DEVELOPMENT OF HYDROGEN TURBULENT FLAME SPEED ANN INTENDED FOR THE CFD APPLICATIONS

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ABSTRACT

During severe accidents in nuclear power plants, hydrogen explosion threatens integrity of the reactor containment building. To prepare effective measures reducing possible risks and manage severe accidents, it is critical to create reliable tools to accurately predict combustion process. For realistic and timely technical computational fluid dynamics simulations simplified approaches are usually used. One of such approaches is avoiding detailed simulation of fast chemical processes by using correlations to evaluate turbulent flame speeds from the mixture composition and conditions (through laminar burning velocity) and turbulence parameters.

The artificial neural networks (ANN) is one of the most used machine learning methods. Recent research indicates that artificial neural networks with a large enough number of neurons and layers can accurately solve challenging problems. While it is computationally costly to use large networks, which would give accurate solutions, it is still possible to obtain very good results with a reduced number of neurons and layers, which in many cases gives better calculations than other similar approaches or known correlations. In recent years, ANNs have achieved great results in various fields, and studies only keep expanding applicability domain of this method. This potential of the ANN method encouraged us to apply it to the simulations of hydrogen combustion.

In previous works we developed an artificial neural network for computational fluid dynamics application, which can predict laminar burning velocities in hydrogen-air mixtures. In present work we start to create analogous neural network for turbulent flame speed prediction. The work is focused on collection and treatment of experimental data required for such neural network and development of initial neural network.

The main result of this study is creation of artificial neural network model, which is light enough to do fast predictions and be implemented in computational fluid dynamics combustion solvers, used for the hydrogen explosion simulations. The paper presents turbulent flame speed data used for the model, preliminary model architecture and its training. Model predictions are compared with the correlation-based results available in the literature.

Keywords: Artificial Neural Networks, Turbulence, Hydrogen

NOMENCLATURE

Nomenclature used in work are explained bello:

- Le Lewis number
- Re Reynolds number
- Ul laminar burning velocity
- Ut turbulent burning velocity
- u′ r. m. s. turbulent velocity
- ANN Artificial Neural Networks
- ML Machine Learning
- TL Transfer Learning
- MSE mean squared error
- MAE mean absolute error
- MAPE mean absolute percentage error
- L1 1st regularization parameter
- L2 2nd regularization parameter

1. INTRODUCTION

Machine learning is major topic currently applied in various research fields. Various ML methods have been suggested to solve complicated structures and behaviors. Multiple works argue that machine learning can be used to predict physics of chemical mixtures as well. In previous paper [1] we have shown that ANN can predict laminar burning velocities of Hydrogen-Air mixtures with high accuracy (mean absolute error approximately 6 cm/s), similar models were developed by Malik [2] and others. On the other hand, were aren’t many works which would do simulations beyond laminar flames area.

Right now, most widely used methods for turbulent burning velocity estimation of Hydrogen-Air mixtures are Bradley
While it is relatively simple and effective, their correlations have some limitations as well. For example, Bradley suggested that his correlation should be used in cases such that multiplication product of dimensionless turbulent quench stretch rate and Lewis number would be in interval (0.14, 0.4), Bray tries to explain results stating that larger scatter not explained by their model can be caused by an increase of flame thickness or curvature of flame, and Zimont correlation was created for high Reynolds numbers and can be less reliable at lower Reynolds numbers.

Some recent works suggest machine learning models such as CFDNN [7] which is based on Convolution Neural Networks (CNN) and can give similar results compared to CFD combustion simulations. However, the disadvantage of such approach is that models require large amounts of data for learning. Also, they often not as well reliable as models created for specific mixtures. However, feeding such networks and merging them with models created for single mixture cases can greatly improve their accuracy and robustness for specific mixtures or cases.

