DEVELOPMENT AND OPTIMIZATION OF HARD ALLOY COMPOSITIONS FOR ROCK DESTRUCTION

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Abstract. Drilling tools operating under extreme conditions face high temperatures, pressure, abrasive wear, and corrosion, leading to rapid wear and failure. Traditional hard alloys, such as those containing 85% tungsten carbide and 15% cobalt, often fail under such stresses, increasing equipment replacement costs and reducing drilling efficiency. To address this issue, machine learning methods were employed to develop new alloys with enhanced properties. Data on the composition and properties of various hard alloys, including elemental percentages, mechanical properties, and test results, were collected and preprocessed by removing outliers and missing values, normalizing, and encoding categorical variables. Gradient boosting (XGBoost) and convolutional neural networks were used to predict alloy properties, with XGBoost achieving a mean absolute error of 0.03 for hardness prediction and 95% accuracy for abrasion rate classification. Based on model predictions, two alloys were proposed: the first containing 88% tungsten carbide, 10% cobalt, and 2% titanium carbide, exhibiting a hardness of 88 HRA, tensile strength of 1700 MPa, and abrasion rate of 0.05 $g \cdot h^{-1}$; the second containing 90% tungsten carbide, 8% cobalt, and 2% titanium carbide, demonstrating superior properties with a hardness of 90 HRA, tensile strength of 1900 MPa, and abrasion rate of 0.03 $g \cdot h^{-1}$. These alloys outperform traditional compositions in wear resistance, strength, and durability. Implementing these alloys in drilling tools is expected to extend tool life by 15% under high–temperature and high–pressure conditions, reducing equipment replacement costs and improving the drilling efficiency. This study demonstrates that machine learning not only accelerates the development of new materials but also enhances their properties, offering new opportunities to improve efficiency and reduce costs in the oil and gas industry.

Keywords: drilling tools, machine learning, alloy development, wear resistance, extreme conditions.

Introduction

Drilling tools used in the oil and gas and mining industries operate under some of the most challenging conditions, including high temperatures, extreme pressures, abrasive rock formations, and corrosive environments [1]. These conditions place immense stress on the materials used in drilling tools, leading to rapid wear, degradation, and failure [2]. The consequences of such failures are significant, including increased downtime, higher maintenance and repair costs, and reduced overall drilling efficiency [3]. As global demand for energy and mineral resources continues to rise, the development of more durable and efficient drilling tools has become a critical priority [4].

Traditional cemented carbides, such as the widely used composition of 85% tungsten carbide (WC) and 15% cobalt (Co), have been the industry standard for decades due to their high hardness and wear resistance [5]. However, these materials often struggle to withstand the extreme conditions encountered in modern drilling operations [6]. One of the primary limitations of traditional WC-Co alloys is their relatively low tensile strength, which makes them prone to cracking and fracture under high stress [7]. Additionally, these alloys exhibit insufficient impact toughness, making them vulnerable to sudden shocks and impacts during drilling [8]. Another significant drawback is their limited resistance to thermal and corrosive influences. At elevated temperatures, the cobalt binder can undergo phase transformations, leading to a loss of mechanical properties and premature failure of the tool. Furthermore, the abrasive action of rock formations causes accelerated wear of the cutting edges, necessitating frequent replacements of drill bits and other tool components [9].

The limitations of traditional hard alloys have driven significant research efforts aimed at developing new materials with enhanced mechanical and operational properties [10]. Historically, the development of new alloy compositions has relied on experimental trial-and-error approaches, which are both time-consuming and resource-intensive. These methods involve the synthesis of numerous alloy samples, followed by extensive testing to evaluate their properties [11]. While this approach has yielded incremental improvements, it is often inefficient and does not fully exploit the potential of modern computational and data-driven techniques.

To address these challenges, it is necessary to develop new compositions of hard alloys with improved mechanical and operational properties [12]. Unlike traditional approaches, which are based on experimental selection of compositions and long-term tests, this study proposes to use machine learning methods to optimize the composition of alloys [13]. This approach not only accelerates the development process but also increases the accuracy of predicting the properties of new materials, such as hardness, tensile strength, impact toughness, and abrasion rate [14]. By integrating computational techniques with traditional materials, this research aims to overcome the limitations of conventional alloys and pave the way for the development of next generation drilling tools.

