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LAMINAR BURNING VELOCITY PREDICTIONS OF SINGLE-FUEL MIXTURES OF C1-C7 NORMAL HYDROCARBON AND AIR

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Abstract

The numerical modelling of combustion phenomena is an important task due to safety issues and development and optimization of engines. Laminar burning velocity (LBV) is one of the most important physical properties of a flammable mixture. Knowing its exact value if crucial for assessment of flame stabilization, turbulent flame structure. It influences strongly safety, probability of knocking combustion and it is one of parameters used for assessment and development of detailed chemical kinetic mechanisms. Hence, the goal of this work is to develop models by means of Machine Learning algorithms for predicting laminar burning velocities of single-fuel C1-C7 normal hydrocarbon and air mixtures. Development of the models is based on a large experimental data set collected from literature. In total more than 1000, LBVs were accumulated for hydrocarbons from methane up to n-heptane. The models are developed in MATLAB 2018a with use of Machine Learning toolbox. Algorithms taken into account are multivariate regression, support vector machine, and artificial neural network. Performance of the models is compared with most widely used detailed chemical kinetics mechanisms' predictions obtained with use of LOFEsoft. These kind of models might be efficiently used in CFD combustion models based on flamelet approach. The main advantage in comparison to chemical kinetics calculation is much shorter computational time needed for computations of a single value and comparable performance in terms of R^2 (coefficient of determination), RMSE (root-mean-square error) and MAE (mean absolute error).

Keywords: *laminar burning velocity, hydrocarbon, machine learning, LOGEsoft, alkane, MATLAB*

1. Introduction

Laminar burning velocity (LBV) is a property of a flammable mixture. Its value depends on mixture composition (fuel, oxidizer), equivalence ratio, pressure, and temperature. Together with ignition delay, time and species concentration is used for development and indirect assessment of detailed chemical kinetics mechanisms. LBV directly influences turbulent flame speed, therefore a knowledge of LBV is crucial in industrial systems (safety, risk of deflagration to detonation transition, DDT) and during design process of gas turbines and piston engines. Turbulent flame speed is a factor affecting i.e. length of gas turbine's combustion chamber, combustion stability, and probability of occurrence of knocking combustion in piston engines.

Combustion models used in computational fluid dynamics (CFD) based on flamelet approach often utilize correlations for laminar burning velocity, where calculations with detailed chemistry are too time-consuming, as well as accessing tabulated chemistry data. The most frequent and the simplest correlation, a so-called power-law equation for LBV are used:

$$LBV_L(EQR, T, P) = LBV_{L0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{P_u}{P_0}\right)^{\beta}, \tag{1}$$

where LBV_{L0} and LBV_L are LBV measured at ambient conditions (temperature T_0, pressure P_0) and LBV sought for, respectively. Factors α and β are temperature and pressure influence exponents and usually they are functions of equivalence ratio (EQR). These power-law

correlations need to be updated, as new experimental data are published continually extending range of conditions.

The objective of this study is to introduce new laminar burning velocity models for a very broad range of hydrocarbon fuels and conditions using machine learning (ML) algorithms. ML 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.

2. Data analysis and simulation

In order to create models following steps are accomplished:

1. Collect data from the literature,
2. Simulate data,
3. Feature Engineering,
4. Normalize data to 0-1 range,
5. Split data into training and test sets (70/30),
6. Apply algorithms,
7. Perform cross validation.

Experimental data

Input of the models are experimental laminar burning velocities collected from literature [1-33]. In total 1073 points are collected for mixtures of air and one of seven hydrocarbons from methane up to n-heptane (normal alkanes only) for different temperatures, pressures and equivalence ratios. A brief summary of the collection is in Tab. 1.

