Ignition delay time model based on a deep neural network

Agnieszka Jach, Mateusz Zbikowski, Konrad Malik, Andrzej Teodorczyk
Insitute of Heat Engineering, Warsaw University of Technology
Warsaw, Poland

1 Introduction

The ignition delay time (IDT) is one of basic properties describing any flammable mixture and it is very important in process safety management. IDT is usually modeled with detailed reaction mechanisms (DRMs), however those calculations might be very time consuming and DRMs are still being developed and refined. The authors of the recent paper accumulated around 1800 IDTs from shock tube experiments for various C1–C7 hydrocarbon–O_2–Ar mixtures. This amount of points becomes sufficient for deployment of one of Machine Learning algorithms - a deep neural network (DNN). Machine Learning is widely used in numerous aspects of life, for instance: self-driving cars, handwriting recognition, anti-spam filtering, web search and rating systems. Now it is becoming more popular in science as well. A DNN is based on an artificial neural network which is inspired by the biological neural networks. The biggest advantage of DNNs is high predictive power and flexibility of application. According to authors' best knowledge IDTs have not been yet modeled with a DNN. Hence, the goal of the recent paper is to introduce a new ignition delay time model based on a DNN technique.

2 Model

A large data set of ignition delay times is collected for C1–C7 hydrocarbon-oxygen-argon mixtures (1789 points in total) from shock tube experiments [1–28]. The data set can be briefly summarized as follows:

- the collected IDT range is from 2.6 μs up to 2.11 ms;
- C1–C7 hydrocarbons are methane, ethane, ethene, acetylene, propane, propene, *iso*- and *n*-butane, *1*- and *iso*-butene, *n*-, *neo*- and *iso*-pentane, *1*-pentene, *n*-hexane, *1*-hexene and *n*-heptane;
- temperature range is 1022–2596 K, pressure 0.3–267 bar, EQR 0.06–4.0, argon molar fraction 54.5%–99.93%.

Correspondence to: agnieszka.jach@pw.edu.pl

The DNN model is developed based on following assumptions:

- the whole dataset of 1789 examples is divided into train and test sets in a proportion of 80/20;
- the number of inputs is equal to 7 (fuel type, fuel molar fraction, oxygen molar fraction, argon molar fraction, initial pressure (bar), initial temperature (K), inverse of initial temperature (1/K), one can note that higher number of inputs is desirable from feature engineering point of view);
- the output is ignition delay time (μs);
- activation function for all hidden layers is hyperbolic tangent;
- identity function is used for the output layer.

The deployment of the model structure presented in Figure 1 (the number of hidden layers, the number of nodes in each layer and the L2 regularization parameter [29]) is described in detail in the paper of Malik et al. [30].

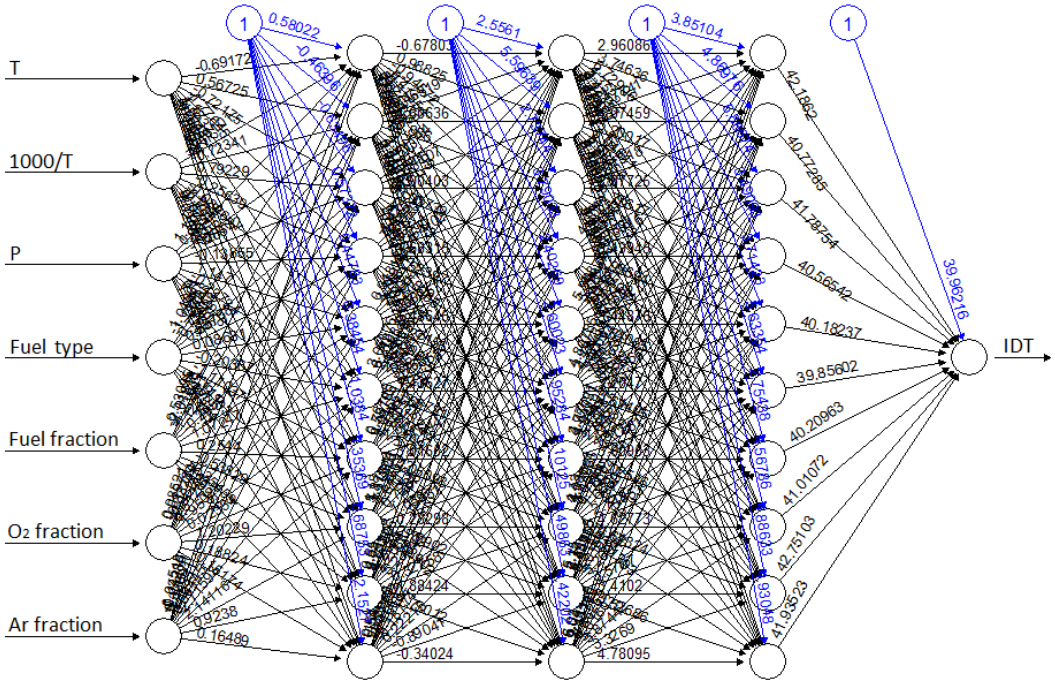

Figure 1: Deep neural network structure used in the present study

3 Results

The performance of the DNN model is measured by Mean Absolute Error (MAE) and the Pearson coefficient (CORR), which measures linear correlation between two sets of values. CORR is defined as follows:

$$CORR(x,y) = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2}} \tag{1}$$

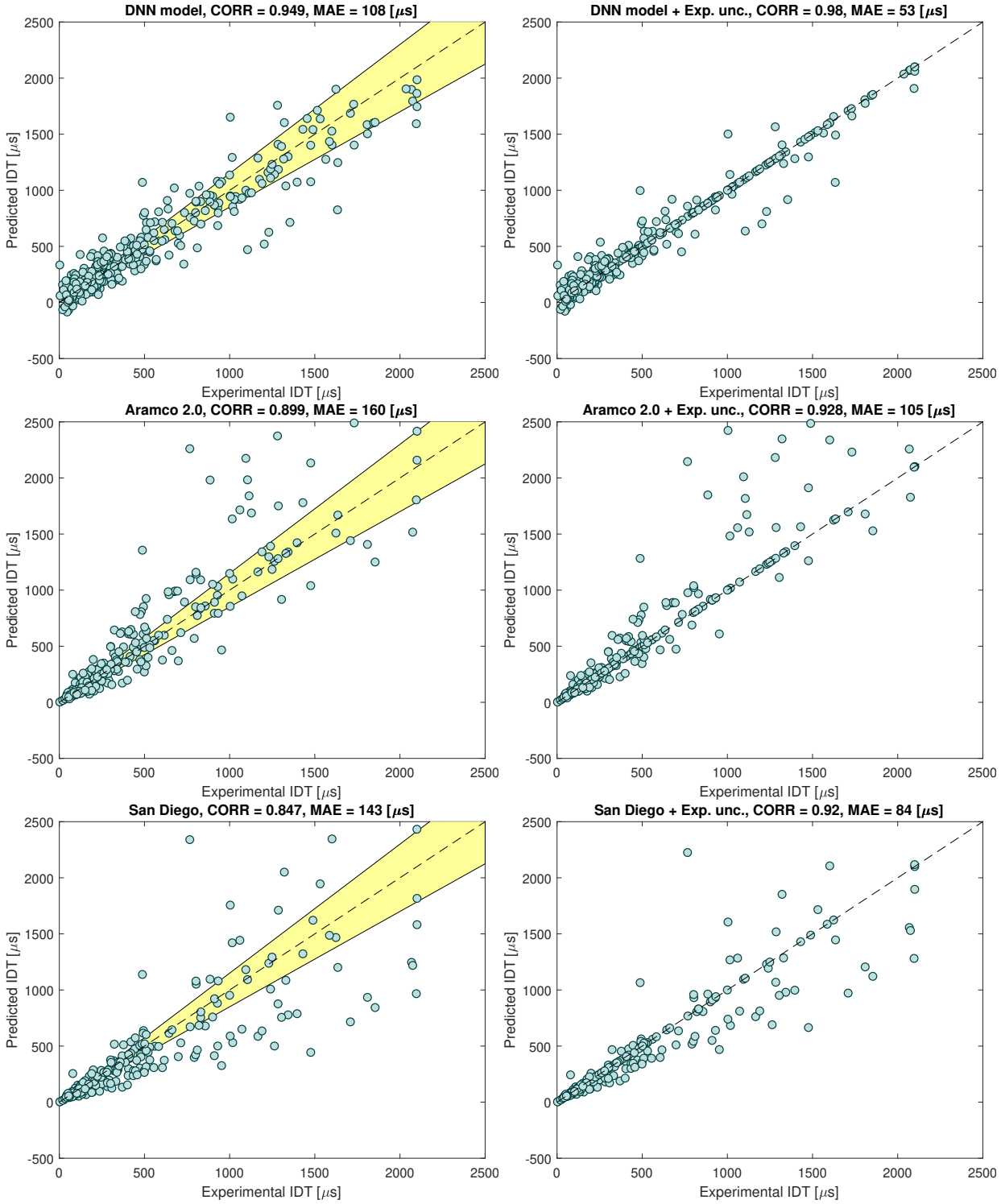

Figure 2: Predicted IDT vs. experimental IDT. Comparison of DNN model to Aramco 2.0 and San Diego 2014. Left: Experimental uncertainty is marked by the yellow area. Right: Experimental uncertainty is taken into account in CORR and MAE calculations.

where x and y are vectors of experimental and predicted ignition delay times, n is the sample size (size of both samples is equal).

In Figure 2 the DNN performance on a test set is presented and compared to two well-known DRMs: Aramco 2.0 [5,28,31–35] and San Diego 2014 [36]. In the left column of Figure 2 experimental uncertainty range (assumed as IDT $\pm$ 15%) is marked by yellow area. Predictions belonging to the *area* are considered as perfect match to experiment. In the right part of Figure 2 experimental uncertainty is taken into account while calculating CORR and MAE. Additionally, in Table 1 the DNN model is compared with NUIG n-Heptane [37] and GRI-mech 3.0 [38]. The DNN model reaches higher CORR and lower MAE than the *best* DRMs' (NUIG n-Heptane: MAE = 85 μs, CORR = 0.933, the DNN: MAE = 53 μs, CORR = 0.98, Table 1).

Table 1: Comparison of DNN model to DRMs.

Metric	DNN	Aramco 2.0	NUIG n-Heptane	GRI-mech 3.0	San Diego 2014
without experimental uncertainties					
CORR	0.949	0.899	0.902	0.645	0.847
MAE	108	160	136	599	143
with experimental uncertainties					
CORR	0.980	0.928	0.933	0.648	0.920
MAE	53	105	85	547	84

4 Conclusion

The DNN model for IDT of C1–C7 hydrocarbon-oxygen-argon mixtures is developed. It results in lower error than the *best* DRM (NUIG n-Heptane) and much shorter computational time (DNN: less than 1 ms, NUIG n-Heptane: 2 min). The model can be easily extended to nitrogen diluted mixtures and to new experimental data as published. In the future work the model for ignition delay times from rapid compression machines and for mixtures diluted with nitrogen will be developed.

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