Such approach comes from so called Transfer Learning. This method application for creation of turbulence combustion models are well analyzed by Subel [8] and Mondal [9]. As stated by Mondal, transfer learning results in better predictions with less data requirement for model training. On the other hand, Sudel suggests that transfer learning can increase neural networks accuracy so that it would even be possible to recreate LES model simulations with high Reynolds numbers.

In theory, it should be possible to obtain fast working model which would still be able to give better predictions than most-applied correlation such as Bradley. One of the ways to achieve that would be to use ML algorithms which would be robust enough to adjust to complex structure of Hydrogen-Air turbulent burning velocities. Such results can be achieved by training model on data with similar physics in order to simplify data and then use obtained results in model which would be made for specific problem (such as Hydrogen-Air combustion).

2. MATERIALS AND METHODS

Next study gives short analysis of data and model structure as well as process of creation.

2.1 Data

In this work data from various literature sources was used [6, 10-17]. Overall we managed to obtain 39 [6, 13, 14, 15] data points for Hydrogen-Air mixtures and 439 data points for other mixtures [10-17]. However, it was problematic to train model to predict turbulent burning velocities at low Reynolds numbers, and additional 10 data points were added for zero Re values and turbulent burning velocity equal to laminar (\(U_t = U_l\)), this way teaching model the transition from laminar to turbulent burning regimes. Considering low amount of information about turbulent burning velocities of hydrogen-air mixtures this data alone wouldn’t be enough to make good model. Therefore, study decided to use data of other mixtures as well, like Bradley did in his work [3]. However, in order to use other mixtures we need to evaluate how both datasets work. For this we evaluate correlations of each dataset. Figures 1 and 2 shows that while Hydrogen-Air mixtures give positive linear relationships for all parameters, same cannot be stated about dataset with various mixtures. Also, Pearson correlation for \(U_t\) gives much higher positive relationships with all other parameters compared to \(U_t\) of dataset without Hydrogen-Air mixtures. Yet, in both cases \(U_t\) has positive linear relationships with other parameters meaning that increase in any parameter’s value should increase turbulent burning velocity as well. Taking that into consideration we can state that both datasets have similar behavior up to some extent, which means that one dataset can at least partially explain another set.
In earlier subchapter we already said that each dataset can partially explain another, which works for models as well. In the beginning study tried to make a model of entire data, however, while results looked well in general (R-Squared around 0.9) it did not give high prediction accuracy for hydrogen-air mixtures dataset alone. Naturally, making ANN model of combined dataset allows ANN to learn behavior of turbulent burning velocities of various mixtures and gives almost linear predictions for various mixtures. However, while predictions for hydrogen-air mixtures are linear-like, they seem to have some kind of constant value as multiplication parameter. This leads to the idea that the model could have been influenced by low amount of data and slightly different physics of various mixtures.

In order to solve the problem of ANN model not predicting \( U_t \) for hydrogen-Air mixture as it should while working relatively well in general case, we decided to imitate Transfer Learning in which case weights or in our case predictions of network trained on much larger database are retrained on small database or smaller model. Yet, even if inspired by TL this approach should be considered as multiple neural networks, as we give prediction of one network as an input to another. For this study we created another ANN which learned from Hydrogen-Air mixtures dataset only, as we give turbulent burning velocity predictions of first ANN as input. Overall, first network (we can name it Generic model (GM)) simplifies physics for second network (which we can call Hydrogen model (HM)) and HM learns how to process that simplified physics for given data. In general, first network might slow down predictions as it has a lot of neurons (arguably) so for future work it should be considered to simplify it or use general correlation which would give similar results which can be used as input to second network.

2.3 ANN models structure

While both networks are similar, we did make some changes in order to obtain better results. First of all, both networks have regularization parameters L1 and L2 where for different layers L1 is in range \((10^{-6}, 10^{-5})\) and L2 is in range \((10^{-6}, 10^{-5})\). Study obtained best results with ANN structures described in Tables 1 and 2. Other numbers of neurons and activation functions also various parameters were tested as well.