Tab. 1. A summary of accumulated experimental LBVs of mixtures of air with one of seven hydrocarbons from methane up to n-heptane

Air +	Methane	Ethane	Propane	n-Butane	n-Pentane	n-Hexane	n-Heptane
T [K]	295-573	295-450	295-650	298-450	353-450	353-460	298-450
P [bar]	0.2-20	1-10	1-7.4	1-3	1-10	1-10	0.5-24.7
EQR [-]	0.5-1.68	0.6-1.5	0.5-1.6	0.7-1.5	0.55-1.7	0.55-1.7	0.55-1.7
LBV [cm/s]	2.2-85.2	7.1-82.4	9.6-162.1	18.4-76.6	8.1-76.2	10.8-76.7	7-77.7
#points	398	123	210	29	44	51	218

Data simulation

Sample size determination is the act of choosing the number of observations or replicates to include in a statistical sample. The sample size is an important feature of any empirical study in which the goal is to make inferences about a population from a sample. In practice, the sample size used in a study is determined based on the expense of data collection, and the need to have sufficient statistical power. Experimental investigation of any physical phenomena is cost and time consuming. In general, tests are repeated 3 to 5 times for the same settings in order to verify that the measure is *more or less the same*. Unfortunately, the size of this sample is not statistically significant. A way to obtain a statistically significant sample is to simulate data based on sample distribution and standard deviation. In this study, data were simulated based on the existing samples assuming beta distribution. The probability density function (pdf) of the beta distribution, for $0 \leq x \leq 1$, and shape parameters α, $\beta > 0$, is a power function of the variable x and of its reflection $(1 - x)$ as follows:

$$f(x;\alpha,\beta) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1} \cdot (1-x)^{\beta-1}. \tag{2}$$

The beta function is a normalization constant to ensure that the total probability integrates to 1. In the above equations x is a realization – an observed value that actually occurred – of a random process X. The expected value (mean, μ) of a beta distribution random variable X with two parameters α and β is a function of only the ratio β/α of these parameters:

$$\mu = E[X] = \frac{1}{1-\frac{\beta}{\alpha}}. \tag{3}$$

Letting α = β in the above expression one obtains $\mu = 1/2$, showing that for $\alpha = \beta$ the mean is at the centre of the distribution: it is symmetric

The simulation procedure is as follows:

1. fit 5th order polynomial into given data points,
2. assume α,
3. calculate β,
4. calculate density, distribution function, quantile function and random generation for the beta distribution with parameters α and β.

Data, which will be simulated, should be correlated with each other or pattern should exists. When doing simulation of laminar burning velocity in a function of equivalence ratio it can be seen that relationship between variables is similar to inverse quadratic.

Figure 2 presents measured values (black dots) with simulated data (blue circles). Simulation of the data is important in order to avoid the over-fitting problem. The larger the data set the more flexible model can be fitted [34].

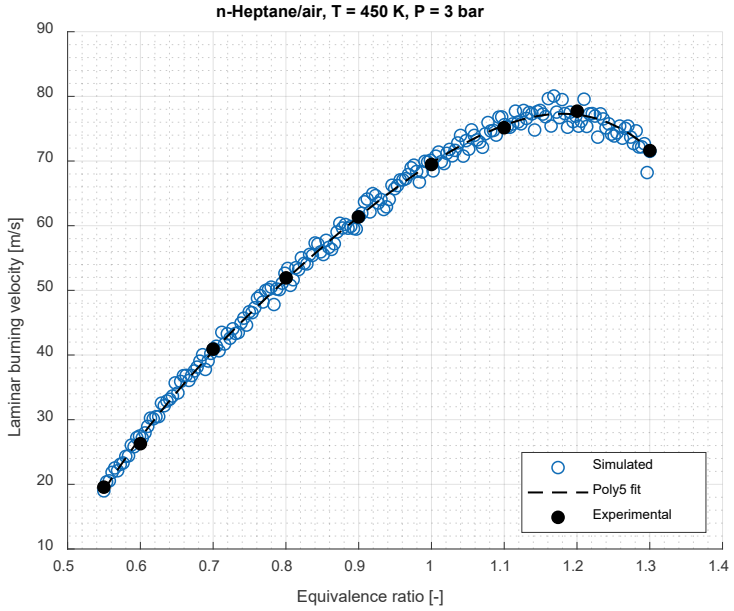

Fig. 1. Experimental LBVs (black dots) with its functional estimate (dashed line) and simulated LBVs (blue circles) of n-heptane/air mixture at 450 K and 3 bar

