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Review

Machine Learning Approaches for Predicting Ignition Delay in Combustion Processes: A Comprehensive Review

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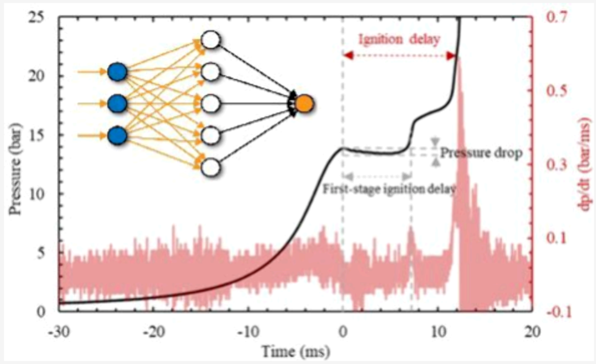
ABSTRACT: This review explores machine learning approaches for predicting ignition delay in combustion processes. Ignition delay is a vital parameter in optimizing the engine design, fuel formulations, and combustion efficiency. The review examines the applications of artificial neural networks (ANNs) and convolutional neural networks (CNNs) in various combustion processes and equipment, such as engines, boilers, and rapid compression machines. The differences between ANNs and CNNs are discussed, highlighting their capabilities and limitations. Numerous studies are presented, demonstrating the successful application of neural networks in predicting ignition delay for different fuels and engines. Overall, machine learning approaches show great promise in accurately predicting the ignition delay and advancing energy utilization.



1. INTRODUCTION

A segment of the scientific community is actively exploring alternatives to hydrocarbon-based fuels in order to address the growing global energy demand. Nonetheless, carbon-based fuels are anticipated to remain the predominant and reliable sources of energy for the foreseeable future. Another promising approach involves the optimization of existing combustion technologies, as substantial endeavors have been dedicated to enhancing the efficiency of fossil fuel utilization. In the pursuit of this objective, a comprehensive understanding of combustion characteristics is imperative. To gain such insights, several experimental investigations and numerical studies, including zero-dimensional (0-D) and three-dimensional (3-D) modeling, have been undertaken.

In recent decades, neural networks have emerged as powerful tools for addressing a wide array of complex scientific challenges, drawing inspiration from principles governing the human mind. This development holds great promise for the research community, offering the potential for highly accurate simulations that demand significantly reduced execution times and computational resources compared to traditional methods. Neural networks have already demonstrated their utility in effectively simulating diverse combustion processes and equipment including but not limited to spark ignition engines,[1] compression ignition engine,[2] chemical kinetics,[3] optical diagnostics,[4] gas turbine,[5] boilers,[6] burners,[7] rapid compression machines (RCMs),[8] and shock tubes.[9]

A thorough comprehension of ignition delay allows engineers and researchers to optimize engine design and fuel formulations, leading to more efficient and environmentally friendly combustion processes. Moreover, ignition delay plays a significant role in ensuring engine safety, preventing knock or detonation and promoting stable combustion, all of which are vital for the automotive and energy sectors. Consequently, a deep understanding of the ignition delay is fundamental for advancing technology and achieving more sustainable and efficient energy utilization. A large amount of experimental and numerical research has been performed to understand the combustion and autoignition processes.[10−12]

The concept of ignition delay carries various definitions contingent on the specific application. It can be defined as the time period between the moment of end of compression stroke and the moment of pressure gradient local maxima as illustrated in Figure 1. It also can include multiple stages based on the sensitivity of the fuel and the physics of the phenomenon. This definition is useful in compression−ignition engines. In the context of spark-ignition engines, the ignition delay can also be defined as the time from spark initiation to the time when 10% of the mass is burned. Figure 1 describes the ignition delay, which is well-suited for premixed fuel/oxidizer blends commonly utilized in rapid compression machines. In the context of combustion devices, such as

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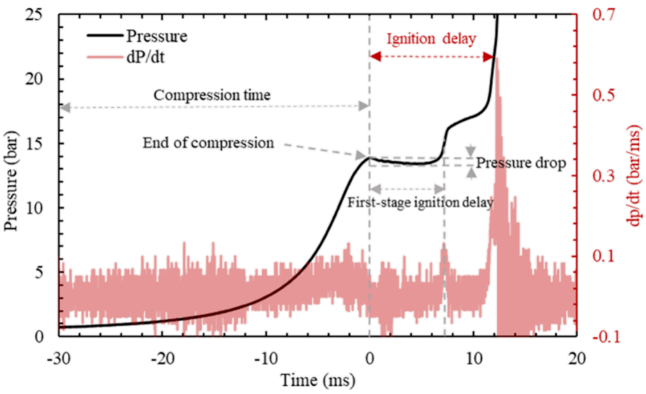

Figure 1. Pressure and pressure gradient of the *n*-heptane/oxygen/nitrogen mixture. The compressed gas temperature was 633 K, and the compressed gas pressure was 13.5 bar.[12] Reproduced or adapted with permission from.[12] Copyright [2021] [ACS].

compression ignition engines, where fuel is introduced into oxidizer during compression, ignition delay is conventionally defined as the duration from the initiation of fuel injection to the moment of ignition (specifically, the peaks of local pressure gradient). This comprehensive definition of ignition delay encompasses both physical delays (such as liquid spray breakup and droplet vaporization) and chemical delays involving fuel oxidization and pyrolysis.

