International Conference on Applied Energy 2021
Nov. 29 - Dec. 5, 2021, Thailand/Virtual
Paper ID: 0368

Enhancing Autoignition Characteristics: A Framework to Discover Fuel Additives and Making Predictions Using Machine Learning

Shahid Rabbani

Mechanical Engineering Department, Khalifa University, Abu Dhabi 12778, UAE

ABSTRACT

Combustion process can become more energy efficient and environment friendly if used with appropriate fuel additive. Discovery of fuel additive can be accelerated by applying hybrid approach of using of chemical kinetics and Machine Learning (ML). In this work we present a framework that takes the robustness of Machine Learning and accuracy of chemical kinetics to predict the effect of fuel additive on autoignition process. We present a case of making predictions for Ignition Delay Time (IDT) of biofuel n-butanol (C_4H_9OH) with several fuel additives. The proposed framework was able to predict IDT of autoignition with high accuracy when used with unseen additives. This framework highlights the potential of ML to exploit chemical mechanisms in exploring and developing the fuel additives to obtain the desirable autoignition characteristics.

Keywords: Fuel additive, machine learning, ignition delay, emissions, renewable energy

1. INTRODUCTION

In the wake of fast changing global climate scenario, a lot of emphasis has been laid on reducing hazardous emissions and using renewable energy solutions. Specially during the last few years, climate change has become a global challenge and many regions have already started experiencing its impact. Fortunately, during the same time period, ML algorithms have come of age and helping researchers in tackling variety of challenges. Also, for climate change, ML is proving to be very helpful in suggesting ways to reduce emissions [1]. For conventional fuels - which have been found to contribute significantly to increase emissions - ML has high potential to find ways to reduce emissions. For example, Li *et al.* used ML approach to explore organic waste to find equivalent renewable energy source of fossil fuels [2]. Badra *et al.* used combined approach of Computational Fluid Dynamics and ML to optimize combustion process [3]. Despite all these applications of ML to minimize effects of climate change and making combustion process more environment friendly, it can be noted that not much attention has been devoted to find fuel additives which can provide desirable emissions related characteristics of burning fuels.

In this work, we present a framework that uses ML algorithm and chemical kinetics to discover fuel additives. First we present the methodology that was employed to obtain data and train the model, and then we present results for fuel additives obtained using the framework.

2. METHODOLOGY

As an application of the framework we present a case of finding IDT for autoignition of n-butanol. The approach of exploring new additives using this framework consist of three main steps:

First step consists of obtaining results of IDT for n-butanol using experimentally validated chemical kinetics mechanism [4] which consists of 6 elements (C, H, N, O, Ar and He), 243 species and 2892 unidirectional reactions. Adiabatic autoignition of butanol at constant-volume was considered for simulations. Apart from n-butanol, total of 50 stable species were found in the

