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Application of deep learning for predicting ignition delay in hydrogen combustion engines

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ABSTRACT

This study investigates the use of deep learning techniques to forecast ignition delays in hydrogen combustion systems, with a focus on optimizing hydrogen combustion processes in industrial applications such as stationary power generation and the automotive industry. The work utilizes experimental data from a rapid compression machine (RCM) and a shock tube. Two large datasets were created through 0-D simulations and experimental measurements, covering a wide range of conditions. The study involves the development of two artificial neural network (ANN) models, one for RCM and another for shock tube data, each with distinct architectures. The ANN models were trained, tested, and evaluated using thoughtfully divided datasets. The results demonstrate the effectiveness of the developed ANN models in predicting ignition delays with remarkable accuracy. Comparative analyses with 0-D simulations and experimental measurements reveal that the ANN models predict ignition delays "1000 times faster" than traditional simulation methods. This speed improvement is crucial for real-time industrial applications, allowing engineers to quickly optimize combustion parameters, adjust engine settings, and make operational decisions in a fraction of the time. The study highlights the potential of these ANN models to optimize hydrogen combustion processes, improving combustion efficiency, reducing operational costs, and enhancing resource utilization in industrial settings. This progress can play a significant role in optimizing hydrogen-powered internal combustion engines by increasing fuel efficiency, reducing emissions, and enhancing overall engine performance. In the automotive and power generation sectors, the quick predictive abilities of ANN models can support more effective energy production, decrease operational expenses, and lessen environmental harm.

1. Introduction

Hydrogen combustion holds significant importance within the realm of alternative energy sources and environmental sustainability. As a zero-carbon emission fuel, hydrogen can generate substantial amount of energy by reacting with oxygen to produce water vapor as its primary emission, thus avoiding the release of greenhouse gases and hydrocarbon pollutants associated with traditional

fossil fuels, making it the most promising candidate for zero-carbon emission future for various applications, including but not limited to stationary power and heat generation [1], transportation [2], and aerospace [3]. Zoldak et. al [4], [5] have demonstrated the benefits of hydrogen combustion in a 1 L boosted opposed-piston four stroke (OP4S) engine. When combined with the Copius intake manifold boost and direct injection of hydrogen. Their lean burn process showed up to 39% brake thermal efficiency.

Hydrogen combustion presents a critical strategy for both energy warehousing [6] and power grid efficiency enhancements [7]. It enables smoother incorporation of renewable energies by establishing a dependable method for stockpiling surplus power during peak production, and subsequently releasing it to meet high demand periods [8]–[14]. Consequently, harnessing hydrogen combustion not only mitigates ecological impact but also fosters the advancement of a more enduring and resilient energy infrastructure.

The time lag preceding combustion, known as ignition delay, is a fundamental metric for analyzing and refining burn sequences in diverse applications. Its significance stems from its immediate impact on combustion efficacy, pollutant generation, and the overall operational effectiveness of combustion systems. The precise determination of ignition delay is context-dependent. However, a prevalent interpretation defines it as the interval between the end of compression and the point of peak pressure rise, as illustrated in Fig. 1. This definition is particularly relevant for compression-ignition engines. Complex chemical reactions can also lead to the observation of multiple ignition delays within a single combustion event. For example, Fig. 1 demonstrates two distinct ignition delays during the combustion of an n-heptane/oxygen/nitrogen blend within a rapid compression apparatus (RCM), under conditions of 13.5 bar compressed gas pressure and 633 K. Due to n-heptane's zero octane rating, it displays a heightened sensitivity to shifts in temperature and pressure during combustion, potentially leading to several sequential ignition phase.

A shorter ignition delay is generally desirable as it leads to more rapid and controlled combustion, improving fuel efficiency and reducing emissions. Therefore, studying and manipulating ignition delay is essential for enhancing combustion technologies, optimizing engine performance, and addressing environmental concerns associated with combustion. The minimal paragraph in the introduction is three paragraphs.

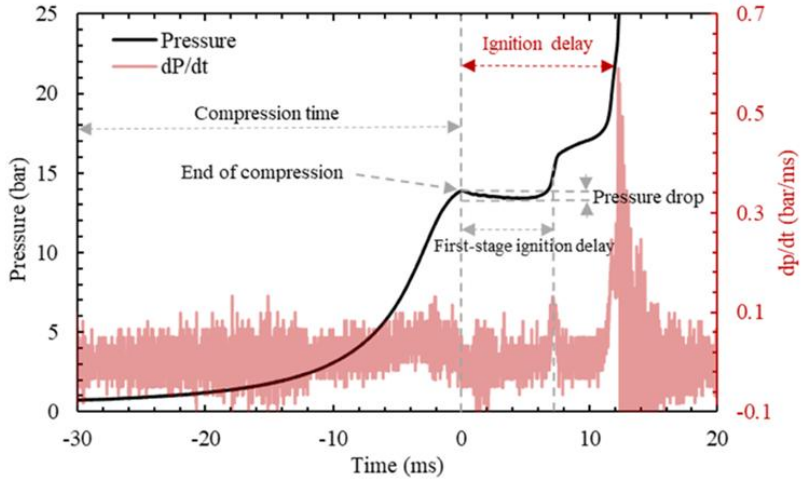

Fig. 1. The pressure profile and pressure gradient of an n-heptane/oxygen/nitrogen mixture at a compressed gas pressure of 13.5 bar and a temperature of 633 K are shown in [15]

An RCM is a specialized experimental apparatus designed for investigating the combustion characteristics and autoignition behaviors of fuels under controlled and highly dynamic conditions. It is useful, particularly for studying the ignition delay, chemical kinetics, and combustion kinetics of various fuels. The RCM typically consists of a high-speed piston-driven compression chamber, allowing to precisely control the compression process and simulate the extreme conditions

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encountered in internal combustion engines. On the other hand, a shock tube has similar capabilities as the RCM but with different designs. A shock tube is a long, narrow tube separated into two sections by a diaphragm. It allows for the generation of shock waves with precise control over their characteristics. The process involves sudden rupture of the diaphragm, causing a high-pressure shock wave to propagate through one section and interact with the lower-pressure gas in the other.

Wagh et al. [16] have performed a simulation-based study on gasoline compression ignition engines and predicting ignition delays using surrogate fuel model of gasoline and have found good agreement with experimental production, however, have observed that the simulation takes over 10 hours to complete for a 1L constant volume chamber model.

Villenave et al. [17] recently conducted an investigation into the time lapse before combustion initiation in extremely diluted hydrogen blends, utilizing empirical techniques. This research spanned a range of post-compression gas temperatures, specifically from 900 to 1030 K, and pressures between 20 and 60 bar. The stoichiometric ratio of the mixtures varied from 0.2 to 0.5. Concurrently, they attempted to replicate the ignition delay through the application of intricate chemical kinetic models. The results demonstrated a high degree of correlation between the experimentally determined ignition delays and those forecasted by simplified, spatially uniform simulations.

