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Nonlinear Prediction of Detonation Velocity in Aluminized Explosives Using Optimized Support Vector Regression

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Abstract- ***Accurate determination of the velocity of detonation (VoD) of aluminized explosives is essential for evaluating explosive performance in military, mining, and engineering applications. Conventional empirical and equation-of-state-based models often exhibit limited predictive capability due to the complex nonlinear interactions among explosive composition, density, oxygen balance, heat of explosion, and aluminum content. In this study, a Support Vector Regression (SVR) machine learning framework is developed for predicting the velocity of detonation of aluminized explosives. The proposed model utilizes key physicochemical descriptors of explosive formulations as inputs and establishes a nonlinear relationship between these descriptors and detonation velocity through kernel-based learning. The effects of important SVR hyper-parameters, including the regularization factor (C), epsilon-insensitive loss parameter (ε), and regularization parameter (λ), were systematically investigated to obtain optimal model performance. Predictive accuracy was evaluated using correlation coefficient (CC), root mean square error (RMSE), and mean absolute error (MAE). The developed SVR model was further compared with existing predictive approaches, including BHWS-EOS-full, BHWS-EOS-partial, and Keshavarz models. Results indicate that the optimized SVR model exhibits superior predictive accuracy, lower prediction errors, and stronger generalization capability than the conventional models. The demonstrated performance of the proposed framework highlights the potential of machine learning techniques as reliable and efficient tools for modeling detonation characteristics of complex explosive systems***

Keywords: Velocity of Detonation, Aluminized Explosives, Support Vector Regression, Machine Learning, Energetic Materials, Predictive Modeling, Data-Driven Modeling, Nonlinear Regression, Explosive Performance, Artificial Intelligence

I. INTRODUCTION

The velocity of detonation (VoD) is one of the most important performance parameters used in the characterization and evaluation of energetic materials [1]. It describes the speed at which a detonation wave propagates through an explosive medium and serves as a fundamental indicator of explosive power, energy release rate, brisance, and overall detonation performance. Accurate determination of VoD is essential in the design, optimization, and safe utilization of explosives for military, mining, demolition, aerospace, and civil engineering applications [2]. Since detonation velocity is directly related to the thermochemical and physical properties of explosive formulations, reliable prediction of this parameter remains a critical aspect of energetic material research. Among various classes of energetic materials, aluminized explosives have attracted considerable attention due to their enhanced energy output and improved blast effects. The incorporation of aluminum powder into explosive formulations significantly increases the total energy released during detonation through secondary oxidation reactions. Aluminum particles possess high combustion enthalpy and contribute substantially to afterburning processes, thereby improving explosive performance in applications requiring high blast energy and prolonged pressure pulses [3]. Consequently, aluminized explosives have found extensive applications in underwater explosives, thermobaric weapons, mining operations, and military warhead systems. Despite their advantages, the prediction of detonation characteristics of aluminized explosives presents significant challenges. The presence of aluminum introduces complex physicochemical interactions that affect the detonation process. Parameters such as explosive

density, oxygen balance, heat of formation, molecular composition, particle size distribution, aluminum content, and reaction kinetics collectively influence detonation behavior. These factors often interact in a highly nonlinear manner, making the development of accurate predictive models difficult using conventional theoretical and empirical approaches.

Over the years, numerous models have been proposed for estimating the detonation velocity of explosives. Traditional approaches include thermochemical calculations, equations of state (EOS), and empirical correlations derived from experimental observations. Models such as the BKW equation of state, Kamlet–Jacobs equations, BHWS-EOS formulations, and the Keshavarz predictive model have demonstrated varying degrees of success in estimating explosive properties [4]. However, many of these models rely on simplifying assumptions regarding reaction mechanisms, equilibrium conditions, and material homogeneity. Such assumptions may limit their predictive accuracy when applied to complex aluminized explosive systems, particularly when significant nonlinear interactions exist among the governing variables [5]. Recent advances in artificial intelligence and machine learning have created new opportunities for modeling complex engineering systems characterized by nonlinear behavior and multidimensional data. Machine learning algorithms possess the capability to automatically learn hidden relationships between input variables and target outputs without requiring explicit mathematical descriptions of the underlying physical processes. These techniques have been successfully applied across diverse scientific disciplines, including materials science, chemical engineering, combustion science, catalysis, energy storage systems, and energetic materials research.

