.34	130.41	−38.93	66.22	8.45	96.18	1.08
Exp. value at 450 °C	238		382		27		74	
Absolute error in pre- diction	238 − 228.85 = 9.15		382 − 373.22 = 8.78		27 − 27.60 = −0.60		74 − 73.69 = 0.31	
Percentage error	3.84%		2.29%		2.22%		0.42%	
Exp. value at 700 °C	89		131		65		96	
Absolute error in pre- diction	89 − 85.73 = 3.27		131 − 130.41 = 0.59		65 − 66.22 = −1.22		96 − 96.18 = −0.18	
Percentage error	3.67%		0.45%		1.88%		0.19%	

3.2. Model Interpretation Using the Index of Relative Importance (I_{RI})

The predictive capability of the developed ANN model was further assessed using the Index of Relative Importance (I_{RI}), which provides quantitative information regarding both the magnitude and direction of the influence of input variables on the predicted mechanical properties [23]. Although several feature importance methods are available for interpreting machine learning models, I_{RI} was adopted in the present study because it provides a simple and computationally efficient means of quantifying the relative contribution of input variables while simultaneously indicating whether their effects on the output responses are positive or negative. Moreover, I_{RI} has been successfully employed in previous ANN-based materials studies for model interpretation [24]. Unlike conventional sensitivity analysis, the I_{RI} enables direct evaluation of whether a particular variable exerts a positive or negative effect on the output response.

Figure 2 presents the variation in YS and EL, together with their corresponding I_{RI} values, at four representative temperatures: 25 °C, 300 °C, 450 °C, and 700 °C. The selected temperatures include ambient temperature, the maximum service temperature, and two intermediate temperatures that are particularly relevant for engineering applications.

As shown in Figure 2, YS exhibits a progressive decrease with increasing temperature, whereas EL initially decreases up to 300 °C and subsequently increases at higher temperatures, resulting in enhanced ductility at 450 °C and 700 °C. Importantly, the trends predicted by the ANN model are accurately reflected by the corresponding I_{RI} values, which correctly capture both the positive and negative influence of temperature on the mechanical response of the steel.

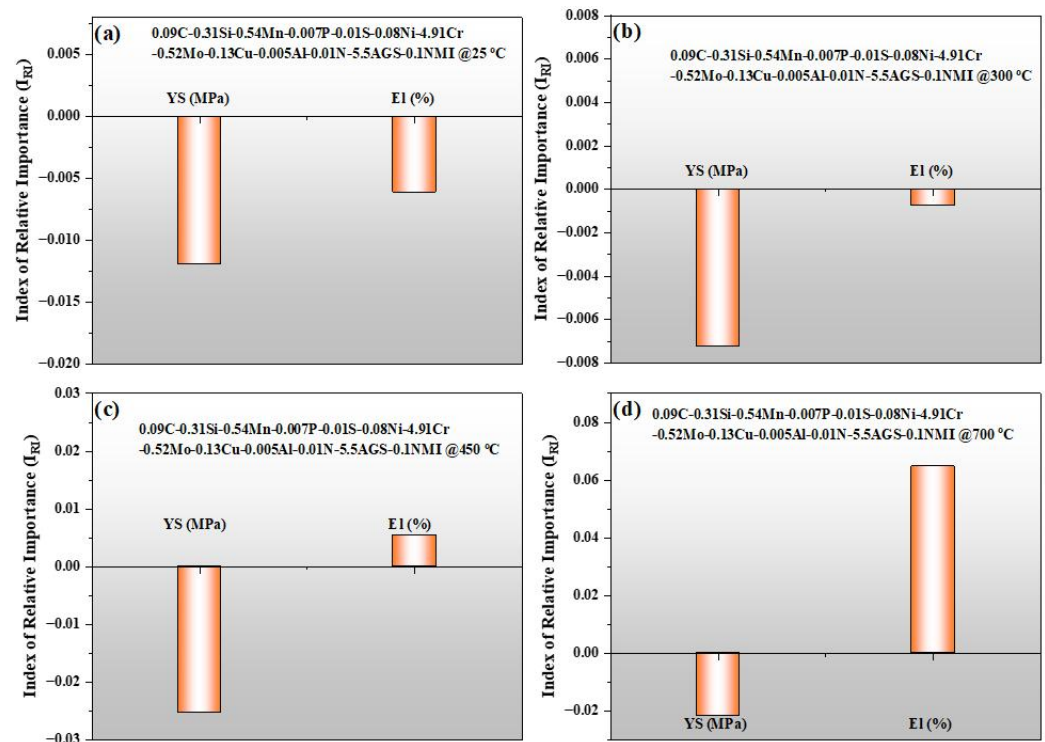


Figure 2. The I_{RI} for the effect of temperature on YS and El: (a) 25 °C, (b) 300 °C, (c) 450 °C, (d) 700 °C.