On the other side, machine learning constitutes a subset within the realm of artificial intelligence, concentrating on crafting algorithms and statistical models. These tools empower computers to acquire knowledge, enabling them to make predictions or decisions that are devoid of explicit programming tailored to specific tasks. Machine learning methods have a wide range of applications, including but not limited to image and speech recognition,[13] natural language processing and text analysis,[14] recommendation systems (e.g., personalized product recommendations),[15] autonomous vehicles,[16] robotics,[17] healthcare (e.g., disease diagnosis and drug discovery),[18] financial modeling,[19] fraud detection,[20] predictive maintenance,[21] climate forecasting,[22] and so on.

A neural network serves as a computational model, drawing inspiration from the structural and functional attributes of biological neural networks, notably those observed in the human brain. Neural networks are a fundamental component of deep learning, a subfield of machine learning that focuses on training deep and complex neural networks. A neural network is comprised of interlinked nodes referred to as neurons, whether biological or artificial in nature, systematically arranged into distinct layers. These layers conventionally encompass an input layer, one or more hidden layers, and an output layer. These layers typically include an input layer, one or more hidden layers, and an output layer. Here is definition of some of its basic concepts:[23]

- Input Layer: the input layer receives the initial data or features (experimental or numerical) that are fed into the neural network. Each neuron in the input layer corresponds to a physical parameter of the data.
- Hidden Layers: Between the input and output layers, there can be one or more hidden layers. These hidden layers perform intermediate computations and are responsible for learning complex patterns and representations in the data. Each neuron in a hidden layer is connected to neurons in the previous and subsequent layers.
- Output Layer: The output layer generates the outcome or prediction, a consequence of computations conducted by the hidden layers. The quantity of neurons within the output layer is contingent upon the unique requirements of the given task, such as classification (where each neuron represents a class) or regression (where each neuron represents a numerical value).
- Weights and Biases: each connection between neurons in adjacent layers has an associated weight, which determines the strength of the connection. Additionally, each neuron typically has an associated bias, which helps in adjusting the neuron's output. These weights and biases are learned during the training process.
- Activation Functions: activation functions are used in neural networks to introduce nonlinearity into the model. Nonlinearity is essential for capturing complex relationships in the data. Common activation functions include the sigmoid function, ReLU (Rectified Linear Unit), and tanh (hyperbolic tangent).
- Training: training a neural network involves the process of learning from input data. The network makes predictions, and the error or loss between its predictions and the actual target values is computed. The back-propagation algorithm is then used to update the weights and biases of the network to minimize this error. This process is repeated iteratively until the network's performance on the training data reaches an acceptable level.

Neural networks can be categorized into several main types based on their architectural characteristics and the types of problems they are designed to solve. The two most important categories are artificial neural networks (ANNs) and convolutional neural networks (CNNs). Each of these has specific capabilities and limitations. Their differences are summarized in Table 1.

In summary, ANNs are more general-purpose neural network architectures that can be applied to a wide range of tasks. On the other hand, CNNs are specialized for tasks involving grid-like data, particularly image-related tasks. When working with images, CNNs are often the preferred choice due to their ability to automatically learn hierarchical features from raw pixel data, reducing the need for manual feature engineering. In this review, the focus was placed on the capabilities and recent advancements of ANNs and CNNs in ignition delay prediction. A general introduction on ignition delay and neural networks has already been presented. The application of ANNs and CNNs in ignition delay prediction is presented in the next two sections. The important studies, their methodology, and results will be discussed.

2. APPLICATION OF AN ARTIFICIAL NEURAL NETWORK IN IGNITION DELAY PREDICTION

The pioneering work on employing neural networks to forecast the ignition delay of diesel fuel was introduced by Basu et al.[24] in 2003. They analyzed 60 commercial diesel samples by using an ignition quality tester (IQT). These experimental results, coupled with specific input parameters, were employed to train the ANN model with Statistica software serving as the computational tool. The outcome of their research demonstrated a remarkably strong correlation between the predicted

Table 1. Differences between ANNs and CNNs in Terms of Five Important Criteria

Criterion	ANN	CNN
Purpose and Specialization	ANNs are versatile and can be applied to a wide range of tasks like classification, regression, and even sequential data processing. They are not specialized for any particular type of data but can be adapted to various data formats.	Designed to process grid-like data, like images, and multidimensional arrays. They are highly effective in tasks that involve extracting hierarchical features from visual data.
Architecture	They consist of layers of interconnected neurons, typically including input, hidden, and output layers. Neurons in ANNs are fully connected to neurons in adjacent layers.	CNNs have a specialized architecture with layers like convolutional layers, pooling layers, and fully connected layers. Convolutional layers use filters to convolve over input data, capturing local patterns and features. Pooling layers reduce dimensionality.
Feature Learning	ANNs require hand-crafted feature extraction in many cases, meaning that feature engineering is often necessary to preprocess the input data effectively.	CNNs can automatically learn hierarchical features from raw input data. Convolutional layers are designed to capture patterns at different spatial scales, making them capable of feature learning.
Image Processing	ANNs can process images but may not perform as well as CNNs when dealing with visual data due to the lack of specialized layers for feature extraction.	CNNs are highly effective for image-related tasks, such as image classification, object detection, image segmentation, and feature extraction.
Training	Training ANNs may require a larger number of parameters and data compared to CNNs for tasks involving visual data.	CNNs are more parameter-efficient and can achieve good performance with smaller data sets, thanks to their ability to learn local features.

and observed cetane numbers, affirming the efficacy of the ANN-based approach in predicting the ignition delay for diesel fuels.

