Progress in the Application of Machine Learning in Combustion Studies

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Abstract

Combustion is the main source of energy and environmental pollution. The objective of the combustion study is to improve combustion efficiency and to reduce pollution emissions. In the past decades, machine learning (ML), as a branch of artificial intelligence, has attracted increasing interests, especially in the combustion field. In the present work, the definition, current status and recent progress in the applications of ML on researches related to combustion are briefly reviewed. Combustion studies combined with ML can be divided into theoretical and industrial aspects. Studies of combustion theory include computational fluid dynamics (CFD) simulation, combustion phenomenon and fuel. ML is used to reduce the cost of CFD, including reducing the scale of combustion mechanism, saving the memory storage of the probability density function table and optimizing Large Eddy Simulation. ML helps in the research of combustion phenomena, such as detecting thermoacoustic combustion oscillation, portioning regimes of ignition and detonation, and reconstructing cellular surface of gaseous detonation. ML has been also applied to study physicochemical properties of fuels and to design the next generation fuels. In the industrial research with respect to combustion, ML is mainly applied to produce electricity and power by power plants or engines, and less to other fields. ML could figure out problems of combustion in various kinds of furnaces and post-combustion emissions in power plants. In addition, ML plays important roles in biodiesel engine, Homogenous Charge Compression Ignition (HCCI), and operation control or monitoring in the engines. Moreover, ML can also be applied to other industrial studies related to combustion, mainly to particulate matters. The methods of the mentioned studies are summarized in details and the potential applications of ML in combustion community are proposed.

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1. Introduction

As the main approach to getting energy, the combustion of fuel is commonly applied to the industry, power generation, heating supply, waste disposal and related fields. About 80 % of world energy comes from combustion of fossil fuels.^[1] Combustion contributes a lot to the electric power. For instance, the installed thermal power capacity of China in 2019 is about 1.19 billion kilowatts, accounting for 59 % of

the total installed power capacity.^[2] Nonetheless, as a main method to supply the most energy that people desire, combustion of fossil fuels is responsible for pollutions, which greatly endanger ecological and people's living environments. Amount of CO₂ causes environmental problems that threaten human survival, such as the greenhouse effect, sea-level rise, global warming and etc. The incomplete combustion of fossil fuels will produce pollutants like nitrogen oxides (NO_x), sulfur oxides (SO_x), volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs) and soot. Efficient and clean combustion plays an important role in relieving energy pressure, ensuring energy security, lowering emissions and keeping sustainable development. The goals of the combustion study are to improve combustion efficiency and reduce emissions. Despite vast applications of combustion in industrial production, the combustion study still remains a lot of gaps. As combustion is a kind of flowing oxidation reactions, it needs to couple the fluid dynamics, chemical

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kinetics, heat and mass transfer, it also requires powerful methods to investigate.

Machine learning (ML), which is subject to constructing models from existing data, is a branch of Artificial Intelligence (AI) and has been applied in many other research fields. For example, many scholars have used it in the design of functional thermal materials and achieved good results.^[3] With ML, researchers are able to predict the thermal conductivity or interface thermal conductivity of various materials,^[4-6] discover the abnormal thermal properties of different nanomaterials^[7,8] and modulate the thermal conductivity of aperiodic superlattices.^[9] Mitchell *et al.*^[10] defined ML as: “A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.” The definition has been accepted by the academic world. The dependence on experience may suggest a shortage of ML. For example, systematic biases in society will lead to biases in data, which will raise questions and make unfair judgements^[11] when using ML in policy decision-making.^[12] Domingos *et al.*^[13] believed that learning = representation + evaluation + optimization. The purpose of representation is to express the model with the language that the computer can handle. More than one classifier will be represented, so the evaluation and optimization functions are needed to score the models and search for high-scoring classifiers.^[13] ML is shifting our power^[14] in social and economic life, whose influence is considered in policy-making.^[14]

According to the learning methods, ML can be categorized into supervised learning, unsupervised learning, semi-supervised learning, reinforcement learning (RL), and etc.^[15] The respective characteristics of these methods are: 1) supervised learning needs to provide labeled sample sets; 2) unsupervised learning does not need to provide labeled sample sets; 3) semi-supervised learning needs to provide a small number of labeled samples; and 4) RL requires a feedback mechanism. Supervised learning^[15] is to use a finite set of labeled training data to build a model through a certain learning strategy to achieve labeling of new instances. Supervised learning requires that the classification labels of the training samples are known. The higher the precision of the classification labels and the more representative the samples are, the higher the accuracy of the learning model predictive for previously unseen data^[16] we can get. Supervised learning, a powerful set of tools that have successfully been used in applications spanning the themes of automation, modeling and discovery,^[16] is often used for classification and regression, with typical algorithms like Decision Tree, random forest, Support Vector Machine (SVM), Naïve Bayes, Artificial Neural Network (ANN), and so on.^[15] Unsupervised learning uses unlabeled finite data to describe the inherent laws of unlabeled data. Instead of telling the computer how to classify data set, unsupervised learning makes the computer learn to classify data by itself, and then

give feedback on those classification behaviors. Common algorithms include clustering, hierarchical clustering, k-means, principal component analysis (PCA), local principal component analysis (LPCA) and association rules.

Semi-supervised learning is a two-stage or multi-stage process that uses supervised (or unsupervised) learning as pre-processing for unsupervised (or supervised) learning.^[17] Its main goal is to use a small number of labeled samples and a large number of unlabeled samples for training and classification, so as to reduce the cost of labeling and improve learning ability. Semi-supervised learning is applied in solving both classification and regression problems. Its algorithm includes some extension forms of commonly-used supervised learning algorithms, like graph inference and Laplacian SVM. RL, different from supervised learning and unsupervised learning, does not require any data in advance. RL obtains learning information and updates model parameters by receiving feedback that includes strengthening effective rules and weakening invalid or bad rules from interactions between the RL system and the environment. Dynamic systems and robot control are the common application fields of RL. Typical algorithms of RL include Q-Learning and temporal difference learning.