Among various machine learning techniques, Support Vector Regression (SVR) has emerged as a powerful and reliable tool for nonlinear regression analysis [6]. Derived from the principles of statistical learning theory, SVR combines strong generalization capability with excellent predictive performance, particularly when dealing with limited datasets and nonlinear relationships [7]. Through the use of kernel functions, SVR effectively transforms input data into higher-dimensional feature spaces where complex relationships can be represented using linear regression functions. Furthermore, the incorporation of structural risk minimization principles enables SVR to achieve robust predictive performance while minimizing over-fitting. Several studies have demonstrated the effectiveness of machine learning approaches for predicting the properties of energetic materials [8]. Artificial neural networks, support vector machines, random forests, ensemble learning methods, and deep learning architectures have been employed to estimate detonation pressure, explosive energy, sensitivity parameters, combustion characteristics, and thermochemical properties. These studies have consistently shown that machine learning models often outperform conventional empirical and theoretical approaches, particularly when modeling systems governed by intricate nonlinear interactions. Motivated by these developments, this study proposes a data-driven Support Vector Regression framework for predicting the velocity of detonation of aluminized explosives [9]. The proposed model seeks to establish a robust nonlinear relationship between selected explosive descriptors and detonation velocity while overcoming limitations associated with conventional predictive approaches. Hyperparameter optimization is performed to enhance model performance and ensure optimal generalization capability. The predictive accuracy of the developed SVR model is evaluated using statistical performance metrics including correlation coefficient (CC), root mean square error (RMSE), and mean absolute error (MAE).

Furthermore, the developed model is benchmarked against established predictive approaches, including BHWS-EOS-full, BHWS-EOS-partial, and Keshavarz models [10], to assess its relative performance. Through this comparative analysis, the study aims to demonstrate the effectiveness of machine learning techniques for improving predictive accuracy in energetic materials research and to provide a reliable computational framework for the rapid evaluation and optimization of aluminized explosive formulations.

The remainder of this paper is organized as follows. Section 2 presents the methodology and theoretical formulation of the Support Vector Regression model.

Section 3 discusses dataset preparation, model development, and performance evaluation procedures. Section 4 presents and discusses the obtained results, including comparisons with existing predictive models. Finally, Section 5 summarizes the major findings and outlines future research directions

II. IMPLEMENTED ALGORITHM

2.1 Description of support vector regression

Support Vector Regression (SVR) is a supervised machine learning technique derived from the principles of Statistical Learning Theory [11]. It is widely employed for modeling and predicting continuous numerical variables, particularly in situations where the relationship between input variables and target outputs is highly nonlinear and complex. Unlike conventional regression approaches that focus primarily on minimizing prediction errors, SVR seeks to achieve a balance between prediction accuracy and model generalization [12], [13]. This characteristic enables the algorithm to perform effectively even when dealing with limited datasets and noisy experimental observations. The fundamental objective of SVR is to identify an optimal functional relationship between a set of input descriptors and a target variable. During the training process, the algorithm learns the underlying patterns embedded within the available data and constructs a predictive model capable of estimating unknown outputs for new observations. Rather than attempting to fit every data point exactly, SVR allows a certain level of tolerance for prediction deviations, thereby reducing sensitivity to experimental uncertainties and preventing over-fitting.

One of the most important strengths of SVR is its ability to handle nonlinear relationships through the use of kernel-based learning. The kernel mechanism enables the algorithm to capture complex interactions among variables without requiring explicit transformation of the original data [14], [15]. As a result, SVR has demonstrated excellent performance in various scientific and engineering applications involving highly nonlinear systems, including materials science, chemical process modeling, energy systems, environmental studies, and nanotechnology. The predictive capability of SVR is strongly influenced by several model hyper-parameters that govern model flexibility, complexity, and tolerance to prediction errors. Appropriate selection of these parameters is essential for achieving optimal performance. Consequently, hyper-parameter optimization is often performed to identify the most suitable model configuration for a given dataset. Another notable feature of SVR is its strong generalization ability. By emphasizing structural risk minimization rather than empirical error minimization, the algorithm reduces the likelihood of memorizing training data and improves its capability to make reliable predictions for previously unseen samples. This makes SVR particularly attractive for scientific applications where experimental data are often limited and expensive to obtain.

In the present study, Support Vector Regression was employed to establish the relationship between the selected descriptors of aluminized explosives and their corresponding velocity of detonation values. The algorithm was trained using experimentally reported data and subsequently validated using independent testing samples. Through its capability to capture complex nonlinear interactions among explosive descriptors, SVR provides an efficient and reliable framework for predicting detonation performance while reducing dependence on laborious and costly experimental investigations.