Choi and Chen[25] aimed to integrate a semiempirical model designed for predicting ignition delay in an HCCI (Homogeneous Charge Compression Ignition) engine with an ANN model to forecast the start of combustion (SOC). The ANN model was trained through the back-propagation algorithm with temperature (790−1270 K), pressure (1−45 atm), equivalence ratio (0.2−1.0), and EGR (exhaust gas recirculation) percentage (0−60%) as inputs. In their ANN architecture, a configuration is explored comprising one or two hidden layers and an output layer featuring a single node to represent the ignition delay, as depicted in Figure 2.

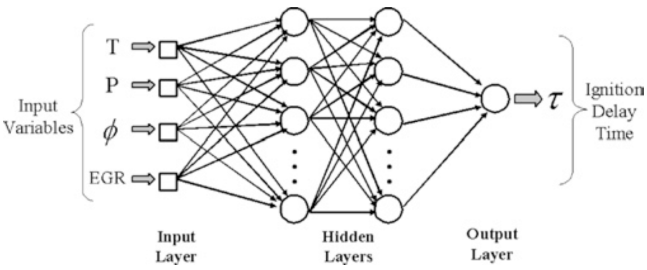

Figure 2. Back-propagation artificial neural network with two hidden layers.[25] Reproduced or adapted with permission from.[25] Copyright [2005] [Elsevier].

Achieving accuracy in the ANN model necessitates fine-tuning of several key parameters. These parameters encompass factors such as the epoch size, the quantity of nodes within the hidden layer, and the frequency at which testing is conducted during training, as quantified by the number of epochs between tests. They found out that the model is capable of providing reasonably accurate predictions of the SOC. It was also found to be much faster than a detailed chemistry solution.

Another interesting study was performed by Kannan et al.[26] They developed an ANN model using injection pressure (220−300 bar) and injection timing (23−28 °bTDC) as inputs to predict several important combustion performance and emissions parameters, including ignition delay of a diesel engine that was burning waste cooking palm oil-based biodiesel. They first performed a series of experiments in a single cylinder, four-stroke direct injection diesel engine. The engine was run at full load condition and a constant speed of 1500 rpm to train the ANN model by using the experimental data based on the back-propagation learning algorithm. They observed that the ANN model predicts the target characteristics very accurately.

Rezaei et al.[27] used experimental data of an HCCI engine to train a feed-forward ANN model by two inputs of butanol volume percentage (6−48.5%) and equivalence ratio (0.30−0.43%) and seven outputs of IMEP (indicated mean effective pressure), indicated thermal efficiency, net total heat released, maximum in-cylinder pressure, total hydrocarbon, NO_x, and CO. They observed that the ANN model predicts HCCI engine performance metrics with less than 4% error (Figure 3).

Huang et al.[28] employed machine learning methods to predict ignition delay of a Jet A-1/hydrogen fuel mixture in a single cylinder heavy duty research compression ignition (CI) engine to reduce the time and cost of experimentations in a wide range of operational conditions including pressure (1.0−

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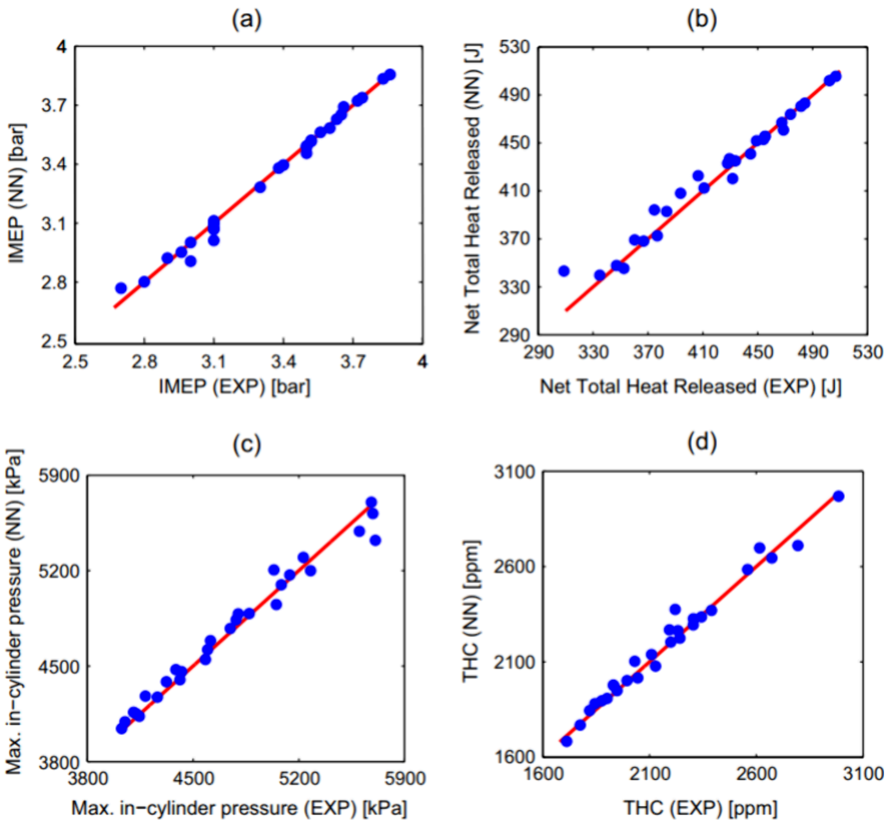