In particular, as a new research direction in the field of ML, deep learning (DL), one of the fastest-growing learning method,^[18] has received a lot of research attention due to the substantial improvement in computing power in recent years. It is closer to the original goal of ML-AI, and has been widely used in related fields including data mining and natural language processing (NLP). Here is a brief introduction to several common models of DL. Convolutional neural network (CNN) is one of the most widely-used models for DL, with applications in image recognition, recommender systems and NLP. CNN is a type of feedforward neural network (NN) that includes convolution calculation and has a deep structure. Its weight-sharing network structure makes it more similar to a biological NN, reducing the complexity of the network model and reducing the number of weights. This advantage allows the image to be directly used as the input of the network, avoiding the complex feature extraction and data reconstruction processes in traditional recognition algorithms, which is conducive to the rapid learning of NNs and reduces the memory overhead during calculation.^[19]

In order to meet the needs of modeling in changes of time sequence during NLP and Automatic Speech Recognition (ASR), Recurrent Neural Network (RNN) appeared. RNN is a kind of recursive NN that takes sequence data as input and performs recursion in the evolution direction of the sequence and all nodes (recycling units) are connected in a chain.^[20] RNN has memory, parameter sharing and Turing completeness, so it has certain advantages when learning the nonlinear characteristics of the sequence. The general RNN has a long-term dependence problem, and the ML field has developed a long-short term memory unit (LSTM), which is a time-recursive NN that realizes the memory function in time

through the switch of the gate. Due to its unique design structure, LSTM is suitable for processing and predicting important events with very long intervals and delays in time series, and has been well applied in the fields of hand writing recognition (HWR) and ASR.

Fig. 1 The variation of paper number about combustion and ML.

ML has been used in several studies related to combustion. This work reviewed the current state of ML in combustion research, especially the recent five years. As can be seen in Fig. 1, the application of ML in combustion field is attracting more and more attention. It should be noted that the paper number published in 2020 was taken into account up to August. The studies of ML in combustion will be divided into theoretical studies and industrial ones. The future development of ML in combustion will be prospected in the end.

2. Theoretical research

As mentioned above, ML has the capacity to find patterns in large sets of data that are incompressible to experimental practitioner,^[21] especially incomplete or uncertain data sets.^[22] ML seems to be able to solve problems where the dependencies are nonlinear relationships between inputs and outputs or insufficiently known to be programmed in a traditional and rigid manner.^[22] The advantages make ML play an important role in studies related to combustion theory, such as Computational Fluid Dynamics (CFD) simulation of combustion,^[23-25] prediction of combustion phenomenon^[26-29] and fuels.^[30-35] ML can help to reduce mechanism scales,^[23] optimize probability density function (PDF)^[24] and Large Eddy Simulation (LES)^[25] method in combustion simulation. When investigating combustion phenomenon, ML algorithms were used to detect thermoacoustic combustion oscillations,^[26,27] distinguish donation and ignition^[28] and reconstruct the detonation surface.^[29] In various fuel studies, ML also played an important role in the investigations about fuel properties,^[30-32] the bio-^[33,34] and next generation^[35] fuels.

2.1 CFD simulation

With the rapid increase of computational resources and data storage capabilities, ML has had a great impact on various fields such as speech, image and text recognition, robotics, health-care and many others. Its ability to learn from data can be used to simulate turbulent and reacting flow, which is

governed by highly non-linear equations and difficult to be predicted. Some scholars have used ML algorithms to solve problems involving combustion in CFD simulation.^[23-25]

Detailed kinetic model is the key factor to simulate laminar and turbulent flames. The computing cost of coupling detailed mechanism with CFD is too high, because detailed models contain too many species and elementary reactions, which recall the simplification of kinetic models. However, to simulate the entire flow field with a sole simplified mechanism may get a result that is significantly different from the one obtained from a detailed mechanism. D'Alessio *et al.*^[23] applied ML to simulate flames, and solve the conflict with Sample-Partitioning Adaptive Reduced Chemistry (SPARC) method. The core of such method is to partition the data-space obtained from detailed simulations in different clusters and to generate a special reduced mechanism for each cluster respectively through Directed Relation Graph with Error Propagation. The last step of SPARC is the CFD simulation of a reacting system. LPCA was used in the second step to partition the datasets into several clusters. The feasibility of the method was proven by the successful simulation of co-flow diffusion methane flame under both steady and dynamic conditions. The CPU time was significantly reduced while the precision of the result almost remained. Compared to the calculation cost for transport step, chemistry was not the biggest computational burden in the flame simulation due to the reduction.

PDF is a common method to simulate turbulent combustion, which needs to tabulate parameters like temperature, density and mass fraction. The traditional way is to perform linear interpolation on a table involving such parameters. However, it will consume a lot of memory despite of its simplicity. ANN can correlate input with output, as shown in Fig. 2. Nonetheless, previous ANN tabulation studies need too much training time and have too many nonlinear activation functions to solve, which enlarge the computational costs and time, offsetting the advantage of memory saving. In combination with multi-layer perception (MLP) neural networks for regression and self-organizing maps (SOM) for clustering data, Ranade *et al.*^[24] developed a small and compact ANN, which is more accurate and cost-saving in training and computation compared to previous ANN. The advantage of MLP-SOM is to find optimum number of neurons and subsequently construct a simpler network that can reduce training and interpolation time. In order to compare MLP-SOM approach with traditional interpolation in solution accuracy and computation time, the Reynolds-Averaged Navier-Stokes Models and LES are used to simulate a turbulent jet diffusion flame which is called DLR-A.^[36] A great agreement is achieved between the linear PDF interpolation and MLP-SOM based ANN according to the simulation result. Compared to linear PDF interpolation approach, MLP-SOM method owns the advantage of easily accommodating more parameterized quantities due to 1000 times smaller memory requirements.