III. DATA-SET PREPARATION AND COMPUTATIONAL DETAILS

3.1 Hyper-parameter optimization of the SVR model

The predictive performance of Support Vector Regression depends strongly on the appropriate selection of its hyper-parameters. Consequently, a systematic optimization procedure was performed to determine the most suitable values of the model parameters. The effects of the regularization parameter, epsilon-insensitive loss parameter, and kernel-related parameters on the prediction accuracy of the model were carefully investigated [16]. The optimization results revealed that model performance varied significantly with changes in hyper-parameter values. At low parameter settings, the model exhibited under-fitting behavior characterized by poor representation of the nonlinear relationships

between explosive descriptors and detonation velocity. Conversely, excessively large parameter values resulted in over-fitting tendencies, reducing the generalization capability of the model when applied to unseen data. An optimal combination of hyper-parameters was therefore identified, providing the best balance between fitting accuracy and predictive robustness [17]. The optimized SVR model demonstrated stable learning behavior and effective capture of the nonlinear interactions governing the detonation characteristics of aluminized explosives. This observation confirms the suitability of kernel-based learning techniques for modeling complex energetic material systems where conventional linear approaches may be inadequate.

3.2 Prediction performance of the developed SVR model

The predictive capability of the developed model was evaluated using both training and testing datasets. The close agreement observed between predicted and experimental detonation velocities indicates that the SVR framework successfully learned the underlying relationships between explosive descriptors and the corresponding velocity of detonation. The high correlation coefficient obtained during model validation demonstrates the ability of the developed model to accurately reproduce experimental trends across a wide range of explosive formulations. Furthermore, the low prediction errors reflected by the root mean square error and mean absolute error values indicate that the developed framework possesses excellent predictive accuracy and reliability. The superior performance of the model can be attributed to the ability of SVR to efficiently handle nonlinear relationships while maintaining strong generalization characteristics. Unlike traditional empirical formulations that often rely on simplifying assumptions, the machine learning framework directly extracts patterns from experimental data, allowing it to accommodate complex interactions among explosive properties.

3.3 Comparative assessment with existing models

To establish the effectiveness of the proposed approach, the optimized SVR model was compared with three established predictive models frequently used for detonation velocity estimation, namely the BHWS-EOS-full model, BHWS-EOS-partial model, and the Keshavarz model. The comparative analysis based on mean absolute error demonstrates that the SVR model consistently produced lower prediction errors than the conventional models. The BHWS-EOS-full and BHWS-EOS-partial models exhibited moderate predictive capability, while the Keshavarz model showed relatively larger deviations from experimental observations. In contrast, the developed SVR framework achieved the smallest mean absolute error, indicating a higher level of prediction precision. A similar trend was observed when root mean square error was used as the performance metric. The SVR model recorded the lowest root mean square error among all evaluated models, confirming its superior capability in minimizing large prediction deviations. The reduced error magnitude suggests that the proposed machine learning framework can more effectively capture the complex nonlinear dependencies associated with aluminized explosive systems. The comparison based on correlation coefficient further highlights the superiority of the developed model. The SVR approach achieved the highest correlation coefficient, indicating stronger agreement between predicted and experimental values than those produced by the conventional models. This result confirms the robustness and reliability of the machine learning framework for detonation velocity prediction. Overall, the comparative study demonstrates that the proposed SVR model substantially outperforms the BHWS-EOS-full, BHWS-EOS-partial, and Keshavarz models in terms of accuracy, consistency, and generalization capability.

3.4 Influence of non-linear descriptor interaction

The improved predictive performance achieved by the SVR model can be attributed to its ability to capture nonlinear interactions among the physicochemical properties of aluminized explosives. The detonation process is governed by multiple interdependent factors including density, energetic content, oxygen balance, and aluminum concentration. These variables interact in a complex manner that is difficult to describe using traditional analytical or empirical models. By employing nonlinear kernel mapping, the SVR framework effectively transformed the descriptor space into a

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higher-dimensional representation where hidden relationships could be identified more easily. Consequently, the model was able to establish accurate predictive relationships between explosive composition and detonation velocity without requiring explicit assumptions regarding the physical mechanisms involved. The results therefore highlight the significant potential of machine learning techniques for modeling energetic materials, particularly when complex nonlinear behavior limits the applicability of conventional predictive approaches.

