Original Article

Use of auto machine learning, artificial intelligence, for predictive modeling of metallurgical properties of hot-rolled steel products

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Abstract

This study aimed at predictive modeling, with Artificial Intelligence (AI), of the mechanical properties of sections produced from High Strength and Low Alloy (HSLA) steel, hot-rolled. The models were based on historical data of mechanical properties, along with the chemical composition of heats and the parameters of the rolling process. An Auto-Machine Learning platform was used. This tool can test dozens of algorithms to achieve the lowest error. Simplified models were built based on statistical analyses of the database, while expanded models were developed using all available data. Despite mathematical precision, the models were developed to be metallurgically coherent with scientific trends. The results aligned well with expected trends in most cases. It was possible to evaluate the isolated effect of variables. The expanded models were able to generate predictions with lower statistical errors. Data variability is an important factor for the success of predictive models. Such models allow alloy design to be defined with greater precision, leading to reduced production costs and a better understanding of the effects of input variables. Data-driven decision-making is enhanced with AI.

Keywords: Artificial Intelligence; Machine learning; HSLA steel; Modelling.

1 Introduction

The rolling process of structural steel sections poses a significant challenge in adjusting the chemical composition to satisfy the metallurgical properties required by various international standards. This challenge stems from understanding the effect of process variables on the evolution of properties throughout the rolling process. Diverse techniques have been applied to model the rolling process, providing predictive capability and a comprehensive understanding of the phenomena involved. Artificial Intelligence techniques are exceptionally efficient in predicting mechanical test results with low error and high correlation, often correlating with the metallurgical phenomena. Applying machine learning techniques in materials science is crucial in accelerating the discovery of novel materials. Over time, as materials science research has progressed, a substantial and steadily growing amount of data from experimental and simulation studies has been gathered [1]. This initiative aims to expedite the research cycle and reduce costs by adopting high-throughput computing, data-driven methods, big data technologies, and more. Methodologically, machine learning methods based on data mining are closely linked to applied statistics, given that machine learning is a pivotal component of data science, primarily focused on statistical data processing [1,2]. Machine learning techniques facilitate the establishment of associations between composition, microstructure, process, and performance, enabling the prediction of new materials with exceptional performance in previously unexplored domains—a common strategy in materials development [1,2].

Further advancements in materials science have led to machine learning techniques based on data-driven approaches emerging as a prominent focus in current materials research [2-12]. Machine learning excels in identifying correlations among multiple data points, making them practical for addressing multivariate nonlinear problems and establishing accurate prediction models based on existing data [13]. Using multi-objective optimization methods alongside neural network adjustments to reduce prediction error and average temperature difference has resulted in a model with enhanced predictability [14]. Applying Genetic Algorithms (GA) has made the alloy discovery and optimization process computationally more affordable [15]. Advances in microstructural observations facilitated by AI technology have paved the way for the automatic recognition of steel microstructures. This represents a significant development in understanding and controlling steel microstructures, offering an effective tool for researchers [16]. Automated Machine Learning, or Auto-ML, refers to tools and services that simplify the technical details and expertise needed to implement machine learning, automating essential ML tasks. Typically, these tasks include data normalization, feature engineering, training diverse types of models with

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varying hyperparameters, and evaluating and comparing results. Auto-ML aims to democratize access to analytical tools for non-data scientists by providing tools that require little to no code [17,18].

The present work focuses on modeling the relationship between the tensile test results, Yield Strength (YS), Tensile Strength (TS), and Elongation (E), of hot-rolled HSLA steel sections, which serve as the models' output data, and the chemical composition data and rolling parameters. The training process utilized historical tensile test data as input for the model.

2 Materials and methods

2.1 The steel section

A High Strength Low Alloy (HSLA) steel section with a nominal thickness of 11.00 mm was selected for the following characteristics:

- Tensile test samples taken from the flange, resulting in lower variability of results.
- A high number of tests were conducted following the ASTM A572/A572M-21e1 (Standard Specification for High-Strength Low-Alloy Columbium-Vanadium Structural Steel) [19]. For the present study, 461 sets of results were used.