Pochet et al. [18] conducted experiments to explore the impact of adding hydrogen to ammonia on ignition behavior in a rapid compression machine (RCM). The tests were performed at gas temperatures of 1000 to 1100 K and pressures between 43 and 65 bar. Their findings revealed that when hydrogen content exceeded 10% by volume, the ignition delays were significantly shortened, enhancing the ignition process. However, their zero-dimensional (0-D) simulation results showed that most of the reaction mechanisms could not accurately replicate the experimental ignition delays.

Pavlov et al. [19] examined hydrogen/argon combustion in a shock tube, covering temperatures of 870–2500 K, pressures of 0.5–1.5 atm, and equivalence ratios from 0.1 to 2.0. Using a detailed kinetic model, they established a relationship between ignition delay and temperature, demonstrating that partial pressure within the stoichiometric portion effectively characterizes ignition, especially at high temperatures. However, at lower temperatures, experimental data deviated from predictions, shifting with pressure increases. They also noted challenges in accurately measuring ignition delay in this range due to interference from the contact surface between driver and test gases.

An analysis of the uneven onset of combustion in hydrogen and n-heptane mixtures, conducted by Huang et al. [20] using a shock tube, incorporated both low-temperature chemical reactions and practical, non-ideal conditions. In contrast to idealized laboratory settings, the emergence of non-uniform ignition is attributed to phenomena such as the expansion of the boundary layer and its interaction with the reflected shock wave. Even when these factors are disregarded, variations in ignition delay across different locations are still observable. Their findings revealed that the time preceding ignition was significantly affected by the proximity to the terminal wall, exhibiting a distinct linear trend. Consequently, they developed a predictive model to characterize these variations, thereby contributing to a more precise understanding of ignition delay dynamics.

Artificial Neural Networks (ANNs) have emerged in recent years as powerful tools in engineering applications, offering versatile solutions to complex problems. In engineering, ANNs find extensive use in tasks such as pattern recognition, system modeling, optimization, and control. Their ability to adapt and learn from data enables ANNs to capture intricate relationships within large datasets, making them particularly valuable in scenarios where traditional analytical methods may fall short. ANNs excel in nonlinear mapping, enabling accurate predictions and classifications in diverse engineering domains. The benefits of employing ANNs in engineering include enhanced modeling accuracy, improved decision-making capabilities, and the ability to handle multidimensional and dynamic systems, as well as reduced computational resources.

In a notable study, to forecast ignition delay for n-butane/hydrogen blends within a rapid compression machine (RCM), Cui et al. [21] developed a back-propagation artificial neural network (ANN) model. While they employed a genetic algorithm (GA) for model optimization, the model's

predictive accuracy was compromised by insufficient training data, resulting in underestimated ignition delay values.

Huang et al. [22] developed an ANN model to predict the ignition delay of a Jet A-1/hydrogen mixture under temperatures of 800–1600 K and pressures of 1–20 bar. Using a dataset of 104,000 samples generated with the HyChem mechanism and Cantera, the model achieved a mean relative error of 1.04% but showed local errors up to 10% for short delays. The ANN method was about 1000 times faster than conventional 0-D simulations.

Sakleshpur Nagaraja and Sarathy [23] created an ANN model with 13 inputs and three hidden layers to predict ignition delay time (IDT) for various natural gas blends. Trained with back-propagation, it proved more accurate than linear regression and successfully predicted IDTs in shock tube experiments for both LNG and commercial natural gas mixtures, demonstrating its applicability to real-world combustion systems.

Sharma et al. [24] investigated the application of machine learning for predicting autoignition and ignition delay time in microscale supercritical water oxidation, a technique considered for waste management in space expeditions. The study aimed to identify operating conditions for hydrothermal flame formation while addressing the challenges of scaling from ground-based setups. Homogeneous ignition calculations were used to develop classification models for autoignition prediction and regression models for ignition delay estimation. A two-step approach was introduced for ignition delay prediction, and the broader application of machine learning in optimizing microreactor design was demonstrated, highlighting its potential beyond mere prediction.

Shejan et al. [25] applied machine learning (ML) techniques to model turbulent combustion, focusing on plasma-assisted ignition. They used Decision Trees (DT) and Random Forests (RF) models to predict the spatio-temporal evolution of ignition kernels based on ionization levels. Trained and validated with Direct Numerical Simulation (DNS) data, the ML models accurately predicted ignition kernel profiles, demonstrating their potential to reduce computational costs while maintaining accuracy in complex combustion systems. This research underscores ML's value in advancing turbulent combustion modeling.

Gerard, Benjamin [26] developed machine learning (ML) models to predict ignition delay times (IDT) for common fuels, addressing the computational expense of traditional combustion simulations. Recognizing IDT as a crucial combustion property, the project aimed to create efficient prediction tools. Using Ansys Chemkin, IDT simulations were performed for hydrogen, jet fuel, and gasoline surrogate mixtures. Subsequently, ML models were constructed in R, incorporating initial composition, temperature, and pressure as input parameters. The models were then validated against new simulated data. The resulting ML models accurately captured the complex relationship between IDT and thermodynamic conditions, demonstrating their effectiveness in providing rapid and cost-effective IDT predictions

Bounaceur et al. [27] created an AI-based tool to predict auto-ignition for hydrogen-compatible gas turbines, aiming to reduce computational costs. The tool was trained on a dataset of over 70,000 ignition delay times (IDTs) generated from a detailed kinetic model, covering various operating conditions and fuel compositions. The AI model achieved a correlation coefficient above 99.91% and a mean absolute error (MAE) of 0.03. While it performed well across various conditions, its accuracy decreased with higher alkane content in natural gas.

MacArt [28] applied a variational data assimilation approach to improve the accuracy of predictive ignition delay calculations by integrating higher-fidelity data into reduced-fidelity models. The method was tested on a one-dimensional Navier-Stokes model of shock-tube experiments for ethylene-air autoignition at subatmospheric pressures. Optimization was performed on an eight-species, three-step chemical-kinetic model to match predictions from a more detailed 23-species, 66-reaction model. Using minibatch gradient descent, the study assessed the impact of optimization time windows on predictive accuracy. The findings highlight the potential of machine learning-augmented kinetics for improving ignition delay predictions while reducing computational costs.