Fig. 2 Schematic diagram of MLP-SOM based ANN (adapted from Ranade *et al.*^[24]).

Seltz *et al.*^[25] used a direct numerical simulation (DNS) database of a turbulent premixed stoichiometric methane/air jet flame to train CNN to predict both the filtered progress variable source term and the unresolved scalar transport terms. Then LES method was used to numerically simulate turbulent premixed stoichiometric methane/air flame. The simulation results proved that the CNN could provide quantitatively accurate predictions of both the source and flux terms. The predictive capabilities networks are weakly sensitive to variations in filter width, which is an important attribute for any sub-grid scale model.

Via using CNN, researchers^[25] are allowed to establish a unified modelling framework for all unresolved terms including source and scalar transport terms in the filtered progress variable transport equation in LES simulations of turbulent premixed flames. Using a database from DNS of a turbulent premixed stoichiometric methane/air jet flame, CNN is well trained and shows quantitatively good predictions of all unresolved terms in a priori study, which is in the context of flame tabulated chemistry (premixed flamelet).

Combustion involved into the coupling of many subjects like fluid dynamics, chemical kinetics, heat and mass transfer and so on. Chemical kinetics plays an important role in deeply understanding the mechanism of combustion, even the formation mechanism of astrochemical species like interstellar enols.^[37] So far, the application of ML in combustion theory study has only involved the reduction of chemical kinetic model and optimization of CFD simulation, and has not been used to develop chemical kinetic models. Only constructing an accurate mechanism, can we correctly simulate combustion phenomenon in combination with CFD? The process of constructing a chemical kinetic model needs to adjust the number of chemical parameters, which can be gotten by solving Schrodinger equation. However, the size of chemical space is still overwhelming to model molecules and smart navigation is required, therefore ML can play an important role because the computational strategies automatically improve through experience.^[38] Advances in computational

chemistry and ML are delivering impacts in new catalysis design^[22] and reaction prediction.^[39] Applying ML to chemical kinetics may construct a perfect mechanism that can accurately predict all species profiles.

2.2 Prediction of combustion phenomenon

ML has severely impacted almost all scientific and engineering subjects, and has great potentials to build a new combustion control system. Therefore, it has been used to study combustion phenomena.

Fig. 3 first-second components feature space borrowed from Hachijo *et al.*^[26] (The reuse permission was granted through Rights Link)

Kobayashi *et al.*^[27] and Hachijo *et al.*^[26] combined statistical complexity and ML for detecting thermoacoustic combustion oscillations to avoid it. By combining PCA to estimate the principal component plane and SVM as a binary classifier, a two-dimensional feature space was made to predict thermoacoustic combustion oscillations, as shown in Fig. 3.^[26] The complexity-entropy causality plane (CECP) is another promising way to evaluate complexity in time series data, potentially useful in detecting a precursor of combustion oscillations. The training data samples were divided into three clusters by k-means clustering, which can minimize the distance between noncentral data points and the centroid of each cluster with an SVM classifier.^[27] The result turned out that the CECP feature space constructed by k-means clustering and SVM was an effective way to capture the subtle changes during a transition from low-amplitude combustion noise state to large-amplitude combustion oscillations state, as shown in Fig. 4.

Grogan *et al.*^[28] used ML algorithm to estimate the predictive capability of different combustion parameters like ignition delay time, heat release, chemical sensitivity and etc. under different facilities, fuels and configurations. By means of experimental and simulation data, an ML method which is logistic regression was utilized to demarcate regime transition in shock tubes and Rapid Compression Machines (RCMs) to distinguish detonation and ignition. The decision boundary between ignition and detonation in acoustic residence-chemical resonance plane is obtained. Moreover, it is found that the increased chemical sensitivity has a regularizing effect when plotted against the heat release rate. The classification

considered the influence of combustion devices and the error is reduced to 11.3 %. However, the technique perhaps cannot be used to guide further theoretical ignition analysis for lack of the most crucial physics.

Fig. 4 CECP feature space borrowed from Kobayashi *et al.*^[27] (The reuse permission was granted by American Physical Society)

In order to extract the main features of the flow field and eventually reconstruct the detonation surface, Zhang *et al.*^[29] combined the proper orthogonal decomposition (POD) with ANN to achieve the goals, instead of inconvenient experimental measuring. The POD method decomposed the detonation flow fields into several basic features along with time-varying coefficients, which were subsequently reduced to release the designing and training process of ANN. ANN was key to reach the eventual goal by establishing the mapping relationship between the reduced coefficients corresponding to full flow field and those of the post-surface subfield, whose feasibility was verified by successfully reconstructing the cellular surface of both normal and unstable oblique detonations.

ML can be used to other studies of combustion phenomenon in the future, such as the negative temperature coefficient (NTC) effect, cool flame, and production of soot. NTC effect is a phenomenon that the fuel and ignition delay time increase while immediate species, products and burning velocity decrease with increasing the temperature during a specific temperature span, which emerges in the oxidation of linear alkanes. A well-behaved kinetic model can accurately predict the NTC effect. Cool flame is a kind of flame emerged at a temperature of several hundred K lower than auto-ignition temperature. The formation of soot is believed to be relevant to PAHs, whose profile is hard to be accurately predicted by the existing mechanism. The aforementioned phenomena can be investigated if ML could be used to establish chemical kinetic models.