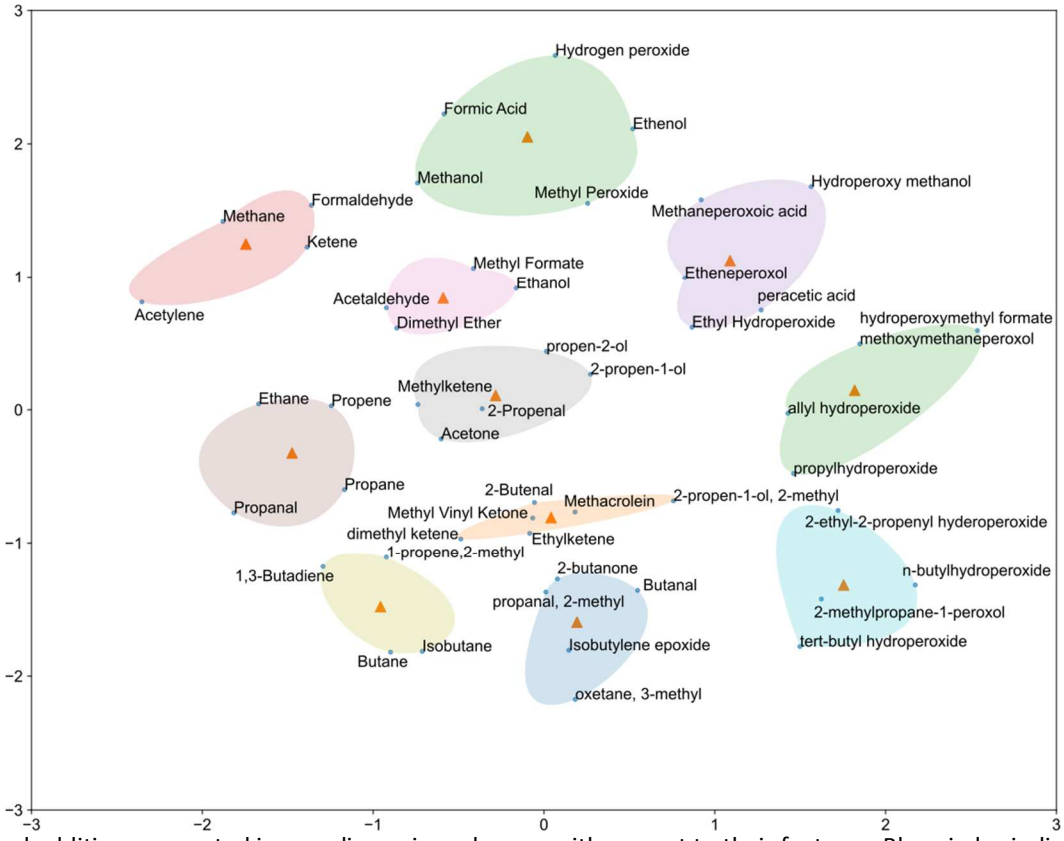

Fig. 1. Clusters of fuel additives presented in non-dimensioonal space with respect to their features. Blue circles indicate spatial position while orange triangles denote centroid of clusters.

mechanism which were used as additive in volumetric ratios of 0.0 (pure n-butanol), 0.01, 0.1, 0.2, 0.4, 0.6 and 0.8. IDT were obtained by running separate simulations for all these additives. For each additive, above mentioned volumetric ratios were considered in combination of different input conditions of temperature, pressure and stoichiometric ratios. Details of these input parameters are given in Table 1.

It should be noted that all these combinations of initial conditions do not necessarily lead to ignition, therefore those simulations that did not result in ignition were omitted from the data such that total number of IDT data points obtained in this work count to 11,732.

Second step comprises of finding the features of all 50 additives used in step 1 to characterize the fuel additive. In this work, we divided features into five categories: (i) Chemical (3D atom count, 3D anion-count etc.), (ii) Physical (Total Polar Surface Area (TPSA), volume of molecule, XlogP etc.), (iii) Compositional (no. of C atoms, molecular weight etc.) and (iv) Structural (bag of bonds such as no. of O-O bonds, number of C=C bonds etc.) and (v) Thermodynamic properties (coefficients of polynomials used to represent thermodynamic data used in NASA chemical equilibrium code [5] etc.). All these features sum up to 46. Figure 1 shows additives plotted using Multi-Dimensional Scaling (MDS) of all features such that similar additives cluster together. For example, butane and iso-butane have many features in common, hence they share lose proximity.

Figure 2 shows distribution of IDT obtained in step 1 when plotted against features obtained in step 2. Although in this figure, IDT is plotted against only six features, yet it can be seen that features of fuel additives relate to IDT with clear patterns. Third step is to exploit such patterns of additive features with IDT using ML. Deep Neural Network (DNN) were employed in this work to fit the IDT with additives features and initial conditions. First a DNN model was generated with full

Input	**Value**
Temperature (K)	1100, 1350, 1600, 1800
Pressure (atm)	1,4,8
Equivalence Ratios	0.6, 1.0, 1.8
Number of Additives	50
Additives Mixing Ratios (vol.)	0.0, 0.01, 0.1, 0.2, 0.4, 0.6, 0.8