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Artificial neural networks (ANNs) have proven valuable in combustion modeling, as demonstrated by Araujo et al. [29] and Huang et al. [30]. Araujo's work, focusing on internal combustion engines, revealed that increased activation energy correlates with prolonged ignition delays, while higher rate constants enhance combustion efficiency. In a separate study, Huang et al. employed ANNs to optimize the reaction mechanism for ammonia/methane combustion in gas turbines. This optimization not only improved the accuracy of predicting ignition delay, flame speed, and NOX emissions, but also significantly increased computational efficiency.

Yang et al. [31] developed a transfer learning-based neural network approach to predict ignition delays for hydrocarbon fuels (C1–C4). They trained ANN and GCN models using a large dataset and applied transfer learning to merge models for smaller molecules (C1–C3) to predict delays for larger molecules (C4). The approach showed high accuracy and robustness, particularly for fuels with limited experimental data.

The objective of this work is to discover the application of the emerging deep learning methods in hydrogen combustion ignition delay parameter. To this end, experimental data from two studies on hydrogen combustion in an RCM and a shock tube will be used to build two large databases of ignition delays. In this scenario, many 0-D simulations will be performed to ensure that the databases include enough data points for model training purposes. In the next step, two ANN models with different architectures will be developed to predict ignition delays in RCM and shock tube. The ANN models will first be trained and evaluated. Then, the predicted ignition delays will be compared with the simulated and measured results.

In this study, we explore the application of deep learning methods for predicting ignition delays in hydrogen combustion. Two distinct artificial neural network (ANN) models are developed for data collected from the rapid compression machine (RCM) and the shock tube, demonstrating their effectiveness in accurately predicting ignition delays. The research contributions are:

- The development of accurate and efficient predictive models using deep learning: We show that ANN models can accurately predict ignition delays in hydrogen combustion, achieving at least a 1000x speedup compared to traditional simulation methods.
- A methodology combining experimental measurements and 0-D simulations for robust model training: We highlight the importance of using both experimental data and 0-D simulations to train neural networks effectively, especially when dealing with labor-intensive and costly experimental measurements.
- A comparative analysis of ANN-predicted ignition delays with 0-D simulations and experimental measurements, emphasizing the capability of ANN models to expedite predictions.
- An exploration of the potential of ANN models to improve the accuracy and prediction of hydrogen ignition delay in small and large hydrogen engines for stationary and automotive industries

2. Method

Two sets of experimental data on the ignition delay measurement of hydrogen mixtures by Villenave et al. [17] for RCM and Hashemi et al. [32] for shock tube were utilized in this paper. Table 1 shows the mixture composition, testing conditions and the databases extracted from these studies. Fig. 2 demonstrates the distribution of the RCM and shock tube measured ignition delays. Both measurements show a long tail distribution profile in which most data are concentrated in the short ignition area. More than 80% of RCM-measured data are shorter than 100 ms. In the same way, more than more than 80% of shock tube-measured data are shorter than 50 µs. In this condition, the model training will be difficult. On the other hand, the number of measured data points is incredibly less than the required data. Therefore, 0-D simulations can be utilized to generate a large dataset for model training purposes.

Table 1. mixture composition, testing conditions and the experimental databases used in this study

Setup	Mixture composition (molar basis percentage				Equivalence Ratio	Pressure (bar)	Temperature (K)	Number of data points
	H_2	O_2	N_2	Ar				
RCM [23]	7.75	19.40	72.85	0.00	0.2	20 - 60	940- 1030	112
	11.20	18.70	70.10	0.00	0.3			
	14.40	18.00	67.60	0.00	0.4			
	17.40	17.40	65.20	0.00	0.5			
Shock Tube [17]	3.47	3.47	0.00	93.06	0.5	0.1-100	1300-1400	50

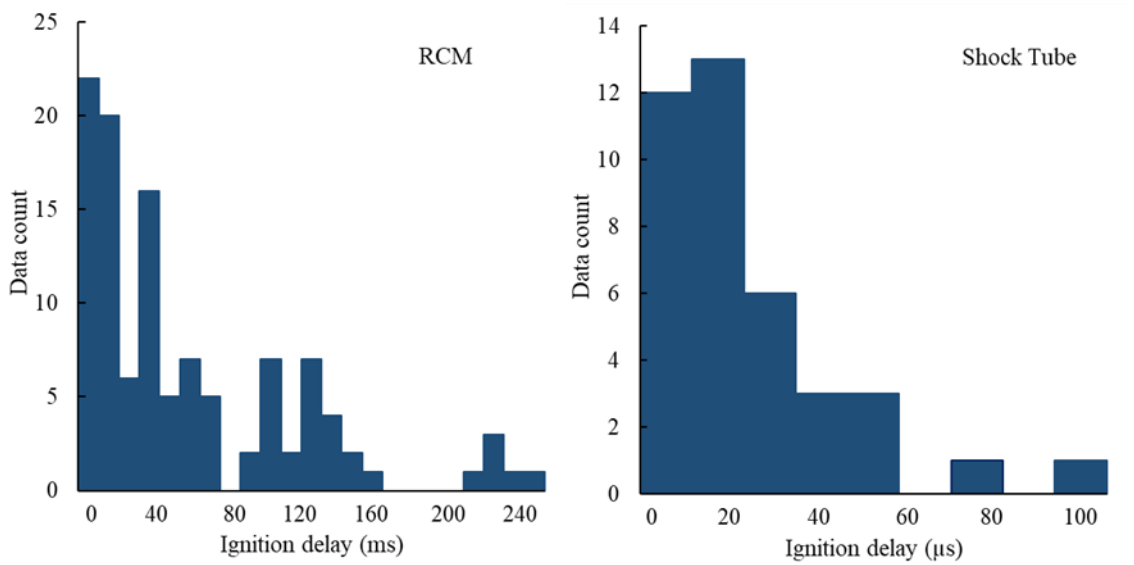

Fig. 2. Long tail distribution of measured ignition delays in RCM and shock tube. Data taken from Villenave et al. [17] for RCM and Hashemi et al. [32]

2.1. Numerical Method

A series of 0-D simulations for lean hydrogen mixtures were conducted using ANSYS Chemkin 17.0 [33] with a homogeneous batch reactor under specific compressed gas temperature and pressure conditions. The detailed hydrogen mechanism by Burke et al. [34] was used for simulating RCM-measured ignition delays, while Conaire et al.'s [35] hydrogen mechanism was applied for shock tube-measured ignition delays. These mechanisms provided good accuracy in simulating ignition delays, particularly for temperatures between 940 to 1020 K in RCM data and pressures between 10 to 100 bar in shock tube data. The results of these simulations will be discussed in section 3.1.