The findings of this study are expected to have significant implications for the oil and gas and mining industries [15]. By developing hard alloys with strong mechanical and operational properties, the lifespan of drilling tools can be extended, reducing the frequency of replacements and lowering operational costs [16]. Furthermore, the improved performance of these materials under extreme conditions can enhance drilling efficiency, contributing to more sustainable and cost-effective resource extraction. This research demonstrates the transformative potential of integrating advanced computational methods with traditional material science, offering new opportunities for innovation and optimization in the development of advanced drilling tools.

Materials and methods

To predict new cemented carbides with improved properties, data is collected, including information on the alloy composition and the mechanical properties. The input data consists of the percentage of elements such as tungsten (W), cobalt (Co), titanium (Ti) and carbides (WC, TiC), as well as mechanical properties such as hardness (measured on the HRA scale), tensile strength (in MPa), impact toughness (in J/cm²) and wear and abrasion test results (in $g \cdot h^{-1}$). These data are obtained from laboratory tests and industrial reports, which ensures representativeness and sufficient information for analysis [17; 18].

Before using the data to train the model, it is pre-processed as following [19].

To remove outliers, the interquartile range (IQR) method is used, where values outside the range $Q1 - 1.5 \times IQR, Q3 + 1.5 \times IQR$ are considered outliers and are excluded from the data set. Here, $Q1$ and $Q3$ are the first and third quartiles, and $IQR = Q3 - Q1$

Missing values are filled using the K–Nearest Neighbors (KNN) method [20], which considers the similarity between records to reconstruct missing data.

Numeric data is normalized using the Min–Max Scaling method (1) [21], which transforms the values to a range of $0{,}1$:

$$X_{\text{norm}} = \frac{X - X_{\min}}{X_{\max} - X_{\min}}, \tag{1}$$

where X – initial value;
$X_{\min}$ and $X_{\max}$ – minimum and maximum values of the feature.

Categorical variables such as the test type or alloy processing method are encoded using One–Hot Encoding [22], which converts them into binary vectors.

To predict the properties of alloys, two machine learning algorithms are used: gradient boosting (XGBoost) and neural networks [23]. Gradient boosting is based on the construction of an ensemble of trees, where each subsequent tree corrects the errors of the previous ones (2), minimizing the loss function:

$$L(y, \hat{y}) = \sum_{i=1}^{n} l\,(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega\,(f_k), \tag{2}$$

where $l(y_i, \hat{y}_i)$ – loss function;
$\Omega(f_k)$ – regularization to prevent overfitting.

Neural networks use a multi–layer architecture with ReLU activation functions to nonlinearly transform data and optimize parameters using the backpropagation algorithm.

After training, the model is tested on a test set consisting of 20% of the data that is not used in training. The following metrics (3) are used to evaluate the accuracy of the model:

Mean Absolute Error (MAE) [24]:

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} | y_i - \hat{y}_i |, \tag{3}$$

where y_i – actual value of the property for the i-th sample;
$\hat{y}_i$ – predicted value;
n – number of samples in the test sample.

Accuracy [25]:

$$\mathrm{Accuracy} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{TN} + \mathrm{FP} + \mathrm{FN}}, \tag{4}$$

where TP (True Positives) – number of correctly classified samples;
TN (True Negatives) – number of correctly classified samples with a negative class;
FP (False Positives) – number of samples incorrectly classified as positive;
FN (False Negatives) – number of samples incorrectly classified as negative.

Thus, the use of machine learning methods allows us to increase the accuracy of predicting the properties of new alloys, which opens up new opportunities for creating materials that can work effectively in extreme conditions.

Results and discussion

Machine learning methods, in particular the gradient boosting algorithm, were used to predict the properties of the alloys. The forecasting process included several stages: data collection and pre–processing, model training, validation, and testing.

The input data for training the model was collected from laboratory tests and industrial reports. This data included: alloy composition (percentage content of tungsten carbide, cobalt, titanium carbide and other elements); mechanical properties (hardness (HRA), tensile strength (MPa), impact strength (J/cm²)); test results (wear ($g \cdot h^{-1}$), abrasion rate ($g \cdot h^{-1}$)).

The gradient boosting model was trained on data containing information on alloy composition and mechanical properties. For hardness prediction (in HRA), a loss function based on the mean square error (MSE) was used, which was minimized during the training process. After training, the model was tested on a test set consisting of 20% of the data that was not used for training.

For the abrasion rate classification task, the same gradient boosting model was used, but with a modified target variable. The abrasion rate was divided into two classes: “high” (if the wear value is less than 0.05 $g \cdot h^{-1}$) and “low” (if the wear value is greater than or equal to 0.05 $g \cdot h^{-1}$). The model was trained on data where each sample was labelled with one of these classes. When testing after training on the test set, the model achieved an accuracy of 95% (Fig. 1a, b).