Table. 1. Range of parameters used to generate data set

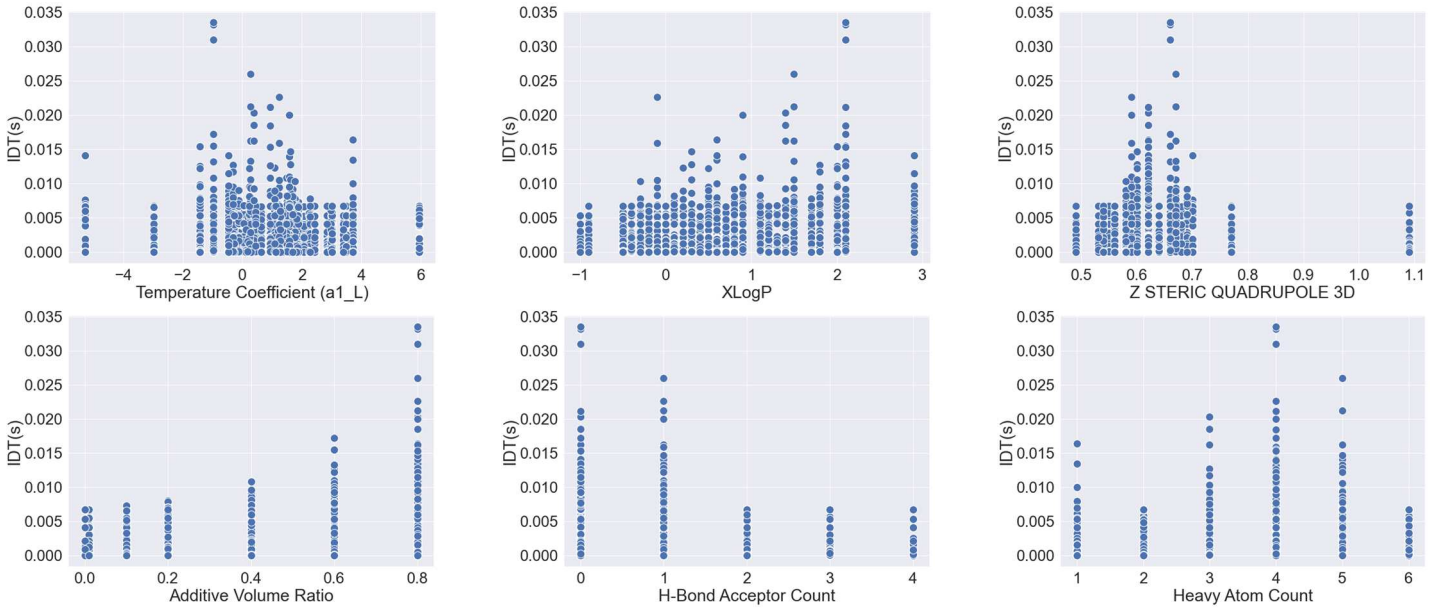

Fig. 2. Scatter plots of IDT with few features of fuel additives.

data of all 50 additives such that 80% of data was used to train the model while 20% data was used for testing purpose. This model was tested to predict the IDT with the different initial conditions of additives for which model was trained.

Once it was established that model can predict the IDT with additives which were part of DNN training, the study was extended to predict the IDT for additives which were not trained in the network so that the capability of this framework to predict the effect of new additives can be assessed. To achieve this objective, another DNN model was trained with only 48 additives and results were tested for two additives which were not part of new trained model.

In the next sections, first the results of trained model for 50 species are presented, followed by the results of DNN model trained on 48 additives to predict IDT for two unseen additives. Here '*unseen*' is referred to the additives which were not part of DNN trained on 48 additives.

3. RESULTS

This section is divided into two parts. In the first part results of the multi-layer DNN are presented where model was trained and tested for 50 additives. The second part relates to the DNN model which was trained for 48 additives and was tested for two unseen additives.

3.1 Evaluation for all 50 additives

Figure 3 shows the comparison between true values of IDT – which were obtained from autoignition simulations - with IDT obtained from DNN model trained on 50 species. This figure shows the predictions against randomly selected test data points which are 20% of all the available data for 50 species.

Overall R2 score for the test data was 0.99. It can be seen that most of the IDT values are below 0.10 s and less than 10 values are above 0.10 s which have relatively high error. This distribution of error can also be seen in Figure 4. This distribution is reasonable because most of the data used for training has IDTs below 0.10 s which leads to high accuracy for region below 0.10 s.

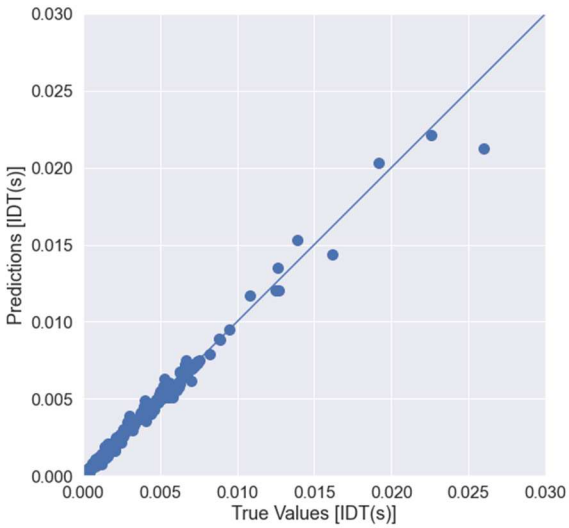

Fig. 3. Comparison of predicted vs true values of IDT for test data using the model trained on 50 additives.