Figure 3. Predicted values by using an ANN model for an HCCI engine versus the experimental data for a) IMEP, b) net total heat released, c) maximum in-cylinder pressure, and d) total hydrocarbon.[27] Reproduced or adapted with permission from.[27] Copyright [2015] [Elsevier].

20.0 atm), temperature (800−1600 K), equivalence ratio (0.5−1.5), and blending molar ratio of hydrogen (0−0.5). To this end, first, they simulated ignition delay times using the HyChem (hybrid chemistry)[29] reaction mechanism.

Following validation against experimental data, an ANN model was trained using a database of ignition delay times. Additionally, a sub-ANN was incorporated into the primary ANN model to enhance the performance under specific local conditions. A comparison of their predicted ignition delay versus the simulated ones at different test conditions is shown in Figure 4. The basic ANN model, featuring five hidden layers, demonstrated proficient predictions of ignition delay times, yielding a mean relative error of 1%. Nonetheless, under

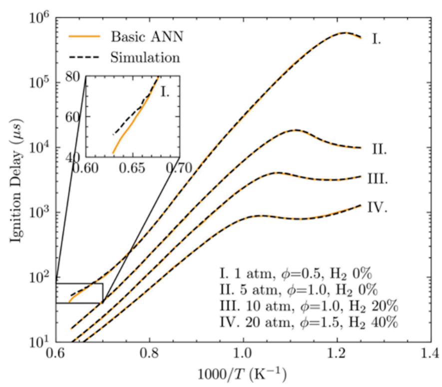

Figure 4. Simulated ignition delays versus the basic ANN predictions.[28] Reproduced or adapted with permission from.[28] Copyright [2022] [Sage].

specific conditions characterized by short ignition delays, the maximum local relative error was extended up to 10%. The introduced nested sub-ANN methodology effectively mitigates the maximum local relative error associated with ANN predictions to levels below 5%. Notably, the proposed data-driven ANN approaches exhibit a computational efficiency approximately 1000 times greater than that of the HyChem simulation method in the context of ignition delay prediction.

In their study, Van Tuan and colleagues[30] harnessed artificial neural networks (ANNs) and support vector machine (SVM) techniques to forecast ignition delay in a single-cylinder compression-ignition engine, focusing on both diesel and biodiesel fuels. To develop their predictive models, they employed a training data set comprising more than 700 experimental data points. The input layer of their models featured four neurons, representing the biodiesel ratio, pressure, temperature, and equivalence ratio. The outcomes of their analysis, which involved training and assessing model accuracy, demonstrated that the SVM model outperformed the ANN model in predicting the ignition delay with greater precision.

Nagaraja and Sarathy[31] developed an artificial neural network to predict ignition delay of natural gas in a homogeneous charge compression ignition engine. The model consists of 13 inputs and utilizes three hidden layers during training, employing a backpropagation approach. To optimize the network architecture, a grid search was conducted to tune the hyperparameters. Each hidden layer of the model contains 1024 nodes, while the output layer contains a single node. In order to prevent overfitting, a dropout fraction of 0.2 is applied to each hidden layer. The database is divided into

60% training data, 20% validation data, and 20% test data. The model was trained using the Keras library with the TensorFlow package.[32]

The inputs were scaled using the standard scaler from the scikit-learn package.[33] The activation function "ReLu" was applied to all hidden layers. For optimization, the Adam optimizer was utilized with a learning rate of 0.0001 and a batch size of 10. The model underwent training for a total of 1000 epochs. The results indicate that the developed model outperforms a multiple linear regression approach and is validated through shock tube experiments.

3. APPLICATION OF CONVOLUTIONAL NEURAL NETWORKS IN IGNITION DELAY PREDICTION

Popov et al.[34] demonstrated an intriguing use of convolutional neural networks (CNNs) in the field of combustion. Their study involved a low-speed wind tunnel, where a flush-mounted jet was directed perpendicularly from the tunnel wall into a turbulent boundary layer. Within this setting, they created a laser-induced optical breakdown (LIB) hotspot. Initially, a comprehensive hydrogen chemical model was employed to simulate the behavior of the radicals and any ensuing chemical reactions. Subsequently, the obtained results were utilized for the training of a CNN model, as depicted in Figure 5.