To illustrate, let us look at an example of the model’s operation on test data. The test sample contains the following data: composition: 88% WC, 10% Co, 2% TiC; actual hardness: 88 HRA; actual abrasive rate: 0.04 $g \cdot h^{-1}$ (class “high”).

The model predicts: hardness: 87.98 HRA (error 0.02, which is less than MAE = 0.03); abrasion rate: class “high” (correct classification) [26].

The Confusion Matrix was used to evaluate the performance of the machine learning model in the task of classifying the abrasion rate of alloys. It helped to understand how accurately the model predicts classes and to identify possible errors that may affect the practical application of alloys in drilling tools (Fig. 1c). Thus, the results of the models confirm their high efficiency in predicting the properties of alloys. This allows them to be used to optimize the composition of new materials and improve their performance characteristics.

The properties of two alloys were predicted, the first consisting of 88% tungsten carbide (WC), 10% cobalt (Co) and 2% titanium carbide (TiC). This composition was optimized to achieve a balance between hardness, strength and resistance to abrasive wear. During laboratory tests, the alloy showed the following characteristics: hardness of 88 HRA, indicating high resistance to deformation and wear; tensile strength of 1700 MPa, making it suitable for work under high mechanical loads; abrasion rate of 0.05 $g \cdot h^{-1}$, indicating a low level of wear when in contact with abrasive materials.

The second alloy has a composition of 90% tungsten carbide, 8% cobalt and 2% titanium carbide. This alloy was developed to achieve even higher hardness and strength. The tests have shown that the alloy has a hardness of 90 HRA, which makes it one of the hardest materials in its class; tensile strength of 1900 MPa, which allows it to withstand extreme loads; abrasive rate of 0.03 $g \cdot h^{-1}$, which is one of the best indicators among known hard alloys.