3.5 Practical implications of developed framework

The developed SVR-based predictive framework offers several practical advantages for explosive design and performance evaluation. First, it provides a rapid and cost-effective alternative to extensive experimental testing, thereby reducing the time and resources required for explosive characterization. Second, the model can assist researchers and engineers in screening new aluminized explosive formulations prior to experimental synthesis and testing. Furthermore, the framework can serve as a decision-support tool during explosive formulation optimization by enabling rapid estimation of detonation performance under varying compositional conditions. Such capabilities are particularly valuable in military, mining, demolition, and aerospace applications where accurate prediction of explosive characteristics is essential. The demonstrated success of the proposed model also suggests that advanced machine learning techniques can play an increasingly important role in future energetic materials research, facilitating data-driven design, optimization, and discovery of next-generation explosive systems.

IV. RESULTS AND DISCUSSION

This chapter presents the results obtained from the Support Vector Regression (SVR) framework developed for predicting the velocity of detonation of aluminized explosives. Particular emphasis is placed on hyperparameter optimization and model performance evaluation. The influence of the regularization factor, epsilon parameter, and hyperparameter lambda on the predictive accuracy of the developed model is discussed in detail. The effectiveness of the optimized SVR model is subsequently compared with conventional predictive approaches.

4.1. Effect of regularization factor on model performance

Figure 1 illustrates the variation of root mean square error (RMSE) and mean absolute error (MAE) with changes in the regularization factor (C) while maintaining the epsilon parameter at 0.1, kernel parameter at 0.3, and lambda.

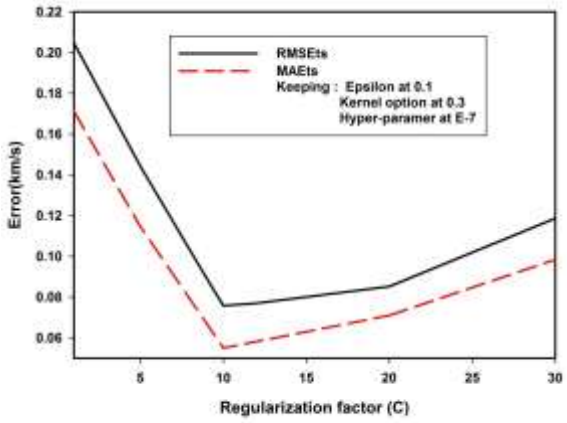

Fig.1: Performance sensitivity of the developed model to regularization factor

The figure reveals that both RMSE and MAE decrease significantly as the regularization factor increases from 1 to 10. The RMSE reduces from approximately 0.205 km/s to about 0.076 km/s, while the MAE decreases from approximately 0.171 km/s to about 0.055 km/s. This behavior indicates that increasing the regularization factor initially improves the learning capability of the SVR model by allowing it to better capture the nonlinear relationships between explosive descriptors and velocity of detonation. However, beyond a regularization factor of 10, both error metrics begin to increase gradually. At higher values of C, the model tends to overfit the training data, leading to deterioration in its generalization performance. The increase in prediction errors observed at C=20C = 20C=20 and C=30C = 30C=30 confirms this tendency. Consequently, a regularization factor of 10 was identified as the optimal value for the developed model. This value provides the best compromise

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between model complexity and predictive accuracy, resulting in minimum RMSE and MAE values.

4.2 Effect of epsilon parameter on model performance

Figure 2 presents the influence of the epsilon parameter on the predictive accuracy of the developed SVR framework. During this investigation, the regularization factor was maintained at 10, while the kernel parameter and lambda values were fixed at 0.3 and 10−710^{-7}10−7, respectively.