Data normalization

Generated data are normalized to 0.0-1.0 range, in order to bring all the features to the same scale. This procedure makes machine-learning algorithms to converge faster and improves their adaptation ability. Data is normalized. Normalization is made based on the following equation:

$$z_i = \frac{x_i - \min(x)}{\max(x) - \min(x)}, \tag{4}$$

where $x = (x_1,...,x_n)$ and z_i is i-th normalized data. Normalized data are divided randomly into training and test set, 70% to 30% accordingly. First set is used to train model, the second set is to

estimate how well the model has been trained. In this work multivariate regression [35, 36], supported vector machine [37, 38] and artificial neural network [39] are applied for the data set and the results are compared.

Feature engineering

Process of feature engineering was used to create additional features with addition to the existing one in order to improve the prediction power of the models. As a result equivalence ratio is presented in the form of the 5th order polynomial and both temperature and pressure additionally as the second power and the root. The final model is a laminar flame speed in function of equivalence ratio, initial pressure and initial temperature and number of carbons in a chemical formula, HC:

$$LBV = HC + (EQR + EQR^2 + EQR^3 + EQR^4 + EQR^5) + (P_0 + P_0^2 + P_0^{0.5}) + (T_0 + T_0^2 + T_0^{0.5}).$$

3. Machine Learning Algorithms

Multivariate Regression

Multivariate regression is a technique that estimates a single regression model with more than one outcome variable [35]. The multivariate general linear model is defined as follows

$$\mathrm{Y} = \mathrm{X}\,\mathrm{B} + \mathrm{E}, \tag{5}$$

where *Y* is a matrix of *n* observations on *m* response variables; *X* is a model matrix with columns for *k* + 1 regressors, typically including an initial column of *1's* for the regression constant; *B* is a matrix of regression coefficients, one column for each response variable; and *E* is a matrix of errors [36]. Fig. 2 summarizes obtained results.

Supported Vector Machine

Supported Vector Machine (SVM) is a method of the optimal separating hyperplane. This algorithm belongs to supervised learning models used for classification and regression analysis. Input vectors *X* are mapped into the high-dimensional feature space *Z* through nonlinear mapping, chosen a priori. In this space, in case of classification, an optimal hyperplane is constructed, which divides the data into the most distinct sets. In case of regression, it creates a hyperplane which is the closest to all observations [37]. In order to improve the performance of SVM the best parameters for the model are selected by the process called hyper parameter optimization [38]. The standard way to do this is a grid search where many models are trained for the different pairs of ϵ and cost, and choose the best one.

Artificial Neural Network

The artificial neural network (ANN) consists of layers of neurons, where the first layer is called input layer and the last layer is called output layer. The layers between input and output are called hidden layers. Input nodes are passive which means that they duplicate received the input value and passes it to each node in the next layer. The connections between nodes contain parameters known as weight, which indicates the influence of a given node on the final output value. Nodes in hidden and output layers hold activation function. Those nodes are being called as active. Sum of input values multiplied by specific weights is passed to the active node's activation function [39]. Additional nodes added to the layers are called bias nodes (b). Those bias nodes hold constant values and support achieving better-fitted results of prediction by shifting the activation function characteristics. Fig. 2 presents structure of the ANN used in this study.