2.2. Dataset construction

To create a suitable dataset for model training, 0-D simulations were performed for RCM data at compressed gas temperatures of 940 to 1020 K and pressures of 20-60 bar. Additionally, another dataset was generated using 0-D simulations at compressed gas temperatures of 1300-1400 K and pressures of 10-100 bar for shock tube data. The shock tube dataset includes two feature channels of pressure and temperature, while the RCM dataset involves five feature channels of pressure, temperature, hydrogen, oxygen, and nitrogen mole percentages. The number of feature channels in these two datasets is different because the equivalence ratio does not change in the shock tube data, while it changes in the range of 0.2 to 0.5 for the RCM data. The RCM and shock tube datasets include 7544 and 9191 data points, respectively. Fig. 3 presents the data distribution of the simulated ignition delays in RCM and shock tube. Both datasets inclined to the left which remarks that the model training will be difficult. In addition, the developed model will probably be more accurate in predicting the shorter ignition delays since there is more data available to use in the model training process.

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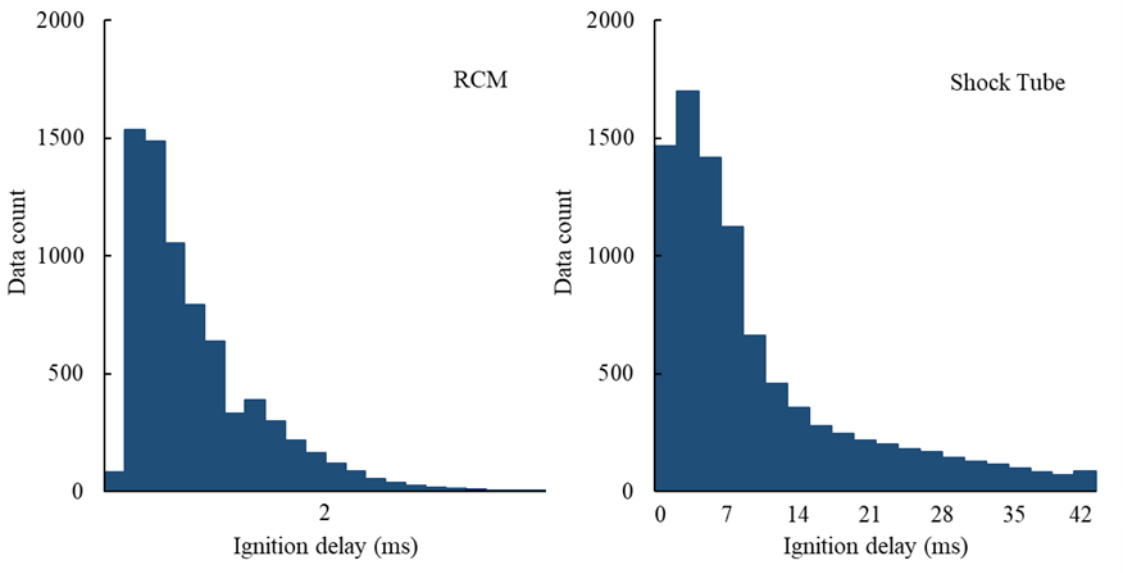

Fig. 3. Distribution of simulated ignition delays in RCM and shock tube

2.3. Artificial Neural Network

Two ANNs were built to predict hydrogen ignition delay in RCM and shock tube experiments [12]–[14], [25], [31], [33], [36]. The RCM model used four layers, with five inputs: pressure, temperature, and hydrogen, oxygen, and nitrogen mole percentages. The first and second hidden layers of the model contain 8 and 16 neurons, respectively, with the predicted RCM ignition delay as the sole feature (response) in the output layer. Fig. 4 illustrates the architecture of the developed ANN model for the RCM data.

The developed ANN model for the shock tube data also includes four layers, while the input layer has only two neurons of compressed pressure and temperature since the equivalence ratio does not change in the dataset built for shock tube. This ANN model has 5 and 9 neurons in the first and second hidden layer, respectively (Fig. 5).

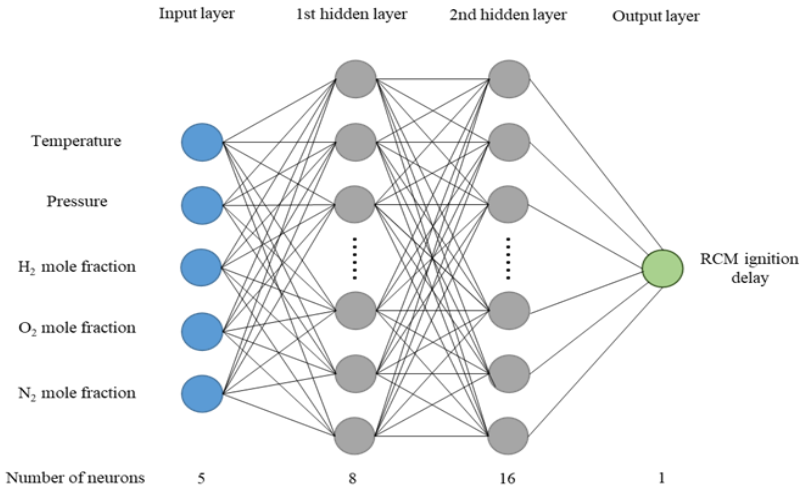

Fig. 4. The architecture of the developed ANN model to predict ignition delay in RCM

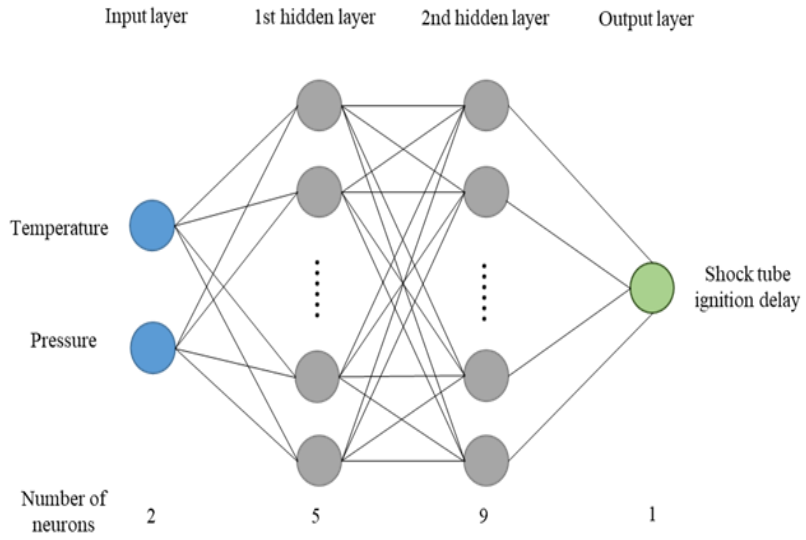

Fig. 5. The architecture of the developed ANN model to predict ignition delay in shock tube