2.3 Fuel

In the theoretical studies of fuels, there are cases of studying fuels properties and designing the next generation fuels. The compositions of jet fuels are too complex and it's difficult to study physical and chemical properties of fuels by constructing physical models. In the context of materials, ML techniques, a new tool in synthetic chemistry,^[40] are often used

for property prediction, seeking to learn a function that maps a molecular material to the property of choice.^[38] Wang *et al.*^[30] built the correlations between mid-Infrared Fourier Transform Infrared (mid-IR FTIR) absorption spectra and physical and chemical properties for 64 hydrocarbon fuels. The least absolute shrinkage and selection operator (LASSO) regularized linear model, which takes FTIR spectra as input parameters, was developed to accurately predict the physical and chemical properties of fuel. Saldana *et al.*^[31] used the ML method to predict melting points and net heat of combustion of fuels like hydrocarbons, alcohols and esters. The consensus model was developed on the basis of molecular descriptors and functional group count descriptors with the use of various statistical algorithms. The algorithms include Genetic Function Approximation (GFA), Partial Least Squares (PLS) regressions, Feed Forward Artificial Neural Networks (FFANN), general regression neural networks (GRNN), SVM and Graph Machines (GM), as shown in Fig. 5. The predicted values of the model agree well with experimental ones. ML could be a facile and efficient way to design the next generation fuels, which was utilized by Li *et al.*^[32] to conduct a proof-of-concept study for discovering high energy density hydrocarbon (HEDH) fuels. The model based on ML, as shown in Fig. 6, identified 28 hydrocarbon molecules with high density, high net heat of combustion, high specific impulse and low melting point from 319, 895 hydrocarbon molecules. The result turned out that this high-throughput screening strategy was a promising technique to search or design new fuels.

Fig. 5 Schematic representation of the methodology followed for the development of the consensus models (adapted from Saldana *et al.*^[31]).

In the theoretical studies of biofuels, ML was used to discriminate the biomass pellets^[33] and predict activation energy.^[34] Liu *et al.*^[33] developed models to discriminate biomass pellets in combination with Laser-induced breakdown spectroscopy (LIBS) technique and several ML

algorithms including PCA, SVM, extreme learning machine (ELM) and so on, and tested the new technique by discriminating ice husk, redwood, pine wood and rubber wood. The accurate discrimination indicated that the newly built approach of LIBS combined with chemometrics methods was reliable. Compared to the five chosen algorithms, the radial basis function neural network model was the most reliable one and used to develop a visual pseudo-color image to discriminate biomass pellets intuitively with different colors. The study would benefit for screening out biomass pellets with good combustion performance to improve the energy utilization. Jiang *et al.*^[34] studied combustion activation energy of alkali-catalyzed straw pyrolytic carbon. The kinds of straw utilized in reference^[34] are wheat straw, corn straw and sorghum straw. The catalysts are NaOH, KOH and their blends. The algorithms include Linear Regression (LR), Support Vector Regression (SVR) and Random Forest Regression (RFR). Fig. 7 is the flow chart of programming. The realistic activation energy was analyzed by thermogravimetric analysis. The result indicated that it is feasible to apply ML to predict the combustion activation energy. The RFR model was the most suitable model to predict combustion activation energy of alkali-catalyzed straw pyrolytic carbon among the models in reference.^[34] Besides the application in biofuels, ML also plays an important role in the combustion study of biowaste. Wen *et al.*^[35] experimentally quantified the co-combustion/pyrolysis performances of textile dyeing sludge and incense sticks in combination with thermogravimetric analysis and regression ML model under different atmosphere, blend ratio, heating rate and temperature. The operational conditions were optimized by using Box Behnken design and general linear model to identify the significant interactions among blend ratio, heating rate, atmosphere and temperature for different thermogravimetric measurements. The two most important predictors for every measuring method were found based on Random Forest model.

Fig. 6 Schematic diagram for discovering new fuels via ML enabled high-throughput screening (adapted from Li *et al.*^[32]).

Besides the mentioned above, ML may also be used to construct surrogate fuels. Real fuels are composed of several hundred compounds. In order to investigate combustion chemical kinetics, researchers usually choose to blend some representative compounds to get a surrogate fuel similar to real one. When constructing surrogate fuels, researchers need to consider physical and chemical properties of real fuels,

chemical reaction kinetics processes and other features. ML, has been successfully used to predict fuel properties^[30,31] and design the next generation fuels,^[32] perhaps will be applied to construct surrogate fuels.

Fig. 7 The flow chart of the programming (adapted from Jiang *et al.*^[34]).

3. Industrial research

Compared to theoretical studies, there are more industrial ones using ML algorithms. This section will introduce application of ML in industrial studies related to combustion, including power plant,^[41–45] engine,^[46–54] fuel^[55–58] and other fields.^[59–64] To reach the goal of efficient and clean combustion in electric generation, ML was used to classify coals,^[41] monitor combustion process^[42] and treat emissions^[43–45] in power plants. Biodiesel engine^[46–48] HCCI combustion^[49,50] and improving operational methods^[51–54] are three branches of engine design where ML made contributions. Industrial studies about fuel, such as coal fuel^[55,56] and predictions of cetane number (CN)^[57] and octane number,^[58] also utilized ML algorithms. Besides, ML was also applied to other studies, including gas turbine,^[59] particulate matters,^[60–62] organic Rankine cycle^[63] and hydrogen array sensor detection.^[64]

3.1 Power plant

The boiler is one of the most crucial devices in power plants, with a responsibility to transfer heat from flame to working fluid. ML was mainly applied to the combustion of furnace and pollutant treatment. The previous studies include fuel classification^[41] based on flame characteristics and control of combustion processes,^[42] while the latter ones focus on the treatment of CO₂^[43] and NO_x.^[44,45]

Annadurai *et al.*^[41] utilized ML such as Trees, Random Forest, Naïve Bayesian, SVM, ANN and Existing algorithm adopted by Bharat Heavy Electrics Limited, to distinguish fuel types by flicker frequency range. It was challenging to correctly predict fuels due to the ambiguity and uncertainty existing in the algorithms. Annadurai developed a new model that is Time Series Analysis with Fuzzy Support Vector Machine (TSA-FSVM), as shown in Fig. 8. The performance criteria like accuracy, Micro-Precision, Micro-Recall and Micro-F-Measure were compared among the algorithms, and the values of TSA-FSVM are the highest. TSA-FSVM

overcome ambiguity and will play an important role in generating electricity more efficiently and conserving energy.