The agreement between the predicted property trends and the corresponding I_{RI} values demonstrates that the ANN successfully learned the underlying temperature–property relationships from the experimental data, despite the absence of explicit metallurgical information during training. From a metallurgical perspective, elevated temperatures promote thermally activated dislocation motion, recovery, and recrystallization processes, thereby reducing resistance to plastic deformation and consequently lowering strength [25]. Simultaneously, the increased mobility of dislocations enhances plasticity, resulting in improved ductility and elongation. The ability of the ANN model to reproduce these well-established metallurgical trends provides additional confidence in its predictive reliability and physical consistency.

3.3. Ten-Fold Cross-Validation

To evaluate the generalization capability of the developed ANN model, ten-fold cross-validation was employed. The dataset comprising 99 samples was randomly partitioned into ten subsets, with nine folds containing 10 samples and one fold containing 9 samples. In each iteration, one fold was used for testing while the remaining folds were employed for model training, ensuring that each sample served as an independent test case exactly once. The fold-by-fold test performance metrics obtained from the ten-fold cross-validation are presented in Figure 3, while the detailed numerical results for the training and test datasets are provided in Tables S1–S4. As shown in Figure 3a, the ANN model for YS exhibited consistently high predictive performance across the ten folds, yielding average test R^2 and Pearson’s r values of 0.9492 and 0.9739, respectively, with an average MAPE of 10.98%. Similarly, the UTS model (Figure 3b) demonstrated excellent predictive capability, achieving average test R^2 and Pearson’s r values of 0.9788 and 0.9893, respectively, with a comparatively lower average MAPE of 6.46%. In comparison, the models for El (%) and RA (%) (Figure 3c,d) exhibited slightly larger fold-to-fold variations in the performance metrics. Nevertheless, the average test R^2 values of 0.8085 and 0.8775 and corresponding Pearson’s r values of 0.8744 and 0.9107, respectively, indicate

satisfactory predictive performance. Overall, the cross-validation results demonstrate that the developed ANN model provides reliable predictions despite the relatively limited dataset size.