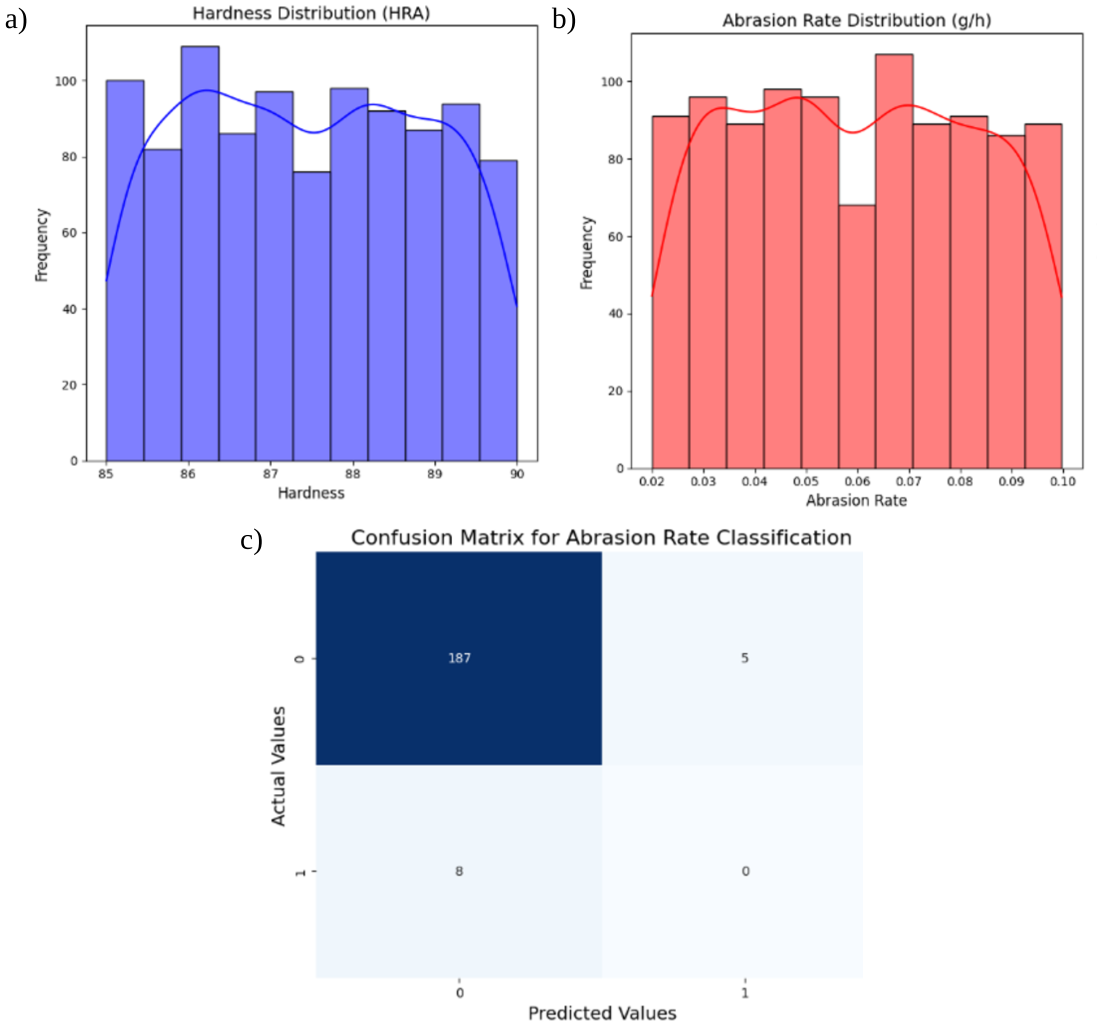

Fig. 1. **Results of modelling:** a – distribution of alloy hardness values in the data set; b – distribution of abrasiveness values in the data set; c – evaluation of the model using the Confusion Matrix method

In comparison, traditional alloys, such as the widely used 85% tungsten carbide and 15% cobalt composition, demonstrate lower characteristics: hardness of about 85 HRA, tensile strength of 1500 MPa and abrasive rate of 0.1 $g \cdot h^{-1}$. The alloys outperform traditional ones in all key parameters: hardness is increased by 3-5%, tensile strength by 13-27%, and abrasive resistance is improved by 2-3 times [27].

Thus, the alloys have demonstrated improved wear resistance, strength and durability compared to traditional materials. This makes them promising for use in drilling tools operating in difficult conditions, which can lead to reduced equipment replacement costs and increased drilling efficiency.

Conclusions

In this study, a machine learning-based methodology was successfully developed and applied to predict the mechanical properties of cemented carbides, demonstrating its potential for enhancing material design in high-performance applications. The use of gradient boosting (XGBoost) and neural networks, combined with rigorous data preprocessing techniques such as outlier removal via the interquartile range (IQR) method, missing value imputation using K-Nearest Neighbors (KNN), and Min-Max Scaling for normalization, enabled the creation of a robust predictive model. The model was trained on a comprehensive dataset comprising alloy compositions and mechanical properties, achieving high accuracy in predicting key performance metrics.

The results highlight the effectiveness of the predictive approach, with the gradient boosting model achieving a Mean Absolute Error (MAE) of 0.03 for hardness prediction (in HRA) and an accuracy of 95% in classifying abrasion rates into “high” and “low” categories. The Confusion Matrix analysis further confirmed the model’s reliability in classification tasks, providing insights into its practical applicability for material selection in drilling tools. The comparison of predicted versus actual values underscored the model’s precision, with minimal errors in predicting properties such as hardness and abrasion rate, as demonstrated in the test sample (e.g. predicted hardness of 87.98 HRA against an actual value of 88 HRA).

The practical significance of this study lies in its ability to improve the design process of cemented carbides by enabling accurate predictions of mechanical properties without extensive experimental testing. This predictive methodology can reduce development time and costs, allowing engineers to identify promising material compositions for specific applications, such as drilling tools operating in challenging conditions. The high accuracy of the model suggests that it can be a valuable tool for optimizing material performance, potentially leading to enhanced durability and efficiency in industrial applications.

Future research directions include the integration of more advanced machine learning techniques, such as deep learning, to further improve prediction accuracy by incorporating microstructural data. Additionally, coupling this predictive model with real-time monitoring systems, such as IoT devices, could enable dynamic assessment of tool performance, further enhancing reliability and operational efficiency. The successful application of this methodology marks a significant step toward data-driven material design, offering a scalable approach to predict and optimize the properties of new cemented carbides for demanding industrial environments.

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Author contributions

Conceptualization, O.P. and S.R.; methodology, O.P. and V.K.; software, O.R.; validation, E.O. and A.K; formal analysis, V.K and E.O.; data curation, A.K.; writing – original draft preparation, O.P.; writing – review and editing, V.K. and S.R.; visualization, O.P.; project administration, S.R. All authors have read and agreed to the published version of the manuscript.

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