Fig. 8 Schematic diagram of TSA-FSVM (adapted from Xu *et al.* [41]).

Fig. 9 Bootstrap aggregated ELM (adapted from Bai *et al.* [43]).

To control the combustion processes in the furnace and minimize the incomplete combustion heat loss. Rahmanta *et al.* [42] optimized the control and monitoring system in Furnace Boiler Prototype at Industrial Steam Power Plant by means of ELM and NN. The result indicated that ELM is better than NN, the former one has less training time and average errors.

ML was also applied to the studies of post-combustion pollutants. As shown in Fig. 9, Bai *et al.* [43] built a bootstrap aggregated ELM model consisting of many ELM models, which were developed on bootstrap re-sampling replication of the original training data to predict CO₂ capture rate and level. Choosing the mean square error of the prediction results of different hidden neurons as a comparing criterion, the bootstrap aggregated ELM model excelled a single ELM model in providing more accurate and reliable predictions and model prediction confidence bounds. The training data (50 %), testing data (25 %) and unseen validation data (25 %) came from operation data of thermal power plant, so the bootstrap aggregated ELM would be a promising way to optimize and control post-combustion CO₂ capture processes.

NO_x emissions mainly come from the combustion of coal and coal-derived fuels (like pyridine) [65] in thermal power plant, and recall an effective way to reduce. Yang *et al.* [44] managed to model the relationship between operational parameters and NO_x emission by ML and applied to a 660 WM boiler. After processed by PCA, the input data were respectively put into

LSTM, RNN and Least Squares Support Vector Machine (LSSVM) to build and compare three NO_x emission models. The optimization algorithms like Stochastic Gradient Descent, Root Mean Square prop and Adaptive Moment Estimation were used in the LSTM model to improve the network performance. Comparison results of the three NO_x emission models proved the superiority of LSTM model in solving the long term memory problem. Selective catalyst reaction (SCR) system is a common and expensive approach to NO_x emission control in coal-fire boiler, which is negative to economic benefit of the power plant. To balance the unit thermal efficiency, SCR reagent consumption and NO_x emissions, Si [45] implemented an integrated combustion optimization scheme by genetic algorithm and accurate on-line SVR to achieve the goal of multi-objective optimization. The relationships between process controllable variables and optimization targets and targets were investigated by means of the scheme via the field case study performed at a 160 MW coal-fired unit. The validity of the integrated combustion optimization approach was proven by the field case study, which obtained the feasible optimal solutions in the first stage and achieved the lowest operation cost in the second stage.

The boiler is a device that transfers the chemical energy of fuel into internal energy of the working fluid. There may be catastrophe like heat transfer deterioration during the transfer of heat in flame into steam. An ML model can be trained by the combination of combustion parameters and steam parameters to predict, monitor and control the operation of boiler. The relevant research is still lacking up to now. Apart from NO_x and CO₂, there are other pollutants like CO, SO_x, VOCs and soot, which can be abated by the appliance of ML in the future. For instance, as an effective way to abate CO and VOCs, [66-69] catalyst can be facilely synthesized with the help of ML.

3.2 Engine

Engine is a kind of important power equipment. In order to solve the problems caused by consumption of fossil fuels, ML has been used to many studies about engine like diesel engine consuming biodiesel, [46-48] Homogeneous Charge Compression Ignition (HCCI) [49,50] and the operation of engine. [51-54]

Biodiesel is an effective way to reduce pollution and enlarge energy source. ML has been used to study engines consuming biodiesel. Aghbashlo *et al.* [46] designed a method based on Extreme Learning Machine with Wavelet Transform (ELM-WT) algorithm to estimate the exergetic performance of a DI diesel engine running on diesel/ biodiesel blends, including fuel exergy rate, exergy rate of exhaust gas, exergy transfer rate to cooling water and ambient, exergy destruction rate, exergy efficiency and sustainability index. Besides ELM-WT, other algorithms like ELM, Genetic Programming and ANN were also used to predict seven parameters. The outperformance of ELM-WT was proved by comparing error statistical indicators of the four models: root mean square error, Pearson correlation coefficient and coefficient of

determination. ELM is a single layer feed forward NN, as shown in Fig. 10. Silitonga *et al.*^[47] used Kernel-based Extreme Learning Machine (KELM) to analyze the performance, emission and combustion characteristics of a turbocharged diesel engine fueled with Jatropa curcas biodiesel-diesel blends. The coefficient of determination of the parameters is within a range of 0.9805–0.9991 for both the KELM model and the experimental data, while the mean absolute percentage error (MAPE) is within a range of 0.1259–2.3838. Silitonga *et al.*^[48] used the same model to evaluate the engine performance exhaust emissions of a single-cylinder diesel engine fueled with biodiesel-bioethanol-diesel blends. Besides, results showed that this algorithm is of a learn speed thousands times faster than the conventional popular learning algorithms. The engine performance parameters evaluated are the brake specific fuel consumption and brake thermal efficiency whereas the exhaust emission parameters evaluated are carbon monoxide, nitrogen oxide, and smoke opacity. The predictive results agree well with experimental ones, which suggests that the KELM model is a reliable technique to predict the engine performance and exhaust emission parameters of biodiesel-bioethanol-diesel blends.

Fig. 10 Single layer feed forward NN (adapted from Aghbashloet *al.*^[46]).

HCCI is a new combustion method that the fuel is burned by autoignition instead of spark. The primary challenge of HCCI autoignition is to ensure that the burn timing is synchronized against the motion of the piston, to avoid noisy combustion and unstable combustion oscillation. HCCI involved nonlinear chemistry, nonlinear physics, period-doubling bifurcation, turbulent mixing and so on, which result in high cyclic variability and difficult prediction of combustion timing. Vaughan *et al.*^[49] proposed a Weighted-Ring ELM, an online adaptive ML model to offer an accurate, causal combustion timing prediction. The algorithm can also enable a new class of real-time model predictive strategies for HCCI, emitting less NO_x and CO₂. Janakiraman *et al.*^[50] developed an ELM model based on stochastic gradients (SG-ELM). Janakiraman *et al.* built the online models by means of

SG-ELM and online sequential extreme learning machines (OS-ELM) respectively, to get HCCI engine state variable and dynamic operating envelope. The results prove that good generalization performance can be achieved by both means and the SG-ELM might have an advantage in terms of stability, crucial for designing robust control systems.