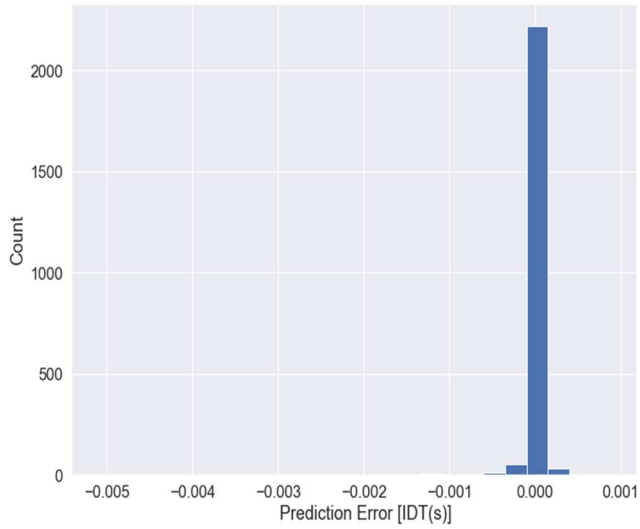

Fig. 4. Error distribution for predictions of test data using model trained on 50 additives.

3.2 *Evaluations for unseen additives*

To test the framework for unseen additives, data points for two additives were completely omitted from the training data and a new DNN was trained on 48 additives. The two unseen additives were ethane (C_2H_6) and methyl-vinyl-ketone ($C_2H_3COCH_3$). It can be seen from Figure 1 that $C_2H_3COCH_3$ has features which are similar to several other close fuel additives such as ethyl ketene and 2-butenal. This shows that although $C_2H_3COCH_3$ is not included in the training data, however training data contains fuel additives which have similar features. Unlike $C_2H_3COCH_3$, C_2H_6 does not share close proximity with other fuel additives. This indicates that training data does not contain fuel additives which have as similar features to C_2H_6 as $C_2H_3COCH_3$. Using this selection of additives will enable to assess the capability of model to predict IDT for unseen additives; irrespective of similarity in features with training data.

Figure 5 shows that result of IDT predictions against true values for C_2H_6 and $C_2H_3COCH_3$. It can be seen that predicted values are close to true IDT values. Similar to Figure 3, most of the data points locate below 0.004 s. Although the points are more dispersed as compared to DNN trained on 50 species, however R2 score is still 0.97 which indicates high accuracy. So, the trained model on 48 additives is found to successfully predict IDT for the unseen additives.

3.3 *Conclusions*

In this work, a framework to predict autoignition characteristics -both for seen and unseen additives - is presented. The framework combines the accuracy of

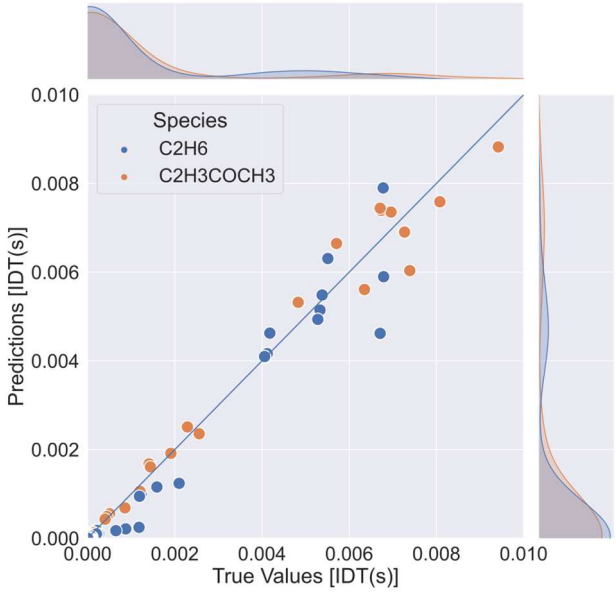

Fig. 5. Comparison of predicted vs true values of IDT for unseen additives using model trained on 48 additives. Top and right plots show distribution of data points.

experimentally validated chemical mechanism and robustness of ML to predict autoignition characteristics. An example of renewable fuel n-butanol is presented to predict IDT for trained and untrained fuel additives. It was shown that the framework was able to capture the chemical kinetics to predict IDT for the additives included in the chemical mechanism. Moreover, framework was also successfully able to predict IDT for species which were not part of DNN trained model. As shown using the case of unseen additives, this work also highlights the applicability of this framework to study fuel additives which are not part of chemical kinetic mechanism, thus opening a new whole new domain to explore and discover new fuel additives to achieve desired autoignition characteristics. In summary, the framework can be used to:

- Study the effect of new fuel additives; irrespective of their presence in chemical kinetics mechanism.
- Predict the effect of new additives on emission such as NO_x, CO, CO_2, CH_2O etc.
- Predict maximum heat generation during autoignition process.
- Predict adiabatic flame temperature during autoignition process.
- Predict flame-type using new additive.

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