The following information was utilized in developing predictive models of mechanical properties: chemical composition, final rolling temperature on the beam flange, the thickness of the test specimen as measured, and historical data for tensile strength (TS), yield strength (YS), and elongation (E). To calculate the percentage of total rolling reduction, the initial thickness was defined as the thickness of the cast raw material in the flange (Equation 1).

$$\%\text{Reduction} = \frac{\left(E_f - E_i\right)}{E_i} * 100 \quad (1)$$

In this equation, E_f denotes the final thickness of the rolled section measured at the sampling location, and E_i denotes the initial thickness of the cast raw material, specifically a beam blank.

2.2 Database statistical treatment

The following analyses and actions were performed to ensure data reliability in the database and final models. Approximately 5% of the data were considered as outliers or non-representative data and were therefore eliminated from the final database.

- Correlation analysis between input variables and output variables.
- Data Treatment: Limiting data within a range of ±3 standard deviations and eliminating outliers.

2.3 Models development

A total of six different models were built, comprising three simplified models and three expanded models. The output variables for all models are YS, TS, and E. The simplified models used a limited set of process parameters (YS, TS, E, %C, %Mn, %Si, %S, %Cr, %Nb, %N, Final Rolling Temperature (TFL) in °C, and total rolling reduction (%)), while the expanded models utilized all available data (YS, TS, E, %C, %Mn, %Si, %P, %S, %Cu, %Ti, %Cr, %Ni, %Nb, %Mo, %V, %B, %Al, %Sn, %W, %Zr, %As, %Ca, %Co, %Sb, %N, %Te, Final Rolling Temperature (TFL), and total rolling reduction (%)). The goal was to determine if simplified models, though less complex, could yield superior results regarding correlation and mean errors. Regressive models were employed using cross-validation with k-fold (using randomized subsets from the training data to reduce training bias) set to 5, on a dataset partitioned into 90% training and 10% testing. The mean absolute percentage error (MAPE) was used as the error metric. With the advantage of Auto-ML software, data quality verification and feature engineering steps were conducted automatically [18]. All modeling stages were visualized, both in descriptive and predictive parts, with adjustment curves and residual analysis also performed.

2.4 Selection of model parameters

- Simplified Models: The selection of input variables was based on the correlation analysis between these and the output variables (YS, TS, and E), involving the construction of a correlation matrix, evaluation of the obtained correlation coefficients, and elimination of chemical elements deemed residual. After this step and the elimination of the outliers, a database was obtained with 461 occurrences of the variables indicated in Table 1(a).
- Expanded Models: The variables shown in Table 1(b) were used in conjunction with the variables shown in Table 1(a) to construct this model:

2.5 Architecture of the AI models

DataRobot software was used, which is market-leading commercial software according to the Gartner quadrant, as it is one of the partner companies of the A10 consultancy that supported the completion of this work. The software in question provides easy use of the most advanced resources regarding the use of Machine Learning models for structured and unstructured data, through Auto Machine Learning with just a few clicks, maximizing the time and results ratio. The Data-Robot® Auto-ML tool features model competition, enabling functions such as mixing models (Blend Models) and modeling in parallel with different families of models. This

Table 1. The input and output variables (YS, TS, and E) included in the simplified models (a) and the expanded models (b)

Variable	Description	(a)	Variable	Description	(b)
Y1	YS, MPa: Yield Strength		X10	P, %	
Y2	TS, MPa: Tensile Strength		X11	Cu, %	
Y3	E, %: Elongation		X12	Mo, %	
X1	C, %		X13	V, %	
X2	Mn, %		X14	Al, %	
X3	Si, %		X15	Sn, %	
X4	S, %		X16	Ti, %	
X5	Cr, %		X17	Ni, %	
X6	Nb, %		X18	Co, %	
X7	N_2, %		X19	Sb, %	
X8	Final Rolling Temperature (TFL), ºC		X20	Zr, %	
X9	Total Rolling Reduction, %		X21	As, %	
			X22	Te, %	
			X23	B, %	
			X24	Ca, %	
			X25	W, %	