Fig. 11 Process of the energy management strategy based on DDQL algorithm (adapted from Han *et al.*^[51]).

Han *et al.*^[51] proposed an energy development strategy based on double deep Q-learning (DDQL) algorithms for a dual-motor driven hybrid electric tracked-vehicle, as shown in Fig. 11. It is easy to lead to an overoptimistic evaluation of the results if the same network is used for both selecting action and evaluating value function. Han *et al.* utilized two deep NNs naming action selecting network Q and target updating network Q' to decouple action selection and evaluation. Han *et al.* also used conventional deep Q-learning (DQL) and dynamic programming (DP) to get driving schedules. The simulation results were compared between DQL and DDQL based on the results gotten from DP. The comparison suggested that the fuel economy of DDQL achieved 7.1 % better than DQL and reached 93.2 % level of DP. The results substantiate the effectivity and robustness of proposed methodology in terms of SOC convergence performance and fuel consumption level.

Li *et al.*^[52] developed an air-fuel ratio (AFR) control method combined with fuzzy feed-forward, intelligent PI feedback and self-learning control, as shown in Fig. 12. The conclusion was drawn from the simulation on Matlab and engine bench test that this technique could perfectly correct the AFR deviation during the compressed natural gas engine stationary and transient operations. The method could rapidly respond to the dynamic changes of engines, improve the AFR control accuracy required by three-way catalyst converter purification rate and reduce exhaust emissions.

Fig. 12 Structure of AFR control method (adapted from Li *et al.*^[52]).

Namigtle-Jimenez *et al.*^[53] proposed a faulty detection and diagnosis scheme that extracted the oil pressure as the only signal for isolating the damaged injector of an internal combustion engine. The arrangement of scheme consisted of three coupled ANNs shown in Fig. 13. ANNs were trained by Levenberg-Marquardt (LM), BFGS quasi-Newton, and Gradient Descent (GD). The offline comparison of the four training algorithms was carried out to select the best one to function online. The results demonstrated that the LM was the best option that reached a 100 % classification offline and near 100 % classification online.

Fig. 13 Neuronal networks final structure (adapted from Namigtle-Jimenez *et al.*^[53]).

Yan *et al.*^[54] obtained a reciprocating motion control strategy of free piston by ML. The control problem was decomposed to the stroke control, the top turning center control and the bottom turning center control, corresponding to a finite-state machine, iterative learning controller and combustion state estimation as control method respectively. A combined simulation model was presented based on the combination of the three methods, including combustion fluctuations and the validity of the model was proved by a

prototype. The simulation and test results suggested that the good control of the stable reciprocating motion was obtained by the strategy.

There are many kinds of engines. The ignition modes of engine include spark ignition, compression ignition, HCCI, Partially Premixed Combustion (PPC) and Reactivity Controlled Compression Ignition (RCCI). Every ignition method has its flaws. The spark ignition will produce CO and HC along with severe detonation. More NO_x and soot will be formed by compression ignition. HCCI cannot control the combustion timing and exothermic rate. PPC and RCCI have low burning efficiency and more HC and CO. ML can be used to solve the problems.

3.3 Fuel

Besides theoretical studies described in Section 2.3, ML was also used to overcome difficulties about fuel in industrial research.

Fig. 14 Diagram of the multilayer NN (adapted from Abdurakipov *et al.*^[55]).

Coal is the most widely used fuel in the world. It is necessary to develop new, economically viable and environmentally friendly technologies for coal combustion. The treatment of coal fuel in high-stress pulverizers on newly formed surfaces forms active centers that can accelerate the progress of physicochemical reactions. Abdurakipov *et al.*^[55] experimentally investigated the influence of high-stress pulverization on the degree of burnout of coal fuel and analyzed the applicability of a neural network-based mathematical model for predicting the degree of burnout of coal fuel treated in high-stress pulverizers. The model of four-layer ANN was developed as shown in Fig. 14, which consisted of an input layer (17 input parameters), three hidden layers (neurons are 64, 32 and 8 respectively) and an output layer (one neuron). Learning data consisted of temperature, heating rate, coal type, and a degree of pulverization, including training (80 %) and testing parts (20 %). A mean absolute percentage error is used as a model error function that is minimized as the NN learns. The results showed that the model of the four-layer ANN quite accurately reproduced the main effects of the influencing parameters and allowed one to highly accurately determine the coal mass loss coefficient

using the given parameters: coal type, pulverization method, temperature, and heating rate.

Coal and its combustion products contain rare earth elements like Eu. The existence of Ba will interfere with the measuring of Eu, there is a threshold value for Ba/Eu beyond which the Eu concentration gotten by quadrupole-based inductively-coupled plasma mass spectroscopy (ICP-Q-MS) is not reliable. Xu *et al.*^[56] implemented LR, regression tree to predict the threshold value of Ba/Eu. The established model predicted that the interference of Ba to the measurement of Eu could be neglected when Ba/Eu values were less than 363.

Fig. 15 Model architecture including inputs, two hidden layers of 32neurons, and an output (adapted from Kessler *et al.*^[57]).

The method to predict the CN which is the measure of ignition quality can accelerate the research process of the next-generation alternative fuels. Derived cetane number (DCN) could be an alternative of CN and obtained by ignition quality tester (IQT). ANN could be used to establish an effective model to predict CN of a fuel,^[70] the structure and key learning variables of which were optimized by Kessler *et al.*^[57] to incorporate more kinds of fuels, especially furans and furan derivatives. The optimized structure consisted of an input layer containing 15 molecular descriptors, two hidden layers of 32 neurons each and an output neuron, as shown in Fig. 15. The optimization effect was validated from the more accurate CN predictions and slightly larger Root-Mean-Square-Error (RMSE) than the previous.