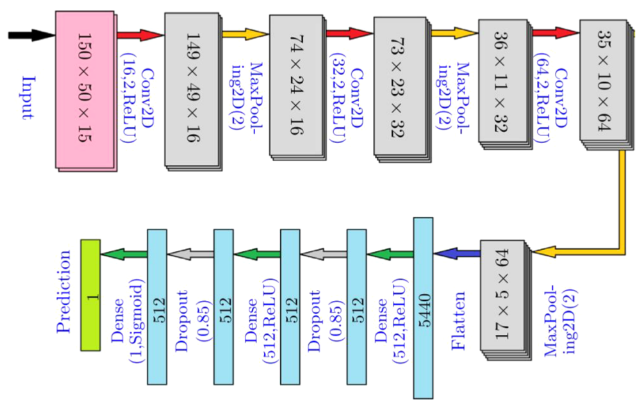

Figure 5. Convolutional neural network used to predict hydrogen ignition in a complex flow.[34] Reproduced or adapted with permission from.[34] Copyright [2019] [Elsevier].

The CNN model follows a layer-by-layer structure using Keras terminology.[35] The initial layer, known as the input layer, accepts a 150 × 50 × 15 input array, representing a discretized 2D field with 15 variables. This input undergoes three sets of convolution and pooling layers, each comprising a 2 × 2 convolutional layer with an ReLU activation function (rectified linear unit), followed by a 2 × 2 max pooling layer. In the subsequent step, the 17 × 5 × 64 tensor is flattened into a 5440-dimensional vector. Following this, two fully connected dense layers are introduced, each with 512 units and ReLU activation. To mitigate overfitting, a dropout layer is added after each dense layer with a dropout coefficient set at 0.85. Dropout involves randomly deactivating a portion (in this case, 85%) of the neurons within a layer, which has been proven to be effective in preventing overfitting.

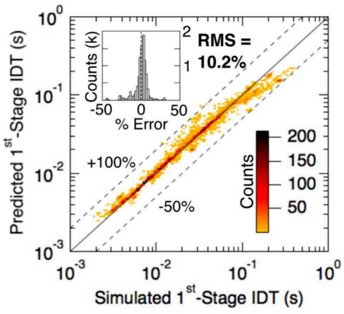

Figure 7. Parity plot and histogram of CNN-derived correlation between the explicitly simulated and predicted first-stage ignition delay using OH/HO_2 PFR training data.[36] Reproduced or adapted with permission from.[36] Copyright [2020] [Elsevier].

Buras et al.[36] explored the potential for predicting the initial ignition delay of highly diluted fuels within a high-pressure plug flow reactor (PFR) by employing a well-trained CNN model. Their approach involved designing a CNN model that took one-dimensional profiles of chemical species such as OH, HO_2, CH_2O, and CO_2 as input and aimed to predict the first-stage ignition delay as its output. This model incorporated several hidden layers to enhance its predictive capabilities.

The CNN models offer a notable advantage in addressing this issue as they make efficient use of fitting parameters, consequently mitigating the likelihood of overfitting. In a CNN convolutional layer, filters comprising a limited set of fitted weights are employed to target specific regions within the input data. These filters are systematically scanned (convolved) across the input, resulting in the creation of fresh images or profiles, known as feature maps.

Feature maps serve as indicators of the regions within the input data where specific features are detected. Typically, before proceeding to the subsequent convolution layer, it is a common practice to perform pooling on the feature maps. This

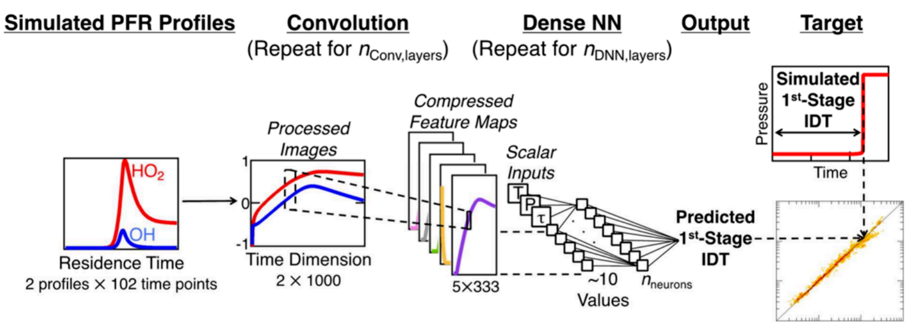

Figure 6. CNN architecture to find correlations between simulated flow reactor profiles and first-stage ignition delay for *n*-heptane at 600 K and 13.5 bar.[36] Reproduced or adapted with permission from.[36] Copyright [2020] [Elsevier].