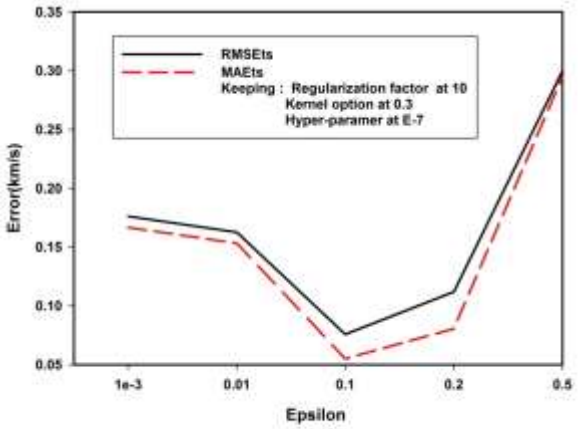

Fig.2: Performance sensitivity of the developed model to epsilon

The figure shows that both RMSE and MAE exhibit a nonlinear dependence on the epsilon parameter. As epsilon increases from 0.001 to 0.1, the prediction errors decrease substantially. The minimum RMSE and MAE values are observed at an epsilon value of 0.1, indicating optimal model performance. The observed reduction in error can be attributed to the ability of the epsilon-insensitive loss function to ignore small deviations and focus on significant patterns in the data. This improves model robustness and reduces sensitivity to experimental noise. However, further increases in epsilon beyond 0.1 result in a noticeable increase in both RMSE and MAE. At epsilon values of 0.2 and 0.5, prediction errors rise considerably because the tolerance region becomes excessively wide, causing important information to be ignored during model training. The results therefore indicate that an epsilon value of 0.1 provides the best balance between noise tolerance and predictive accuracy and was consequently selected for the final SVR model.

4.3 Effect of hyper-parameter lambda on model performance

Figure 3 shows the influence of hyperparameter lambda on the predictive capability of the developed SVR model. During this analysis, the regularization factor and epsilon parameter were fixed at 10 and 0.1, respectively, while the kernel parameter was maintained at 0.3.

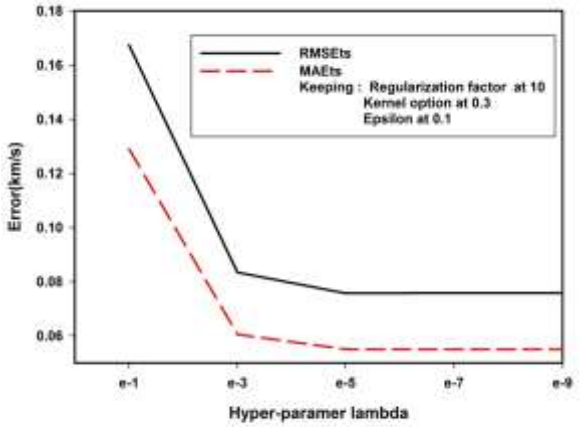

Fig.3: Performance sensitivity of the developed model to hyper-parameter lambda

The RMSE decreases from approximately 0.168 km/s to about 0.076 km/s, while the MAE decreases from approximately 0.129 km/s to about 0.055 km/s. The substantial reduction in error demonstrates the importance of lambda optimization in enhancing model accuracy. Smaller lambda values improve the flexibility of the regression function and enable the model to capture subtle nonlinear interactions among explosive descriptors. Beyond 10−5, the RMSE and MAE values remain essentially constant, indicating that further reductions in lambda provide negligible improvements in prediction accuracy. This plateau suggests that the model has reached its optimum learning capacity. Based on these observations, a lambda value of 10−710^{-7}10−7 was selected for subsequent model development because it yields minimum prediction errors while maintaining numerical stability.

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4.4 Comparative evaluation of predictive models using absolute error

Figure 4 compares the mean absolute error values generated by the developed SVR model and three existing predictive approaches

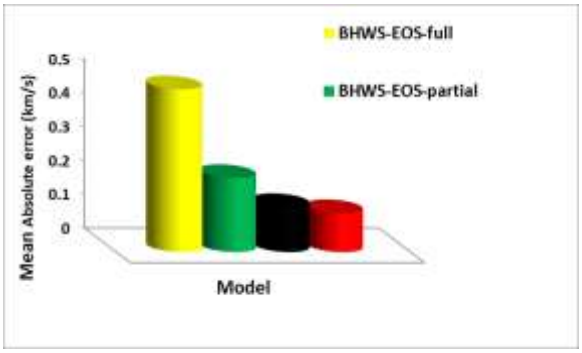

Figure 4. Comparison of mean absolute error obtained using BHWS-EOS-full, BHWS-EOS-partial, Keshavarz, and SVR-based models.

The figure clearly shows that the SVR-based model produces the lowest mean absolute error among all investigated models. This demonstrates its superior capability in accurately predicting the velocity of detonation of aluminized explosives. The BHWS-EOS-full model exhibits lower prediction errors than the BHWS-EOS-partial and Keshavarz models, indicating the importance of incorporating complete thermodynamic information into predictive calculations. However, all conventional approaches produce larger prediction errors than the developed machine learning framework. The improved performance of the SVR model can be attributed to its ability to learn nonlinear relationships directly from experimental data without relying on simplifying physical assumptions.

4.5 Comparative evaluation of predictive models using root mean square error

Figure 5 presents a comparison of the root mean square error values obtained from the different predictive approaches.