Wang *et al.*^[58] applied the ELM, OS-ELM, Self-adaptive evolutionary Extreme Learning Machine (SaDE-ELM) respectively to predict the octane number and compared the three models by means of the statistical parameters like RMSE, Correlation Coefficient, R^2 and the execution time. The prediction accuracy, generalization ability and stability of the ELM were improved by OS- and SaDE-ELM in different levels. Besides, many other ML algorithms have been used to analyze and predict gasoline components like ANN, RBFNN, Adaptive Neuro-Fuzzy Interface Systems and SVM.

The incomplete combustion will result in the formation of HC and CO which is responsible for pollution. ML has not been used to study incomplete combustion yet.

3.4 Other industrial studies about combustion

There are amount of other fields about combustion or post-combustion disposal where ML was applied, such as studies of gas turbine,^[59] particulate matter (PM),^[60-62] organic Rankine cycle^[63] and detection of hydrogen sensor.^[64]

Yan *et al.*^[59] proposed a deep Semi-Supervised Anomaly Detection (deepSSAD) combining DL and semi-supervised learning algorithms to detect gas turbine combustor anomalies. The model was composed of two steps: using DL to learn representations or features from multivariate and time-series sensor measurements and using one-class classification to model normality in the learned feature space. The approach achieved a good performance comparing the data collected from a real-world gas turbine combustion system. This method outperformed others too.

Fig. 16 Endpoint forecasting network of composite regeneration due to coupling cerium-based additive and microwave for diesel particulate filter (adapted from E *et al.*^[60]).

With the help of Fuzzy Least Squares Support Vector Machines (FLS-SVM), E *et al.*^[60] developed a mathematical model which is shown in Fig. 16 to investigate the major factors affecting the time of composite regeneration of diesel particulate filter. The regeneration was affected by the coupling cerium-based additive and microwave. The simulation results with the relative error less than 3.5 % for endpoint forecasting indicated that main factors affecting the regeneration time are the oxygen concentration of exhaust gas, the mass flow rate of exhaust gas, the microwave power, the temperature of exhaust gas and the amount of cerium-based additive.

Siegel *et al.*^[61] built a classification model by decision tree, which can detect filter contaminant loading from audio data collected by a smartphone or stand microphone. The robustness of the model was verified by changing vehicle type (Hondo and Mazda), loading states (clean, dirty and filthy) and microphone type (iPhone and TASCAM). The results showed that 80 % of accuracy can be achieved.

Rutherford *et al.*^[62] combined excitation emission matrix (EEM) fluorescence spectroscopy and CNN to identify PM source. PM came from wood burning, diesel exhaust and cigarettes using filters, with the limits of detection being 0.7,

2.6 and $0.9 \mu\text{g}/\text{m}^3$, respectively. The overall classification accuracy for all three sources was 89%.

Xu *et al.*^[63] applied ML to optimize organic Rankine cycle waste heat recovery system. Three real-time implementable power optimization methods respectively based on Proportional-Integral-Derivative (PID), Nonlinear Model Predictive Control (NMPC) and Dynamic Programming Random Forest (DP-RF) were compared. Xu *et al.* adopted random forest model to extract rules for DP, as shown in Figs. 17 and 18. The comparison results showed that the DP-RF method had similar performance to NMPC method and outperformed the PID method while the computation costs of DP-RF were less than NMPC.

Fig. 17 Diagram of DP-RF optimization method training process (adapted from Xu *et al.*^[63]).

Fig. 18 Schematic of RF model in DP rule extraction (adapted from Xu *et al.*^[63]).

Song *et al.*^[64] utilized moving window principle component analysis and extreme learning machine (MWPCA-ELM) to propose a novel fault diagnosis and reconfiguration strategy for hydrogen sensor array. The effectiveness and feasibility of the strategy were illustrated by the decreased average relative error from 1.18% to 0.82% of hydrogen concentration estimated from a monitoring experimental system.

4. Summary

The appliances of ML to combustion studies were reviewed in the paper. Among the combustion theory studies, most of

which are relevant to fuels,^[30-35] part of which are targeted to study combustion phenomenon,^[26-29] and only a few of studies concentrate on CFD simulation.^[23-25] In industrial studies, ML has been used to study power plant boiler,^[41-45] engine,^[46-54] fuel^[55-58] and other fields.^[59-64]

ML can be used to reduce mechanism, save PDF table memory and predict terms filtered by LES, in order to balance computation costs and accuracy of CFD combustion simulation. In the combustion phenomenon studies, ML is used to construct feature space, to predict thermoacoustic combustion oscillations, distinguish detonation and ignition in RCMs and shock tubes, and reconstruct the detonation surface. ML also plays an important role in studying chemical and physical properties, designing the next generation fuel and studying biofuels.

Compared with theoretical studies, ML is more widely used in industrial ones. ML in power plant studies focused on monitoring combustion in furnace and disposing post-combustion pollutants. In the engine studies, ML was used to study the performance of diesel, combustion timing and dynamic operating envelope of HCCI and operation or control of engine. In the industrial studies about fuels, ML was utilized to investigate the influence of high-stress pulverization on the degree of burnout of coal fuel, obtain the threshold value of Ba/Eu in coals and combustion products, predict the CN of biofuels and octane number of gasoline. Apart from those fields, ML can also be used in PM, monitoring gas turbine combustor anomalies, fault diagnosis and reconfiguration of hydrogen sensor array and optimization of organic Rankine cycle waste heat recovery system.

5. Perspectives

As a powerful instrument to build model, ML is attracting more and more attention in combustion investigations recently. This paper reviewed the applications of ML in theoretical and industrial combustion studies, and some recommendations will be given here.