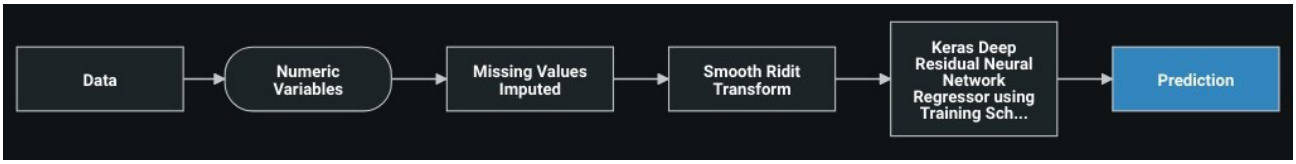

Figure 1. Blueprint for the expanded TS Model, illustrating the model's architecture and processes.

architecture allowed for the optimal results to be obtained in just a few minutes. The adjustment of missing data had already been carried out automatically, and following the widely used modeling methodology (cross-validation), appropriate metrics were achieved for models in applications found in the literature and academic works, as noted in the master's thesis of one of the authors. Figure 1 illustrates the high-level end-to-end procedure for fitting the model, encompassing pre-processing, algorithmic, and post-processing steps. It illustrates the various steps transforming input predictors and targets into models. Each element (or 'node') in the blueprint may represent multiple steps.

The following elements connect to create the blueprint:

- Imputation of Missing Values: For numeric features, missing value rows are credited with the median of the existing data;
- Smooth Ridit Transform: This method replaces the categories of an ordinal variable with scores between -1 and 1. It aims to reduce complex mass data to a more straightforward form, allowing researchers to visualize the data and answer the research question more simply;
- Keras Deep Residual Neural Network Regressor (KDRNNR) uses a training schedule with three layers (512, 64, 64 units): Keras is a high-level library for building neural networks with the TensorFlow framework. Keras provides flexibility for rapidly incorporating state-of-the-art deep learning models into Auto-ML. It supports sparse data, especially for text-heavy or high-cardinality categorical data.

2.6 Training of the models: expanded TS model

The blue 'Forecast' line in the Lift Chart (Figure 2a) displays the average prediction score for the rows in that bin. The orange 'Actual' line displays the actual percentage of the lines in that bin. A strong correlation between these two lines signifies the model's predictive accuracy. Additionally, a steadily increasing line indicates satisfactory model performance. Figure 2b illustrates the impact of several product and process variables on the TS parameter. The variables that impact TS the most are %C, %Mn, %Al, %Nb, %Ti, and Total Rolling Reduction (%). Mn has approximately 60% of the influence of C. The variables with the least impact on TS are %S, %Cu, %N, %Si, and %P. These results align with metallurgical expectations. Figure 2c presents the Matrix Plot, which shows the association between the process variables (input and output data). A higher opacity in a pair indicates a weaker association between the variables, while a lower opacity indicates a stronger association. TS is strongly associated with Al, C, Cr, Mn, N, Nb, P, S, Si, Mo, Ni, Ti, V, As, and Sn.

The correlation between the real TS and the calculated TS was 0.7698. The average percentage error between the real TS and the simulated TS values was 1.11%.