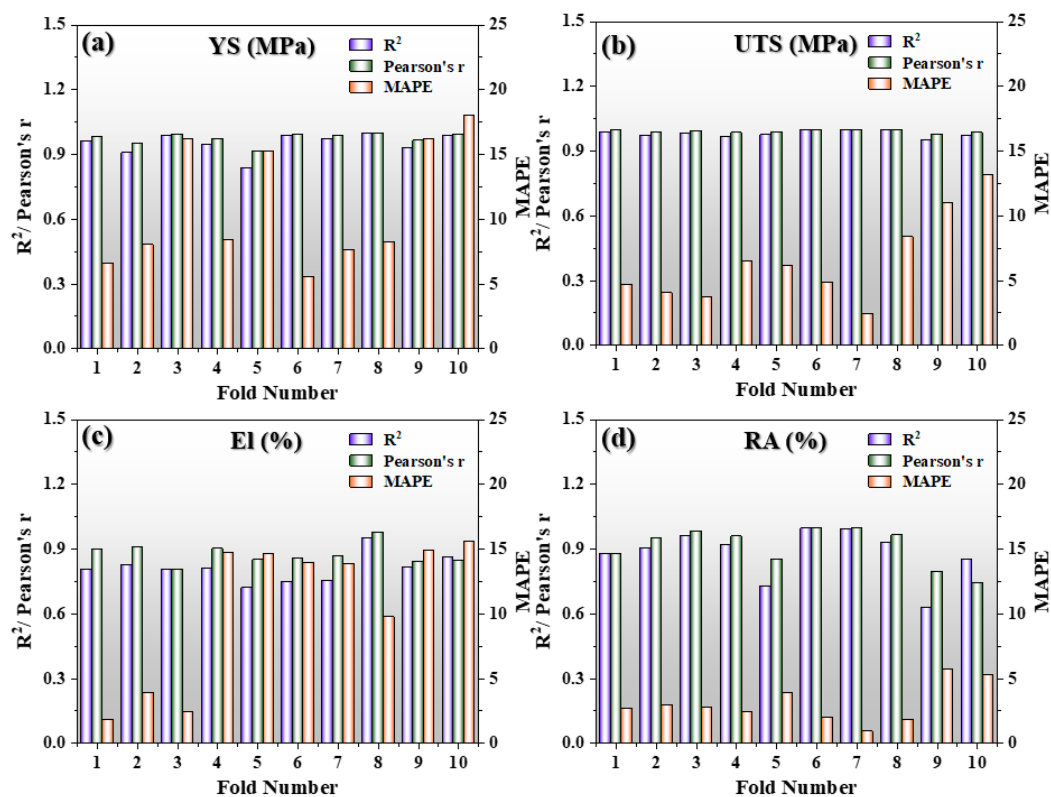


Figure 3. Fold-by-fold test performance metrics from ten-fold cross-validation, showing the test values of R^2 , Pearson's r , and MAPE for the prediction of (a) YS (MPa), (b) UTS (MPa), (c) El (%), and (d) RA (%).

3.4. Graphical User Interface

A user-friendly graphical user interface (GUI), shown in Figure 4, was developed to facilitate the practical implementation of the ANN model for predicting the mechanical properties of 5Cr–0.5Mo steel. The interface allows users to input key variables, including chemical composition, austenite grain size, non-metallic inclusions, and testing temperature and subsequently obtain predictions of YS, UTS, EL and RA. To ensure reliable predictions, the GUI restricts user inputs to the compositional and processing ranges encompassed by the training dataset. Once the input parameters are specified, the predicted mechanical properties can be generated instantaneously through a single calculation step. The interface also includes functionalities for parametric analysis, enabling users to investigate the influence of temperature and other input variables on the predicted mechanical response.

Figure 4. User-friendly GUI developed for ANN-based prediction of YS, UTS, EL, and RA of 5Cr–0.5Mo steel as a function of composition, austenite grain size, nonmetallic inclusions, and testing temperature.

Additional features include customizable data-point generation, selection of random seeds for visualization, plot saving, and export of predicted data for further analysis. The integrated visualization tools provide rapid assessment of composition–microstructure–property relationships, making the developed framework a useful supportive platform for the preliminary evaluation and visualization of temperature-dependent mechanical behavior in heat-resistant steels.

4. Conclusions

An artificial neural network (ANN) model was successfully developed to quantitatively predict the temperature-dependent mechanical properties of 5Cr–0.5Mo steel. The model accurately captured the influence of service temperature on yield strength (YS), ultimate tensile strength (UTS), elongation (El), and reduction in area (RA) over the investigated temperature range. Validation against independent experimental data demonstrated excellent predictive performance, with errors of only 3.68%, 0.45%, 1.88%, and 0.19% for YS, UTS, El, and RA, respectively, at 700 °C.

The Index of Relative Importance (I_{RI}) analysis further confirmed the capability of the model to identify both the magnitude and direction of the influence of temperature on the mechanical response of the steel, yielding trends that are consistent with established metallurgical principles. In addition, a user-friendly graphical user interface (GUI) was developed to facilitate rapid prediction and visualization of mechanical properties under different service conditions. Ten-fold cross-validation further confirmed the generalization capability of the developed ANN model. The models consistently exhibited high coefficients of determination and Pearson’s correlation coefficients, together with low normalized RMSE and MAPE values across all predicted properties, demonstrating reliable predictive performance despite the relatively limited dataset size.

Overall, the proposed ANN framework provides an efficient and reliable approach for the quantitative assessment of temperature-dependent mechanical behavior in 5Cr–

0.5Mo steel. The developed model and GUI demonstrate the potential of machine learning approaches as supportive tools for the preliminary evaluation of material performance under high-temperature conditions. However, further validation using larger and more diverse datasets is required before extending the framework to broader materials design and engineering decision-making applications.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/pr14132208/s1>, Detailed ten-fold cross-validation results for YS, UTS, El and RA predictions (Tables S1–S4).

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Abbreviations

The following abbreviations are used in this manuscript:

ANN	Artificial neural network
YS	Yield strength
UTS	Ultimate tensile strength
El	Elongation
RA	Reduction in area
I _{RI}	Index of relative importance
GUI	Graphical user interface

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