1) From the present results, ML applies more to industrial studies of combustion and less on theoretical ones. Theoretical studies need more assistance from ML, especially combustion chemical kinetics. Combustion kinetic study will help us deeply understand combustion process, and give guidance to efficient combustion and low pollution emissions. The most important thing in kinetic research is to construct the kinetic models. A perfect mechanism can accurately predict profiles of reactants, products and intermediate species. A chemical kinetic model usually contains hundreds of species and thousands of reactions, which means a large number of parameters need to be adjusted. Determination of parameters is a task depending on experience. ML is good at building a model or function from data, which may help to build an efficient mechanism if applied in chemical kinetic studies.

2) NTC effect and cool flame will emerge in combustion of linear alkanes. It's an important criterion to judge kinetic models that whether the NTC effect can be accurately

predicted. The current chemical kinetic models can hardly get an accurate prediction of PAHs, which are precursors of soot, therefore the mechanism can't predict soot satisfactorily. If a well-behaved chemical kinetic model is developed based on ML, then the phenomena like NTC effect, cool flame and soot will be successfully investigated.

3) The realistic fuels like gasoline, kerosene, diesel and so on are usually composed of hundreds of components, which makes it impossible to simulate real fuels. The popular method is to simulate surrogate fuels having similar properties like carbon-hydrogen ratio, molar mass, combustion heat and so on. ML has been used to predict fuels properties and design the next generation fuels, which means it will play important roles in constructing surrogate fuels in the future.

4) The effects of furnace are to function as a combustion chamber and transfer heat from flame to working fluid. Heat transfer deterioration will cause catastrophes, damage boiler and hurt people. ML can be used to develop a strategy to monitor boiler parameters and furnace parameters meanwhile to avoid tragedies like heat transfer deterioration.

5) The combustion methods of engine include spark ignition, compression ignition, HCCI, PPC and RCCI. Low-temperature combustion exists the problems like low efficiency and high emissions of HC and CO. The high temperature will produce more NO_x and soot. HCCI cannot control combustion timing and exothermic rate. ML has been widely used in engine research, but more efforts will be paid to solve the mentioned problems.

6) As for study with respect to the post-combustion pollutants, ML has only been applied to deal with CO₂, NO_x and particulates up to now. However, the emissions formed in combustion are far more than the 3 species. CO and PAH will emerge during incomplete combustion of fuels, harming the environment and the human body. ML will be helpful in the disposal of other pollutants.

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Supporting information

Not applicable.

Conflict of interest

There are no conflicts to declare.

Nomenclature

AFR	Air-Fuel Ratio
ANN	Artificial Neural Network
ASR	Automatic Speech Recognition
CECP	Complexity-Entropy Causality Plane
CFD	Computational Fluid Dynamics
CN	Cetane Number

CNN	Convolutional Neural Network
DCN	Derived Cetane Number
DDQL	Double Deep Q-Learning
DL	Deep Learning
DLR	Deutsches Zentrum für Luft- und Raumfahrt
DNS	Direct Numerical Simulation
DP	Dynamic Programming
DP-RF	Dynamic Programming Random Forest
DQL	Deep Q-Learning
EEM	Excitation Emission Matrix
ELM	Extreme Learning Machine
ELM-WT	Extreme Learning Machine with Wavelet Transform
FFANN	Feed Forward Artificial Neural Networks
FLS-SVM	Fuzzy Least Squares Support Vector Machines
GD	Gradient Descent
GFA	Genetic Function Approximation
GM	Graph Machines
GRNN	General Regression Neural Networks
HCCI	Homogenous Charge Compression Ignition
HEDH	High Energy Density Hydrocarbon
HWR	Handwriting Recognition
ICP-Q-MS	Inductively-Coupled Plasma Mass Spectroscopy
IQT	Ignition Quality Tester
KELM	Kernel-based Extreme Learning Machine
LASSO	Least Absolute Shrinkage and Selection Operator
LES	Large Eddy Simulation
LIBS	Laser-Induced Breakdown Spectroscopy
LM	Levenberg-Marquardt
LPCA	Local Principal Component Analysis
LR	Linear Regression
LSSVM	Least Squares Support Vector Machine
LSTM	Long-Short Term Memory
MAPE	Mean Absolute Percentage Error
mid-IR FTIR	mid-Infrared Fourier Transform Infrared
ML	Machine Learning
MLP	Multi-layer Perception Neural Networks
MWPCA-ELM	Moving Window Principle Component Analysis and Extreme Learning Machine
NLP	Natural Language Processing
NMPC	Nonlinear Model Predictive Control
NN	Neural Network
NO _x	Nitrogen Oxides
NTC	Negative Temperature Coefficient

OS-ELM	Online Sequential Extreme Learning Machine
PAHs	Polycyclic Aromatic Hydrocarbons
PCA	Principal Component Analysis
PDF	Probability Density Function
PID	Proportional-Integral-Derivative
PLS	Partial Least Squares
PM	Particulate Matter
POD	Proper Orthogonal Decomposition
PPC	Partially Premixed Combustion
RBFNN	Radial Basis Function Neural Network
RCCI	Reactivity Controlled Compression Ignition
RCMs	Rapid Compression Machines
RDR	Random Forest Regression
RL	Reinforcement Learning
RMSE	Root-Mean-Square-Error
RNN	Recurrent Neural Network
SaDE-ELM	Self-adaptive evolutionary Extreme Learning Machine
SCR	Selective Catalyst Reaction
SG-ELM	Stochastic Gradients Extreme Learning Machine
SOM	Self-Organizing Maps
SPARC	Sample-Partitioning Adaptive Reduced Chemistry
SSAD	Semi-Supervised Anomaly Detection
SVM	Support Vector Machine
SVR	Support Vector Regression
TSA-FSVM	Time Series Analysis with Fuzzy Support Vector Machine
VOCs	Volatile Organic Compounds

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