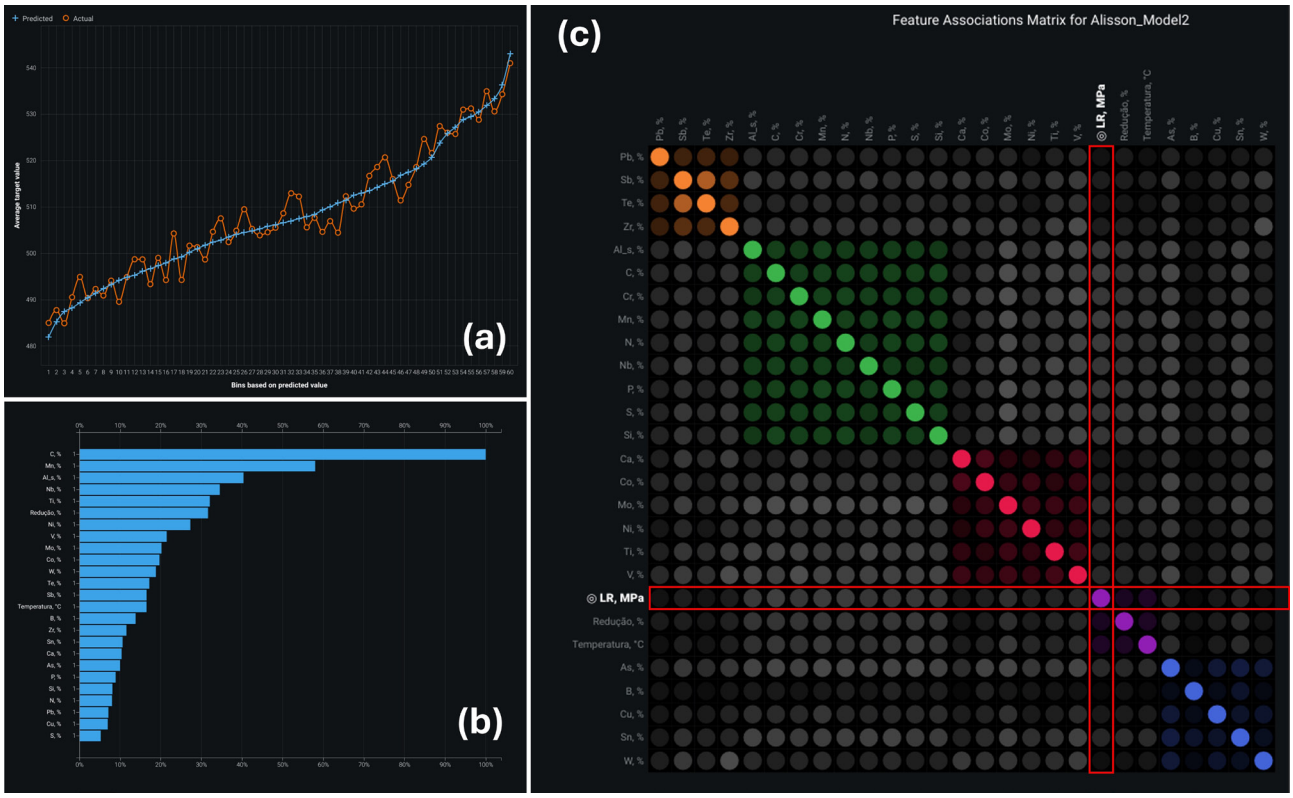

Figure 2. Training results for the expanded TS Model: (a) Lift Chart, (b) Variable Impact, (c) Matrix Plot. In these plots, LR has the same meaning as TS (Tensile Strength).

3 Results

3.1 Influence of input variables on output variables

The impact of input variables, including each chemical element and process parameter, on YS, TS, and E was assessed. This assessment was performed using partial dependence plots (Figure 3), which illustrate the average partial relationship between a set of predictors and the predicted output. The yellow partial dependence data indicate the marginal effect of a feature on the target variable, after accounting for the average effects of all other predictive features. This indicates how the value of this feature affects the prediction while keeping all other variables constant. The figure below presents examples of these plots specifically for the expanded TS model:

3.2 Comparison of model performance metrics

Table 2 compares the output variables (TS, YS, and E) between simplified and expanded models.