Using the open-source machine learning platform TensorFlow 2.4.1 [37], implemented within Python, a range of artificial neural network (ANN) architectures, varying in both breadth and depth, were constructed and evaluated. While all demonstrated similar levels of predictive precision, a streamlined network configuration, characterized by a reduced neuron count but maintained high accuracy, was selected for implementation. More intricate network designs were excluded to prevent potential issues related to prolonged training durations and model overfitting. Table 2 provides a detailed overview of the ANN models developed. Each layer, with the exception of the input layer, is classified as a dense layer, also known as a fully connected layer. In these layers, every neuron is interconnected with all neurons in the preceding and subsequent layers. The output of each neuron within a dense layer is derived by calculating a weighted summation of the inputs, which are the outputs from the preceding layer, followed by the application of an activation function. Activation functions, including sigmoid, tanh, and ReLU, introduce non-linear transformations into the neural network, enabling the model to learn complex relationships within the data. ReLU, a function frequently employed in regression tasks, outputs the input value directly when positive, and zero otherwise.

$$ReLU(x) = \max(0.x) \quad (1)$$

Table 2. Summary of the developed ANN models in this study

Setup	Mixture composition (molar basis percentage				Equivalence Ratio	Pressure (bar)	Temperature (K)	Number of data points
	H_2	O_2	N_2	Ar				
RCM [23]	7.75	19.40	72.85	0.00	0.2	20 - 60	940- 1030	112
	11.20	18.70	70.10	0.00	0.3			
	14.40	18.00	67.60	0.00	0.4			
	17.40	17.40	65.20	0.00	0.5			
Shock Tube [17]	3.47	3.47	0.00	93.06	0.5	0.1-100	1300-1400	50

Before training each model, 10% of each dataset has been selected randomly, removed for the data and saved as another dataset to evaluate the performance of each ANN model in predicting

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ignition delays. The reason for this is to ensure that the developed ANN models are not getting evaluated with the same dataset which was used for training. The reason behind the randomness of the selection is to avoid any kind of biases in the model evaluation procedure. The remaining data points then have been divided to two different datasets by ratio of 80% for training and 20% for testing. It should be noted that testing was performed by the developed ANN models to calculate the model metrics, while the evaluation was conducted by the authors to compare the ANN predictions with the simulated ignition delays.

There are several network metrics for neural networks. In this study, mean square error (MSE) was selected as a loss function. MSE can be defined as.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad (2)$$

In this equation, y_i and $\hat{y}_i$ are simulated and predicted ignition delays of the i-th data point, respectively. n also represents the number of data points. The mean absolute error (MAE) also was selected to ensure network accuracy. Obviously, lower MSE and MAE values indicate better predictive performance.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (3)$$

To minimize the loss function during training, the Adam (Adaptive Moment Estimation) optimizer was used to adjust the ANN's weights and biases

The training process requires careful execution with key hyperparameters like epochs, batch size, and learning rate. An epoch is one complete pass through the dataset, and 100 epochs were used in this study. Training continues through all epochs until the loss function no longer decreases, indicating convergence.

Training with too few epochs may cause underfitting, while too many can lead to overfitting. Early stopping helps prevent overfitting by halting training when performance on a validation set stops improving. Batch size refers to the number of data points used in each training cycle, such as 100 data points per epoch.

The learning rate controls the step size during optimization and affects how quickly the neural network converges to an optimal solution. Initially, larger learning rates and batch sizes are used, with continuous monitoring of the loss. Once convergence is reached, both the learning rate and batch size are gradually reduced to fine-tune the convergence.

While achieving a minimal loss metric is a primary objective, it's imperative to avert model over-specialization. To gauge the potential for overfitting within the neural framework, one must examine the loss metric observed on the validation dataset. A cessation in the loss's downward trajectory, followed by an upward trend during training, signals the onset of overfitting. As an illustration, the initial model constructed for the RCM data employed a complex design, incorporating 64 and 128 neurons within its first and second hidden layers, respectively. This configuration yielded highly effective training, reducing the loss to 0.0059 and achieving a Mean Absolute Error (MAE) of 0.0576. The average deviation in predicted ignition delays was a mere 0.78%, suggesting an exceptionally well-trained ANN. However, this sophisticated architecture was subsequently replaced by a significantly simplified model, featuring only 8 and 16 neurons in its respective hidden layers. The reason was the overfitting experienced for the more complex developed model. Fig. 6 shows the loss variation during the training for the simple (optimized) and complex (non-optimized) models. One can see that the loss value of the non-optimized model decreased abruptly to a small value and then started to fluctuate. This is evidence of an overfitting issue. In contrast, the loss value in the simpler model (which is labeled as the optimized model) decreases during training and settles down to an acceptable low value. The MAE, loss, and average error for the selected optimized model are 0.2445, 0.1138, and 2.76%, respectively.

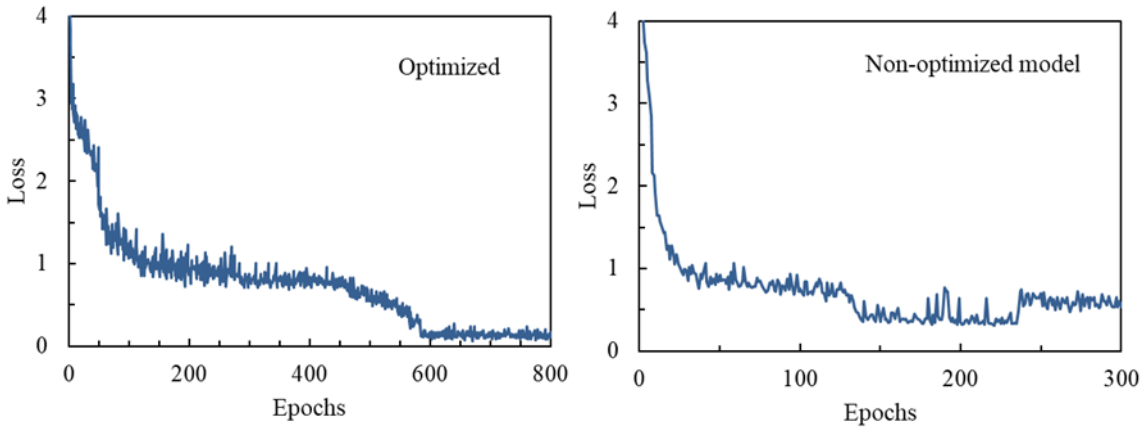

Fig. 6. The loss variation during training for optimized and non-optimized ANN models

3. Results and Discussion

The results of ignition delay simulation, prediction, and the comparison with the measured data will be presented and discussed for RCM and shock tube, separately:

3.1. Ignition delay simulation

Fig. 7 illustrates the comparative analysis between spatially uniform (0-D) modeled and empirically derived ignition delay values for a hydrogen blend, characterized by a 0.4 equivalence ratio, within a Rapid Compression Machine (RCM) across compression pressures of 20, 30, 40, and 60 bar. The experimental data points are represented by circular markers, while the corresponding simulation results are depicted by continuous lines. Consistent with established principles, both the modeled and measured ignition delays exhibit a reduction in duration with increasing pressure and temperature. The computational methodology demonstrated a strong capacity to replicate the observed ignition delay phenomena. However, the fidelity of the simulation diminishes at compressed temperatures exceeding 1020 K, leading to a divergence between the simulated and measured values beyond the designated blue region. Consequently, a selective subset of the simulation data was employed for model training, validation, and performance assessment.