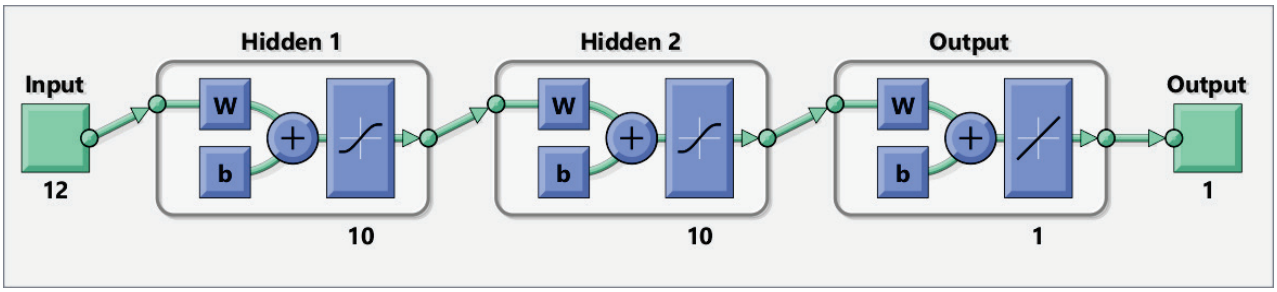

Fig. 2. Structure of ANN used in this study: two hidden layers with 10 nodes each

Each iteration of the neural network training process consists of two steps: forward and backward propagation. Forward propagation is a simple forward pass of input values through all the neurons, and it outputs a result, called a prediction value. Backward propagation method is a part of artificial neural networks supervised machine learning algorithm and it minimizes the neural network error, called the cost function, in each iteration by adjusting the weights in all nodes. The value of the error is the difference between the predicted value obtained in the forward pass and the actual output value taken from the training set. After the training, when the error is small enough, only the forward propagation is used to obtain predictions.

4. Results

Figure 3 presents a summary of obtained models' performance. True LBVs against predicted LBVs for all 3 algorithms is shown in the left part of Fig. 3. The most common metrics for measuring accuracy, R^2 (coefficient of determination), RMSE (root-mean-square error) and MAE (mean absolute error) are in titles. Diagrams on the right side in Fig. 3 show error higher than 3 cm/s.

The model obtained with the multivariate regression has the lowest accuracy and the highest R^2, RMSE and MAE. The ANN performs best across all 3 algorithms and for this model; coefficients are differentiated for each hydrocarbon in Tab. 2. Generally, the model predicts very well investigated LBVs. The lowest metrics are for methane. However, one need to keep in mind that methane has the biggest experimental data set (Tab. 1) and it was investigated for a long span of time. It could result in high spread of experimental data and at last worse predictability of models.

Tab. 2. R^2, RMSE and MAE for each hydrocarbon for ANN model

	CH_4	C_2H_6	C_3H_8	C_4H_{10}	C_5H_{12}	C_6H_{14}	C_7H_{16}
R^2	0.975	0.990	0.993	0.998	0.990	0.995	0.991
RMSE	2.154	1.317	3.126	0.642	1.658	1.022	1.217
MAE	1.397	1.007	1.708	0.543	1.074	0.756	0.851

Tab. 3. Comparison of performance of detailed reaction mechanisms and ANN in reproduction of methane LBV

	ANN	GRI-mech 3.0	San Diego	CaltechMech	POLIMI	AramcoMech
R^2	0.975	0.934	0.867	0.936	0.914	0.973
RMSE	2.154	3.497	4.977	3.466	4.017	2.370
MAE	1.397	2.161	3.829	2.113	2.685	1.555

In Tab. 3 the ANN's performance of methane's LBV is compared to detailed reaction mechanisms (DRMs): GRI-mech 3.0 [40], San Diego 2014 [41], CaltechMech [42], POLIMI C1-C3 LT HT [43] and AramcoMech 2.0 [44]. LBVs were obtained with use of LOGEsoft [45]. One