The expanded model demonstrates superior results for most of the evaluated statistical parameters, particularly regarding the correlation coefficients and standard deviation. The R^2 values for elongation are considerably lower when compared to the YS and TS values. The method of obtaining elongation, since it depends on a manual procedure (measurement of the total length of the test specimen after rupture), is subject to numerous factors, such as operator skill, calibration of the measuring equipment, and perfect fit of the ruptured segments of the test specimen. For this reason, there is greater variability in the elongation data obtained.

4 Discussions

The partial dependence plots shown in Figure 3 provide interesting information regarding how each input variable impacts the output variables YS, TS, and E. Table 3 interprets these plots specifically for TS.

Table 3(a) shows the impact of the input variables on the output variable TS. Input variables, such as C, Mn, Nb, Final Rolling Temperature (TFL), and Total Rolling Reduction, significantly influence on the output variable. Table 3(b) presents the analysis results of the variables' influence (or impact) on TS for the expanded model and whether this influence aligns with the available technical literature. For instance, in microalloyed steels, microalloying elements such as niobium can interact with the movement of austenite grain boundaries in two diverse ways. Firstly, the dispersion of Nb-containing precipitates exerts a retarding pressure on the grain boundaries, which has a pronounced effect on the growth of the austenitic grain. The magnitude