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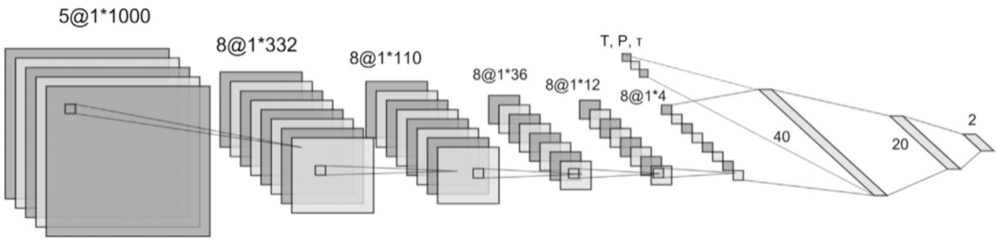

Figure 8. Schematic of the CNN architecture employed for predicting RON and MON numbers based on the profiles of 5 species. Initially, the 5 input species profiles undergo a convolution process, resulting in 8 feature maps. Throughout the convolution process, the number of channels remains constant, while the pooling layer gradually reduces the size of the feature maps. In the final block of the CNN, all the feature maps are flattened into a one-dimensional vector and connected to the subsequent Artificial Neural Network (ANN) along with inputs comprising T, P, and τ.[44] Reproduced or adapted with permission from.[44] Copyright [2023] [Elsevier].

pooling operation involves amalgamating neighboring data points within a specified pooling width, resulting in a condensed feature map. These condensed feature maps then serve as inputs to the next convolutional layer. Once the final convolutional layer is reached, the ultimate collection of feature maps needs to be transformed into a single label or value (first-stage ignition delay) (Figure 6).

Figure 7 shows their results of predicted first-stage ignition delay by using a CNN model versus simulated ones. The graph is generated through a process involving ten distinct CNN training fits, employing a 10-fold cross-validation approach. The data sets were organized by their target ignition delay times, dividing all PFR ignition delay simulations into ten equally sized batches, arranged in ascending order of their first-stage ignition delay values. Within each fold, one of these batches was designated as the test data, while the remaining nine batches were used for training purposes. To clarify, in the first fold, the CNN model was trained on the least reactive 90% of the simulations (those with the longest ignition delays) and subsequently tested on predictions for the most reactive 10% of the simulations.

In Fold 2, the CNN model was trained using data from the least reactive 80% and the most reactive 10% of the simulations, while the test set encompassed data falling between 10% and 20% in terms of decreasing reactivity. This graph illustrates that CNN-derived ignition delay predictions, based on the PFR simulations, generally align well with the simulated values, although the level of agreement does exhibit some minor variations across the different fits. The most demanding challenge emerged during extrapolation to the longest ignition delays, as indicated by the largest deviation from parity in Figure 8. Nevertheless, the overall distribution of errors centers around 0%, with a root-mean-square (RMS) error of just 10.2%. This level of error is comparable to the typical uncertainties reported for ignition delays measured in either shock tube or rapid compression machine (RCM) experiments.

Yang et al.[37] trained ANN and GCN (graph convolutional network) models to predict ignition delay of different short-chain fuels in a homogeneous reactor. A GCN model shares similarities with the traditional CNN in its approach to feature learning through examination of neighboring nodes. It encompasses the aggregation of node vectors, forwarding the outcome to a dense layer, and the application of nonlinearity via an activation function. In essence, it comprises key components: a graph convolutional step, a linear layer, and a nonlinear activation function, collectively contributing to its functionality.

To access to a large data set for training, they performed a series of autoignition simulations at different temperatures (800−2000 K) and pressures (10−600 kPa) by using Cantera[38] and the USC-II detailed mechanism.[39] They observed that the simple ANN model can predict ignition delays for 4 carbon atom fuels with high accuracy, by only incorporating a very small amount of data points. Then, they established the transfer learning framework by merging the neural network models (both ANN and GCN) trained on different fuel data sets and applying transfer learning to a new fuel data set. It is shown that transfer learning with GCN is able to predict ignition delays with better prediction accuracy while it also demonstrates lower stability and training speed than transfer learning with the ANN model.

Li et al.[40] conducted an experimental investigation involving solid fuel combustion within a laminar flow reactor, employing high-speed laser diagnostics. Their primary objective revolved around advancing image analysis methodologies for precise identification of ignition events in individual solid particles using optical measurement data. Remarkably, they achieved the visualization of the homogeneous ignition of individual bituminous coal particles through the concurrent application of planar laser-induced fluorescence of OH radicals (OH-LIF) and diffuse backlight-illumination (DBI) techniques, all at a rapid sampling rate of 10 kHz.

They constructed an extensive experimental data set comprising a total of 1518 single-particle events, complete with high-quality ground truth labels for ignition delay times. This data set was meticulously curated to facilitate the training of a Convolutional Neural Network (CNN) model. To process the images, they employed deep residual learning techniques, specifically based on the Residual Network (ResNet)[41] architecture, progressively increasing the network depth with variants featuring 18, 34, 50, and 101 layers. The primary objective was to classify the OH-LIF images into two distinct categories: ignition and no ignition.