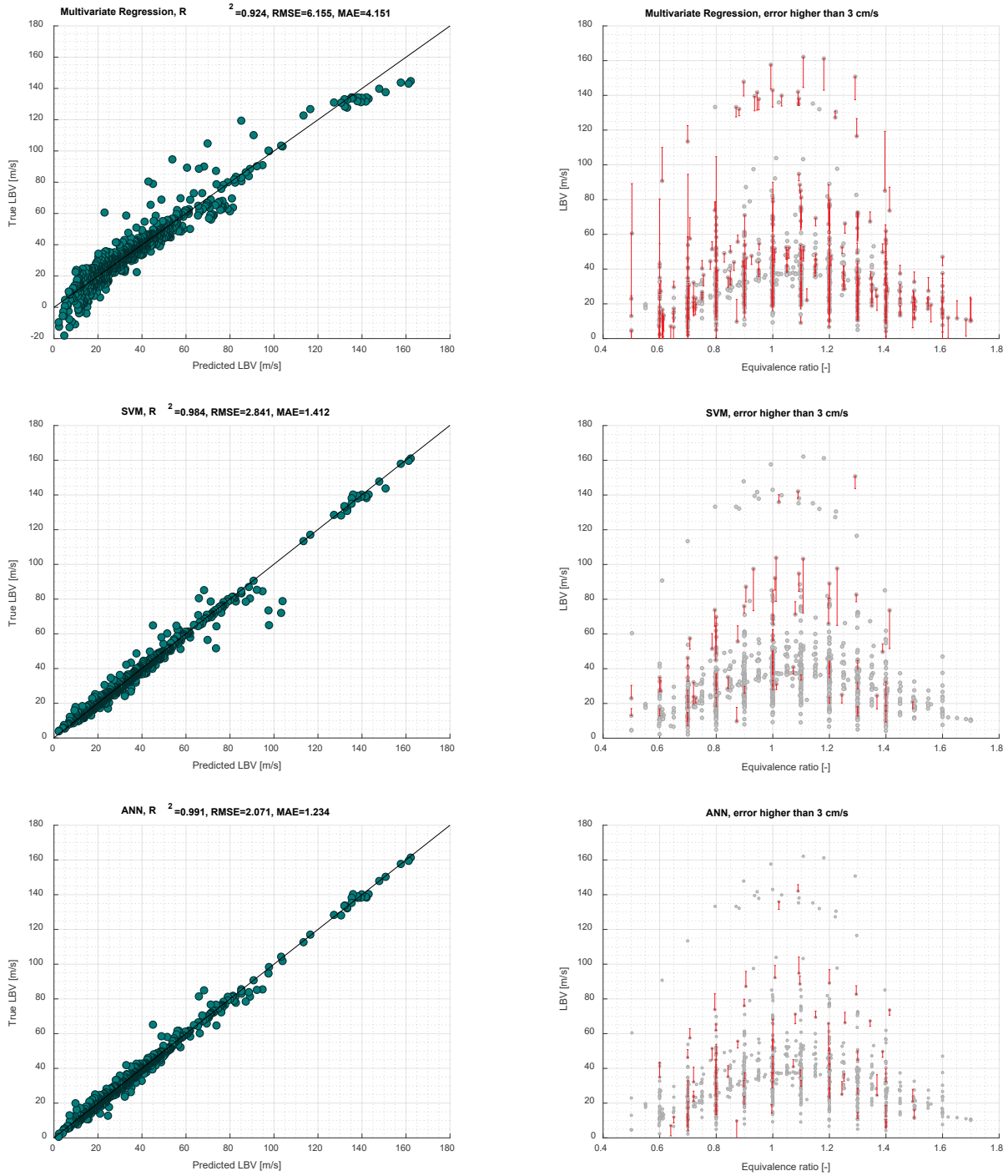

Fig. 3. Results for multivariate regression, SVM and ANN: left – true LBV against predicted LBV, right – experimental LBV against EQR. Model error bars higher than 3 cm/s are marked by red colour

can notice that ANN model is the most accurate and comparable to AramcoMech 2.0. However, due to a high number of species and reactions in the mechanisms computational time is long (average from all calculations with AramcoMech 2.0 is 5.2 h, where for ANN model it is an order of seconds).

5. Conclusions

In the article, 3 models of laminar burning velocity of mixtures of air with one of seven hydrocarbons from methane up to n-heptane were created. Machine learning algorithms, such as

Multivariate regression, Supported Vector Machine and Artificial Neural Network were used. The best performance is obtained by ANN model in terms of R^2, RMSE and MAE. Good performance is constant across all seven hydrocarbons. ANN model performance for methane LBVs was compared to well establish detailed reaction mechanisms. It was shown that ANN model is more accurate than the DRMs and also it is much less computationally expensive.

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