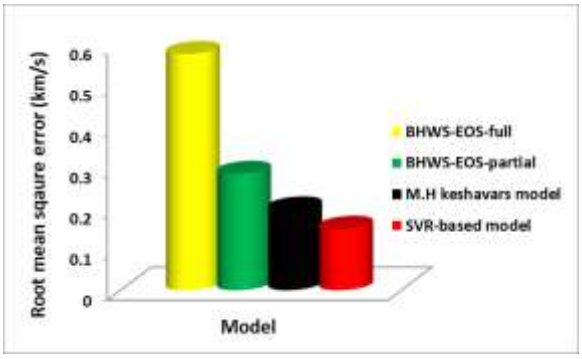

Figure 5. Comparison of root mean square error obtained using BHWS-EOS-full, BHWS-EOS-partial, Keshavarz, and SVR-based models.

The developed SVR model demonstrates the lowest RMSE value, indicating superior prediction accuracy and improved capability for minimizing large prediction deviations. Since RMSE places greater emphasis on larger errors, the low value obtained by the SVR framework confirms its robustness and reliability. The BHWS-EOS-full model exhibits the second-best performance, followed by the BHWS-EOS-partial model, while the Keshavarz model records the highest RMSE value among the investigated approaches. These observations further confirm that machine learning techniques can provide more accurate predictions than traditional empirical and equation-of-state-based models for complex energetic material systems.

4.6 Comparative evaluation of predictive models using root mean square error

Figure 6 compares the correlation coefficients achieved by the investigated predictive models.

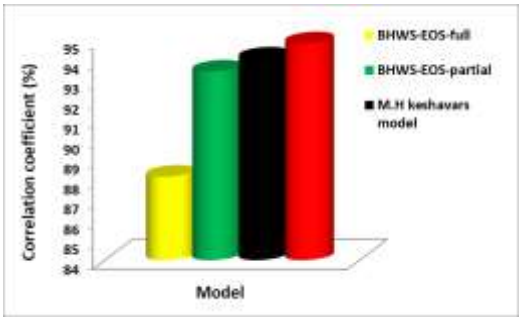

Figure 6. Comparison of correlation coefficient values obtained using BHWS-EOS-full, BHWS-EOS-partial, Keshavarz, and SVR-based models.

The SVR-based framework exhibits the highest correlation coefficient, demonstrating the strongest agreement between predicted and experimental velocity of detonation values. This result confirms the excellent generalization capability of the developed model. Although the BHWS-EOS-full and BHWS-EOS-partial models also produce reasonably high correlation coefficients, their performance remains inferior to that of the SVR framework. The Keshavarz model exhibits the lowest correlation coefficient, indicating weaker predictive consistency. The high correlation coefficient achieved by the developed model demonstrates that the selected explosive descriptors successfully capture the underlying factors governing detonation behavior and that the optimized SVR framework effectively extracts these relationships.

V. CONCLUSIONS

This study successfully developed a Support Vector Regression (SVR)-based computational framework for predicting the velocity of detonation of aluminized explosives. The increasing complexity associated with experimental characterization of energetic materials, coupled with the nonlinear relationships existing among explosive descriptors, necessitates the development of reliable data-driven predictive tools. The proposed machine learning approach was therefore employed to establish accurate functional relationships between selected explosive descriptors and the corresponding velocity of detonation. A systematic hyperparameter optimization strategy was implemented to enhance the predictive capability of the developed model. The effects of the regularization factor, epsilon parameter, and hyperparameter lambda were carefully investigated. The optimization process resulted in significant improvements in model performance by minimizing prediction errors and enhancing generalization capability. The optimum hyperparameter combination produced the lowest root mean square error and mean absolute error values while maintaining excellent agreement with experimental observations. Comparative evaluation of the developed model against established predictive approaches, namely the BHWS-EOS-full model, BHWS-EOS-partial model, and Keshavarz model, demonstrated the superiority of the proposed framework. The SVR model consistently achieved lower prediction errors and higher correlation coefficients than the conventional approaches. These results confirm that machine learning techniques possess greater capability for capturing the complex nonlinear interactions that govern detonation behavior in aluminized explosives. The developed framework offers a practical alternative to labor-intensive and costly experimental investigations. By providing rapid and reliable predictions of detonation velocity, the model can facilitate explosive formulation design, performance evaluation, and optimization. The study therefore demonstrates the significant potential of artificial intelligence and machine learning methodologies in advancing energetic materials research and development.

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