To complement the ResNet models, the original grayscale images underwent a transformation, being cropped and resized into pseudocolor images with uniform dimensions of 224 × 224 pixels, which served as input data. The initial convolutional (conv) layer, irrespective of the network's depth, featured 64 filters measuring 7 × 7, with a stride of 2, and was succeeded by a 3 × 3 max-pooling operation. Following this, four sets of stacked convolutional layers (conv2/3/4/5) were progressively integrated, with an expanding filter dimension represented by N. Each group of layers comprised multiple residual blocks interconnected by shortcut connections. For the purpose of object detection, they harnessed

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Table 2. All Published Studies on the Application of ANNs and CNNs in Ignition Delay Prediction

	Author(s)	Target	Neural Network used	Publish year	Finding(s)
1	Basu et al.[24]	Prediction of cetane number of a diesel fuel	ANN	2003	The developed ANN was able to predict cetane number accurately.
2	Choi and Chen[25]	Prediction of start of combustion in an HCCI engine	ANN	2005	The proposed ANN model is fast and accurate (less than 6%).
3	Kannan et al.[26]	To study the effect of injection pressure and timing on the engine performance and ignition delay in a diesel engine	ANN	2013	The ANN model was very well correlated.
4	Sánchez-Borroto et al.[45]	Cetane number and ignition delay prediction of biodiesel in a four-stroke diesel engine	ANN	2014	The networks demonstrate utility in forecasting the cetane number and ignition delay of biodiesel fuels.
5	Rezaei et al.[27]	Ignition delay prediction of oxygenated fuels in an HCCI engine	ANN	2015	The ANN model can predict HCCI engine performance metrics with less than 4% error for butanol and ethanol fueled engines.
6	Sakthivel et al.[46]	Prediction of performance and emission characteristics of a diesel engine	ANN	2017	The results show the efficiency of the model to predict the performance, emission, and combustion parameters.
7	Abdul Jameel et al.[47]	Prediction of octane number using magnetic nuclear resonance spectroscopy	ANN	2018	ANN was very accurate in predicting the octane number.
8	Jaliliantabar et al.[48]	Sensitivity analysis of a compression ignition engine burning biodiesel fuel	ANN	2018	It was found that all studied factors are vital in creating a model.
9	Bi et al.[49]	Ignition delay prediction	ANN	2019	The ANN model is capable of reproducing experimentally measured ignition delay.
10	Popov et al.[34]	Ignition prediction of a hydrogen jet in air crossflow	CNN	2019	The neural networks were found very useful in predicting the experimental data.
11	Joshi and Thipse[50]	Performance prediction of compression-ignition engine using algae biofuel blend and diethyl ether	ANN	2019	The ANN model was able to satisfactorily predict the engine performance.
12	Cui et al.[8]	Ignition delay prediction *n*-butane/hydrogen in a rapid compression machine	ANN	2020	The ANN model underestimated the ignition delays due to the training data set lacking an "acceleration feature".
13	Zhang et al.[51]	Ignition delay and lift-of-length prediction of a large eddy simulation of spray combustion of *n*-heptane	ANN	2020	The FGM-ANN model is able to predict ignition delay more faster than the conventional FGM models.
14	Sharma[52]	To predict the emission and performance features of a diesel engine	ANN	2020	The ANN-based model can predict engine characteristics very well.
15	Veza et al.[53]	Prediction of cetane number of ABE-diesel blends	ANN	2020	The ANN model based on Levenberg−Marquardt predicts the cetane number very accurately.
16	Messerly et al.[54]	Ignition delay prediction of iso-octane and PRF80 in a constant volume combustion chamber	ANN	2020	Neural networks can be used for sensitivity analysis.
17	Buras et al.[36]	Prediction of first stage ignition delay in high-pressure plug flow reactor (PFR)	CNN	2020	The accuracy of the model is 10−50%. This accuracy level is enough for a quick fuel screening.
18	Abdul Jameel et al.[55]	Prediction of ignition quality	ANN	2021	ANN shows a good capability in prediction of the characteristics.
19	Kefalas et al.[56]	Knock detection in a spark-ignition engine	CNN	2021	The CNN model shows a very accurate performance in knock detection.
20	Huang et al.[28]	To predict the performance of a heavy-duty spark ignition engine burning natural gas	ANN	2022	The ANN model is very efficient to predict the emission and performance characteristics.
21	Huang et al.[57]	Ignition delay prediction of Jet A-1/hydrogen	ANN	2022	The increase of hydrogen blending ratios accelerates the autoignition except at very low temperatures. ANN is able to predict this trend.
22	Cui et al.[58]	To predict the ignition delay of a surrogate	ANN	2022	The computational time for a single 0-D simulation case is 28 s. Upon integration of the BP-ANN, the computational time for 176 cases is markedly reduced to 3.2 s, demonstrating a substantial enhancement in computational efficiency.
23	Tajima et al.[59]	Knock prediction in a spark-ignition engine on a cycle-by-cycle basis	CNN	2022	The CNN prediction accuracy was 91.4%.
24	Ofner et al.[60]	Knock detection in an internal combustion engine	CNN	2022	The model accuracy was 89% after training on a small number of exclusively nonknocking cycles.
25	Aliakbari et al.[61]	Performance prediction of a single-cylinder diesel engine	ANN	2023	The ANN model predicts the emission parameters and engine performance accurately.
26	Minh et al.[62]	Prediction of biodiesel ignition delay	ANN	2023	The ANN model predicts the ignition delay very accurately.