The same trend was observed when the compressed pressure in an RCM is constant at 30 bar and the equivalence ratio varies, which is shown in Fig. 8. At the same compressed temperature, the leaner (lower equivalence ratio) mixture yields the longer ignition delay due to the lower ratio of fuel to the oxidizer/diluent. The numerical method also was able to mimic this effect.

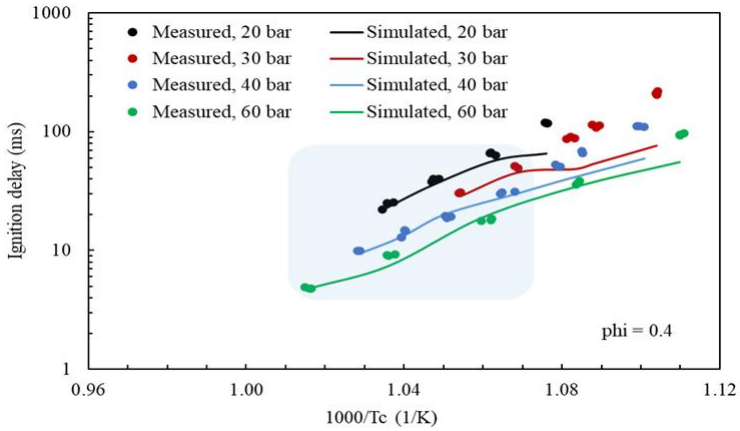

Fig. 7. Comparison of simulated and measured ignition delays of hydrogen mixture at equivalence ratio of 0.4 in an RCM [17]

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The comparison of the simulated and measured ignition delays at two compressed temperatures of 1300 K and 1400 K and different compressed pressures in a shock tube is shown in Fig. 9. As anticipated, a higher compressed temperature yields shorter ignition delay times. The ignition delays are also shorter at higher pressure except for the compressed pressure range of 50 to 100 bar. In this region, any pressure rise leads to a longer ignition delay. This odd trend is explained very well by Hashemi et al. [32]. The numerical method was able to mimic these trends accurately in the pressure range of 20 to 100 bar.

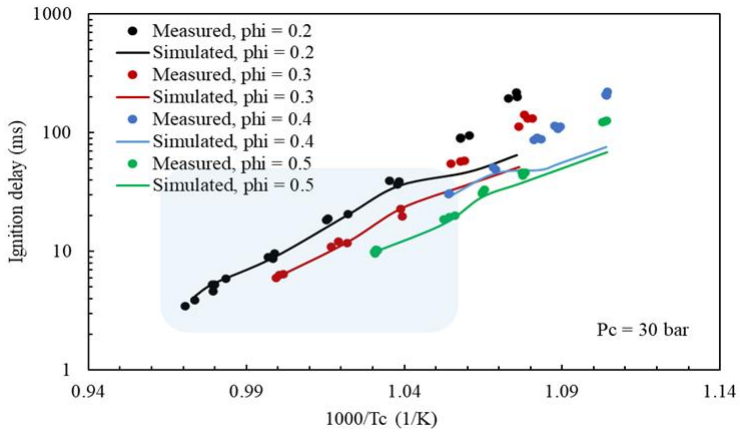

Fig. 8. Comparison of simulated and measured ignition delays of hydrogen mixtures at a compressed pressure of 30 bar and different equivalence ratios in an RCM. [17]

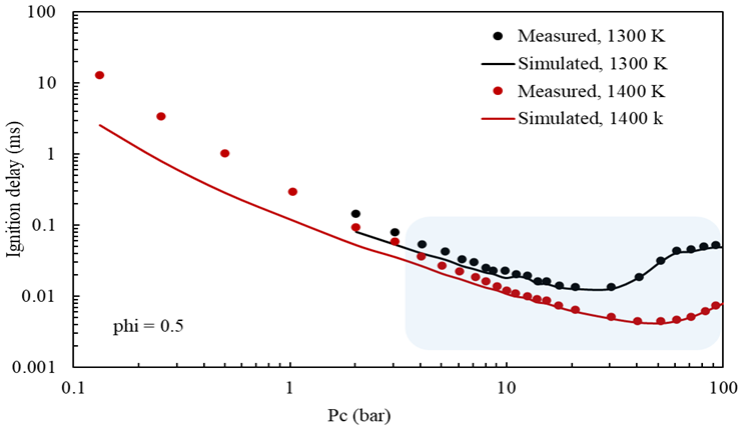

Fig. 9. comparison of simulated and measured ignition delays for a hydrogen mixture at an equivalence ratio of 0.5 and compressed temperatures of 1300 K and 1400 K in a shock tube is presented in [23]

3.2. Ignition delay prediction

Fig. 10 presents the ignition delay durations estimated by the Artificial Neural Network (ANN) model for hydrogen-based mixtures within the Rapid Compression Machine (RCM). These estimations are showcased at a consistent compressed pressure of 20 bar, encompassing a spectrum of equivalence ratios, and juxtaposed against the respective simulation outputs. A notable increase in predicted ignition delay times is observed at elevated equivalence ratios, a pattern consistent with empirical observations (Fig. 8). The underlying chemical kinetics are effectively represented, as evidenced by the minimal disparity between the predicted and simulated ignition delay values. Nonetheless, a significant deviation emerges at compressed temperatures below 970 K. A parallel trend is discernible in Fig. 11, which displays the results at a compressed pressure of 20 bar. Similarly, Fig. 12 illustrates the ANN-generated and simulated RCM ignition delay times at an equivalence ratio of 0.5, across varying compressed pressures. As anticipated, an inverse relationship exists between compressed pressure and ignition delay duration. This was also observed in the

measurement (Fig.7). Again, the numerical method was able to mimic the simulated ignition behavior, accurately.