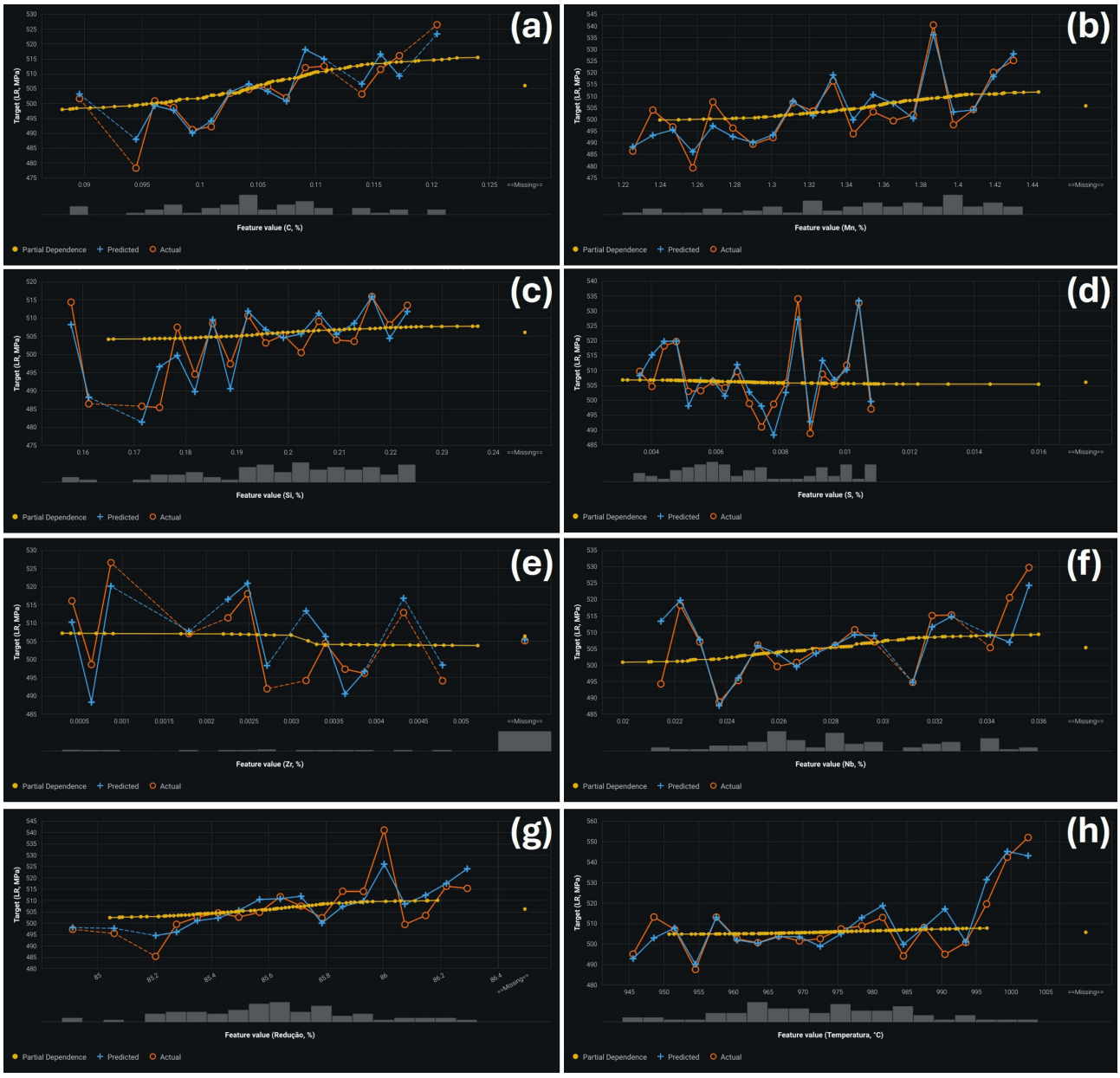

Figure 3. (a) to (h): TS Partial Dependence Plots according to: (a) C, %; (b) Mn, %; (c) Si, %; (d) S, %; (e) Zr, %; (f) Nb, %; (g) Total Rolling Reduction, %; and (h) Final Rolling Temperature (TFL), °C. In these plots, LR has the same meaning as TS (Tensile Strength).

Table 2. Statistical Comparison between the Simplified and Expanded Models

Model	Parameter	Residuals Average	Correlation Coefficient, R^2	Standard Deviation
Simplified	YS	-0.170	0.627	9.392
	TS	-0.126	0.709	8.285
	E	-0.435	0.252	2.615
Expanded	YS	0.049	0.678	8.725
	TS	-0.285	0.770	7.357
	E	-0.079	0.394	2.384

of this effect depends on the size, shape, and volume fraction of these precipitates, typically Nb(C,N) or Nb carbonitrides.

Secondly, a moving interface drags an atmosphere of solute elements, which exerts a retarding force on this interface. Thus, elements in solution can significantly reduce the mobility of austenitic grain boundaries.

This phenomenon is known as the solute drag effect [20]. Both phenomena collaborate to increase TS

Table 3. (a) Impact of the Input Variables on Tensile Strength (TS); (b) Alignment of the Impact with Technical Literature for TS

Input Variables	TS, MPa		(a)	TS Analysis for the Expanded Model			(b)
	Simplified	Expanded		Alloy-Design Range, %	Impact, MPa	Literature aligned?	
C, %	↑	↑		0.01	**5.00**	**Yes!**	
Mn, %	↑	↑		0.01	**0.60**	**Yes!**	
Si, %	↑	↗		0.01	0.62	**Yes!**	
P, %	-	↗		0.001	0.17	**Yes!**	
S, %	→	↘		0.001	**-0.17**	**Yes!**	
Cu, %	-	→		0.001	0.00	**No (Residual)!**	
Ti, %	-	↘		0.0001	-0.16	**No (Residual)!**	
Cr, %	↘	↘		0.001	-0.07	**Yes (Residual)!**	
Ni, %	-	↓		0.001	-0.17	**No (Residual)!**	
Nb, %	↗	↑		0.001	**0.56**	**Yes!**	
Mo, %	-	↗		0.001	0.21	**Yes (Residual)!**	
V, %	-	↗		0.0001	0.21	**Yes (Residual)!**	
B, %	-	↘		0.00001	-0.10	**No (Residual)!**	
Al, %	-	↑		0.001	0.24	**Yes!**	
Sn, %	-	↓		0.0001	-0.11	**Yes (Residual)!**	
W, %	-	→		0.001	0.67	**Yes (Residual)!**	
Zr, %	-	↘		0.0001	-0.09	**No (Residual)!**	
As, %	-	→		0.0001	0.05	**No (Residual)!**	
Ca, %	-	→		0.0001	0.14	**Yes (Residual)!**	
Co, %	-	↗		0.001	0.45	**Yes (Residual)!**	
Sb, %	-	-		0.001	0.00	**?**	
N, %	↗	↗		0.001	0.29	**Yes (Residual)!**	
Te, %	-	↘		0.0001	-0.17	**?**	
TFL, °C	↑	↑		1	**0.04**	**Yes!**	
Redução, %	↑	↑		0.1	**0.58**	**Yes!**	