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Table 2. continued

	Author(s)	Target	Neural Network used	Publish year	Finding(s)
27	Van Tuan et al.[30]	Ignition delay prediction of diesel and biodiesel	ANN	2023	ANN shows a good capability in prediction of the ignition delay.
28	Yang et al.[37]	Ignition delay prediction of long-chain hydrocarbon fuels using a transfer learning approach based on ANN and GCN	ANN CNN	2023	The proposed transfer learning method can predict ignition delays for different fuels with large molecules with prior knowledge from small molecule fuels.
29	Li et al.[40]	To predict the ignition delay of solid fuel in a laminar flow reactor by using high-speed laser diagnostics	CNN	2023	The hierarchical feature extraction of the convolutions networks clearly facilitates data evaluation for high-speed optical measurements and could be transferred to other solid fuel experiments with similar boundary conditions.
30	Wang et al.[44]	Octane number prediction	CNN	2023	The CNN method yields a very acceptable accuracy in predicting the ON number of single component fuels and fuel mixtures.
31	Nagaraja and Sarathy[31]	Ignition delay prediction of natural gas blends in HCCI engine	ANN	2023	The ANN model predicts all experimental data very accurately with a considerably higher accuracy compared to the multiple linear regression approach.

scale-invariant feature pyramid networks (FPNs)[42] in conjunction with Faster R-CNN[43] to identify objects across various scales.

Their investigation revealed that the accuracy of traditional image processing techniques relying on intensity thresholds is highly sensitive to parameter choices. The adoption of deeper networks and pretraining techniques offered marginal enhancements in the training process and subsequently improved ignition prediction. Their overall findings indicated that the hierarchical feature extraction capabilities of convolutional networks significantly aid in data analysis for high-speed optical measurements. Moreover, these insights suggest that such methods can be effectively transferred to other experiments involving solid fuel combustion under similar boundary conditions.

Wang et al.[44] developed a multilayer convolutional neural network for predicting octane number using time-resolved information from species profiles in a constant volume autoignition process. The CNN architecture, shown in Figure 8, consists of convolutional blocks with a 1D convolutional layer, batch normalization, activation function, and pooling layer. Each convolutional layer has a kernel size of 3 and generates eight feature maps. The ReLU function is used as the activation function to introduce nonlinearity.

As the convolution layer deepens, the feature map transitions from local to semantic features, causing a gradual reduction in size. Hence, each convolutional block concludes with a pooling layer of size 3, reducing the feature map by two-thirds. Positioned between the convolutional and activation layers, batch normalization is pivotal in enhancing the training speed and performance of convolutional neural networks. Throughout the training, the convolutional layer parameters are updated, leading to a shift in the input data distribution of the subsequent network.

The researchers validated their approach by employing data sets encompassing fuel blends and diverse single components, including alkanes, esters, and alcohols, among others. The findings illustrate the method's capacity to achieve elevated accuracy in predicting the Octane Number (ON), not only for individual fuel constituents but also for blended fuels, representing a mean absolute error of less than 2. The neural network optimally employs parameter sharing, effectively utilizing a limited set of parameters while extracting noteworthy high-level semantic features. Furthermore, the method exhibits the capability to make predictions for a wide range of fuels, even those lacking information about physical parameters and molecular structure in fuel blends.

Table 2 shows all published studies on the application of ANNs and CNNs in ignition delay prediction in different combustion processes. The goal of study and the main finding of each study was presented.

4. CONCLUSION

In conclusion, this comprehensive review has highlighted the significant potential of machine learning techniques, particularly artificial neural networks (ANNs) and convolutional neural networks (CNNs), in advancing the prediction of the ignition delay for various combustion processes. Through the examination of multiple studies, it has been demonstrated that these computational models can offer precise and rapid predictions, thus providing a valuable tool for optimizing engine design and fuel formulations. Potential applications of this technique could be for optimizing engine design for

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various fuel formulations, model-based control of an engine, multifuel engine calibration, emission calibration development, and fuel economy prediction.

The distinct advantages of ANNs and CNNs have been showcased, with CNNs showing particular strength in handling grid-like data, such as images (of the combustion chamber's inside, for example), and ANNs exhibiting versatility across a broader range of applications. Moreover, the application of machine learning extends beyond mere prediction, offering insights into the complex dynamics of combustion phenomena and contributing to more efficient, safe, and environmentally friendly energy use. The convergence of combustion science and machine learning opens new pathways for innovation in energy technology with the potential to meet the growing energy demands while addressing environmental concerns. Future research may further refine these models, expand their applicability, and integrate more diverse data sources to continue improving the accuracy and efficiency of combustion systems. As suggestions for future work, the community may investigate the applicability of using machine learning for prediction of the ignition delay in the NTC (negative temperature coefficient) region, the ignition delay as a function of the number of carbon atoms for different hydrocarbons, and providing support for optical diagnostic methods.

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Notes

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