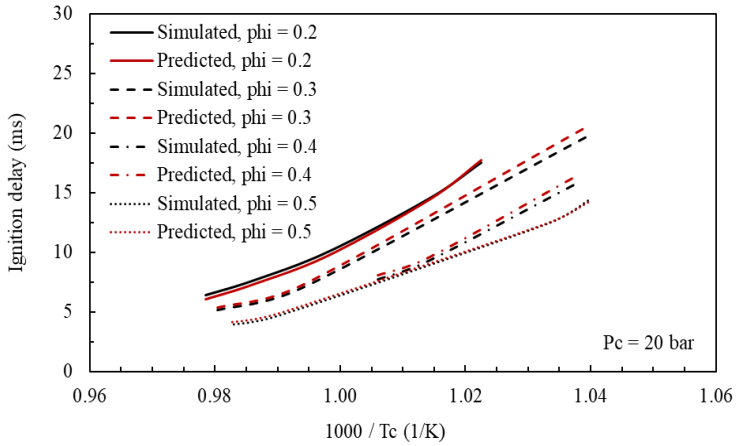

Fig. 10. Predicted and simulated ignition delays in the RCM at compressed pressure of 20 bar and different equivalence ratio

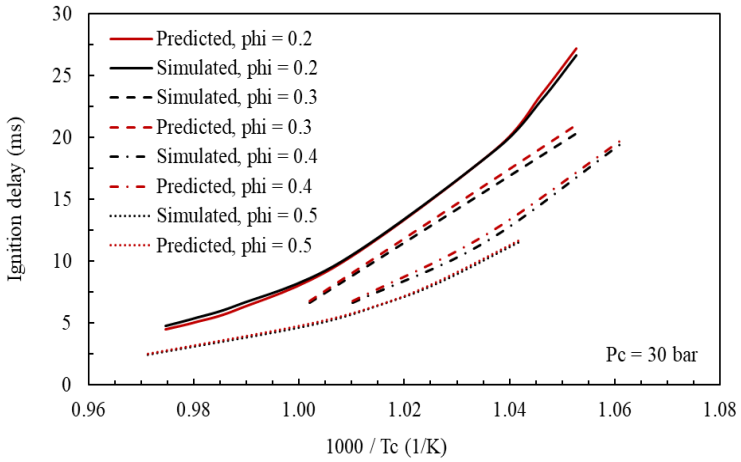

Fig. 11. Predicted and simulated ignition delays in the RCM at compressed pressure of 30 bar and different equivalence ratio

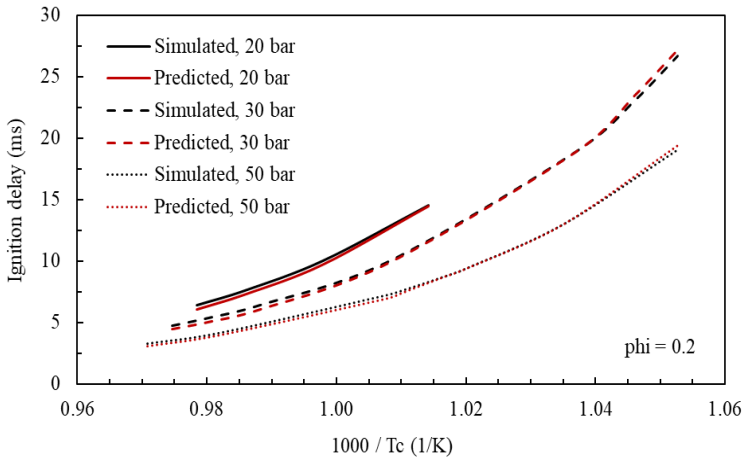

Fig. 12. Predicted and simulated ignition delays in the RCM at equivalence ratio of 0.2 and different compressed pressures

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Fig. 13 contrasts ANN predictions, 0-D simulations, and measured ignition delays. Higher temperatures shortened delays, accurately reflected by both the model and simulation. Increasing pressure from 10 to 20 bar reduced delays, but above 20 bar, delays increased—a trend the ANN model successfully captured, indicating robust training .

All predicted ignition delays for RCM and shock tube versus simulated results are shown in Fig. 14. The graphs show a very good accuracy of prediction, especially for the RCM data. The prediction error for the ANN-predicted ignition delays for RCM and shock tube is 2.76% and 5.04% respectively. The correlation coefficient R2 of predictions for RCM is 0.9985, while an R2 of 0.9958 for the shock tube ANN model was achieved.

The outcomes of this effort show that neural networks can be trained to extremely high accuracy for the prediction of ignition delay over a variety of conditions. The predictions can be performed at least 1000 times more rapidly than 0-D simulation and much faster than experimental measurement. Note that, as far as the authors know, deep learning is not a great substitute for experimental measurement. Experimental measurements remain unbeatable when it comes to providing data that is essential for training neural networks. As experimental measurements are costly and time-consuming, getting a large enough dataset from these measurements is realistically impossible. In this regard, the next best alternative appears to be utilizing 0-D simulations. Provided the numerical method is determined to simulate measurements accurately, it can be utilized to get a large dataset for training a model.

Fig. 10 displays the ANN model's estimations of hydrogen mixture ignition delays in the RCM, maintaining a 20 bar pressure while varying equivalence ratios, and compares them to simulations. Notably, greater equivalence ratios correlated with extended predicted ignition delays, mirroring empirical observations (Fig. 8). The kinetic model showed strong alignment with physical reality, exhibiting minimal divergence from simulations, except at temperatures below 970 K. A similar pattern emerged at 20 bar (Fig. 11). Fig. 12 further illustrates ANN-predicted and simulated ignition delays at a 0.5 equivalence ratio across varying pressures, where increased pressure reduced delay, consistent with measurements (Fig. 7). The simulation effectively replicated the observed ignition trends.

A comparison with previous studies further highlights the contribution of the developed ANN models. Cui et al. [21] designed a refined back-propagation artificial neural network (ANN) model to estimate the ignition delay time of a mixture containing n-butane and hydrogen within a rapid compression machine (RCM). To improve the precision of the predictions, they incorporated a genetic algorithm (GA) as an optimization technique. Their model achieved a mean relative error of less than 5%, but the limited availability of experimental data led to an underestimation of ignition delays in certain conditions. Similarly, Huang et al. [22] utilized a deep learning-based ANN model trained on a large dataset of 0-D simulated ignition delays for Jet A-1/hydrogen mixtures, achieving a mean relative error of 1.04%. However, their model exhibited localized prediction errors of up to 10% under short ignition delay conditions.

In comparison, the present study achieves prediction errors of 2.76% and 5.04% for RCM and shock tube ignition delays, respectively, which are within the accuracy range of previous works. Moreover, unlike Cui et al. [21], who optimized their ANN model using GA, the present study adopts a simpler architecture with carefully tuned hyper parameters to balance accuracy and computational efficiency. Additionally, while Huang et al. [22] relied solely on 0-D simulation data, our approach incorporates both experimental measurements and simulation-generated datasets, ensuring more robust training and validation. This comparative analysis demonstrates the effectiveness of the developed ANN models in predicting ignition delay with high accuracy while maintaining computational efficiency, reinforcing the significance of deep learning methods in combustion modeling.