Table 4. Average prediction error for each model. algorithm, and output variable

Model	Info	Output Parameters		
		YS	TS	E
Expanded Model	Average error, %	1.65	1.11	6.36
	Algorithm	eXtreme G. Boost	KDRNNR, 3 Layers	Adaboost A
Simplified Model	Average error, %	1.89	1.33	6.41
	Algorithm	eXtreme G. Boost	eXtreme G. Boost	eXtreme G. Boost
ANN (MatLab)	Average error, %	2.26	1.57	4.76
	Algorithm	ANN, 3 Layers	ANN, 3 Layers	ANN, 3 Layers
MLR	Average error, %	2.27	1.73	4.86
	Algorithm	MLR (Excel)	MLR (Excel)	MLR (Excel)

when the content of Nb is increased. The TS results for the expanded model show that Nb contributes 0.56 MPa for every 0.001% addition, aligning with the known resistance increase mechanism. In other words, the addition of Nb contributes to the increase in mechanical strength. Both the expanded model and the simplified model demonstrate this trend. According to different authors [21,22], the Zr addition plays a dubious role in improving the mechanical resistance of steel. The constructed model indicates a reduction in TS of 0.09 MPa for each addition of 0.0001% of Zr, noting that there was no intentional addition of Zr to this HSLA steel.

The same dataset was subjected to modeling to construct predictive models [23], utilizing both Artificial Neural Networks and Multiple Linear Regression (MLR). The results are presented in Table 4.

The simplified model outperforms the ANN model in most cases, except for variable E, where the ANN yielded superior results. Additionally, the expanded model performs better than the simplified model across all output parameters.

5 Conclusions

- The Auto-ML tool enables virtual alloy design before actual production, reducing both the product

development cycle and total costs. This approach minimizes heat disqualifications that can arise from design errors during research;

- The models are strongly aligned with metallurgical trends and reflect previously observed patterns from the statistical analyses. They can be used to isolate the effects of individual variables;
- The expanded model, utilizing most available data, achieved lower mean errors and higher correlation coefficients in its predictions;
- In comparison with simulations using other algorithms, the Auto-ML models exhibited greater accuracy, with lower error rates and higher correlations (specifically in the expanded model);
- The tool verified the influence of all input variables on the final results. It can recognize new patterns across a broad range of input variables, showcasing the potential to explore unknown relationships and facilitating innovative approaches for product development and research;
- While the current database contains many variables, it lacks critical ones, including reductions based on the pass schedule, interpass times, temperatures for each rolling pass, and cooling rates post-rolling.

The Automated Machine Learning (Auto-ML) tool is a strategic asset for alloy design, particularly for structural applications and other steel-based products. This tool streamlines research and development (R&D) by simulating various alloy design scenarios in a virtual environment, allowing for process optimization before production begins. By conducting virtual production trials before physical implementation, significant reductions in development costs and project lead times are possible. The empirical models demonstrate commendable predictive accuracy, evidenced by minimal prediction errors (less than 2% for both YS and TS). As a result, these models play a pivotal role in data-driven decision-making processes, fostering innovation and substantial cost savings within the steel industry.

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