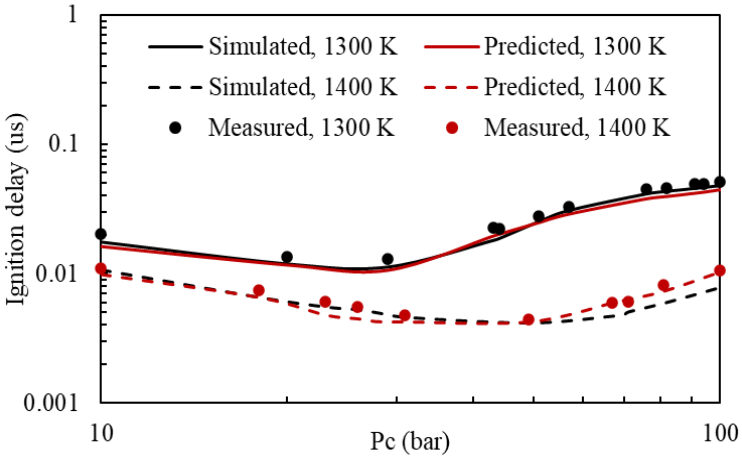

Fig. 13. Predicted, simulated, and measured ignition delays in the shock tube at equivalence ratio of 0.5 and different compressed temperatures

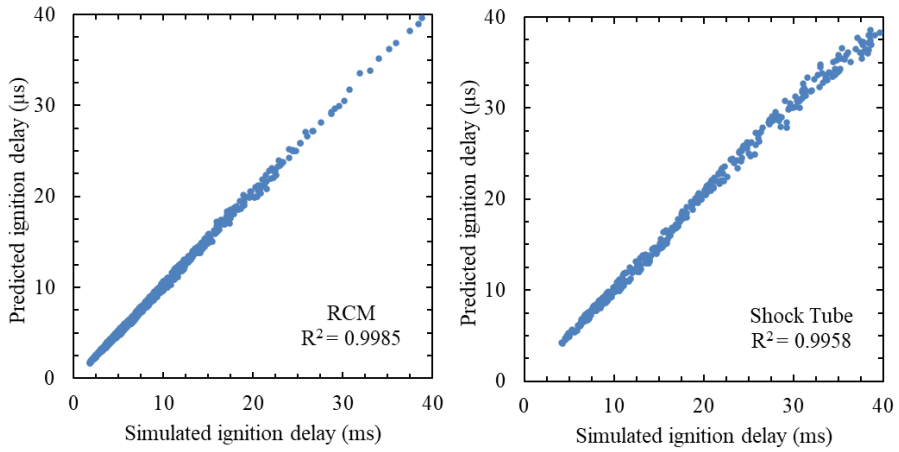

Fig. 14. Simulated versus precited RCM (left) and shock tube (right) ignition delays

4. Conclusion

This research applies deep learning techniques to predict ignition delay times for hydrogen mixtures in both rapid compression machines (RCM) and shock tubes. The RCM dataset includes pressure levels from 20 to 60 bar and temperatures between 940 and 1020 K, while shock tube predictions are conducted within a pressure range of 20 to 100 bar and temperatures from 1300 to 1400 K. First, two series of 0-D simulations were conducted and compared to the experimental data. Since the simulations were performed with acceptable accuracy, they were used to generate two large datasets for neural network training purposes. The datasets produced by the numerical method were partitioned into three subsets for training, testing, and evaluation purposes. Subsequently, two artificial neural networks (ANNs) were constructed, each comprising four layers (with two hidden layers). These networks were trained and deployed to predict ignition delays. The outcomes indicate that the developed ANN models possess the capability to accurately predict both measured and simulated ignition delays in a significantly expedited manner.

4.1. Comparison with Traditional Methods

Traditional approaches to predicting ignition delay, such as simulations of computational fluid dynamics (CFD) and detailed chemical kinetics, require extensive computational resources and time. These methods, while accurate, are often impractical for real-time applications due to their high computational cost and scalability limitations. The proposed ANN models significantly reduce

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computational time by at least 1000 times, enabling rapid predictions that are essential for real-world industrial applications.

In industrial settings, such as engine design and optimization, real-time decision-making is critical for improving efficiency, reducing emissions, and optimizing fuel use. While traditional simulation-based methods may take hours or even days to produce results, ANN models can deliver accurate predictions almost instantaneously. This reduction in computational burden translates into significant cost savings, as less computational infrastructure is required, and optimization cycles can be executed more frequently. Additionally, while conventional models require extensive tuning and recalibration for different fuel compositions and operating conditions, the ANN models demonstrate greater adaptability, making them more suitable for large-scale industrial deployment

4.2. Industrial Implications

This work contributes to the broader field of industrial optimization and simulation by demonstrating how machine learning techniques, specifically ANNs, can be applied to optimize key parameters in industrial systems. By leveraging machine learning models, improvements in the efficiency of combustion processes, reductions in operational costs, and optimization of resource utilization are achieved. The predictive capabilities of ANNs provide a more accurate understanding of system behavior, which can be used to fine-tune industrial operations for enhanced performance and reduced waste.

Furthermore, the introduction of a comprehensive simulation framework offers a more effective tool for evaluating various operational scenarios. This framework enables the prediction of critical performance metrics, which can inform the design and optimization of industrial processes. The integration of machine learning with simulation tools provides significant benefits in decision-making, process optimization, and overall system performance, aligning with the journal's focus on industrial optimization.

The real-world applications of the developed ANN models are particularly valuable in industries such as automotive, aerospace, and energy, where ignition delay is crucial in engine design, enhancing fuel efficiency, and optimizing performance. These models can be integrated into combustion simulation systems, enabling manufacturers to optimize engine parameters and fuel formulations in a cost-effective manner. The scalability of the ANN models further enhances their applicability, as they can be adapted to different engine types, fuel compositions, and operational conditions with minimal retraining.

In addition, the use of ANN models reduces the need for expensive experimental testing, leading to significant cost savings in research and development processes. By providing accurate predictions without the need for costly experimental setups, the models help reduce both time and financial resources spent on traditional testing. Real-time predictions from these models also support efficient decision-making, allowing industries to adjust engine parameters quickly and precisely, optimizing performance and reducing operational inefficiencies.

4.3. Future Work

Future work could extend neural network applications to challenges such as ignition delays in NTC (Negative Temperature Coefficient) regions, facility-independent ignition delay prediction in rapid compression machines and shock tubes, modeling ignition delay based on fuel carbon count, and supporting optical diagnostics

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