<table>
<thead>
<tr>
<th>TABLE 1: GENERIC MODEL STRUCTURE</th>
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<tbody>
<tr>
<td>Number of neurons in layer</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>ReLU</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>ELU</td>
<td></td>
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<tr>
<td>30</td>
<td>ReLU</td>
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</tr>
<tr>
<td>7</td>
<td>ReLU</td>
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</tr>
<tr>
<td>3</td>
<td>ReLU</td>
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<tr>
<td>1</td>
<td>ReLU</td>
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<table>
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<tr>
<th>TABLE 2: HYDROGEN MODEL STRUCTURE</th>
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<tbody>
<tr>
<td>Number of neurons in layer</td>
<td></td>
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<tr>
<td>3</td>
<td>ReLU</td>
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<tr>
<td>5</td>
<td>ELU</td>
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<tr>
<td>3</td>
<td>ReLU</td>
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Another difference between models is that both have different loss functions. However in both cases those are just weighted averaged of mean squared error (Equation 1) and mean absolute error (Equation 2).

\[
MSE = \frac{\sum(y_i - \hat{y}_i)^2}{n} \\
MAE = \frac{\sum|y_i - \hat{y}_i|}{n}
\]

\[
Loss_1 = 0.6 * MAE + 0.2 * MSE
\]

\[
Loss_2 = 0.5 * MAE + 0.5 * MSE
\]

Generic model uses Equation 3 as loss function which has more influence from mean absolute error and Hydrogen model was trained using Equation 4 which is just average of MAE and MSE errors. Such functions were selected as they gave better results and statistically better evaluated expected values.

3. RESULTS AND DISCUSSION

Considering that most of the database points were taken from works related to Bradley, study decided to compare ANN model predictions with Bradley correlation. Figure 3 shows results obtained with developed ANN versus original data gathered from literature. Majority of those points are the data on which Bradley created his correlation. Therefore, these results should clearly show if ANN can give adequate predictions compared to one of the more popular correlations.

As we can see in Figure 3, ANN predicts majority of points well, with only few data points farther from the line which marks identical values. Overall, model obtained R-Squared value of over 0.92 which can be interpreted as a good prediction since model explains around 92% of data points. However, it is worth noting that these results are obtained on a small dataset.

**FIGURE 3: ORIGINAL DATA OF HYDROGEN-AIR MIXTURES VERSUS PREDICTIONS OF ARTIFICIAL NEURAL NETWORK [6, 13, 14, 15]**
The same comparison was made for Bradley correlation. From Figure 4, which shows comparison of original data versus predictions with Bradley correlation we can see that predictions are very good for slow turbulent burning velocities and became slightly inaccurate in areas around 5 m/s and 9 m/s. It is worth to point out that Bradley correlation for this dataset has R-Squared value of 0.88, which means that model explains around 88% of the points.

![FIGURE 4: ORIGINAL DATA OF HYDROGEN-AIR MIXTURES VERSUS PREDICTIONS OF BRADLEY CORRELATION [3, 6, 13-15]](image)

Deeper investigation (Figure 6) shows that Bradley correlation gives better predictions for \( U_t > 10 \) m/s while ANN model shows much better predictions for turbulent burning velocities in the region of \( 6 < U_t < 10 \) (m/s). Meanwhile, for other areas results obtained with both models are very similar.

Considering all results obtained by this study, it can be said that ANN model gives slightly better results overall. However, as noticeable from Figure 6, these results requires deeper investigation and more data. In general, gathering more data is required for evaluation of models as much as better training of Artificial Neural Networks model. As for now, till more data will be gathered, it is better to use both models, in which case Bradley can be used for high burning velocities and ANN for lower burning velocities (6-10 m/s).

![FIGURE 5: COMPARISON OF PREDICTIONS MADE BY ANN AND BRADLEY CORRELATION [3, 6, 13-15]](image)

![FIGURE 6: COMPARISON OF BRADLEY CORRELATION AND ANN PREDICTIONS RATIOS WITH \( U_t \) (AGAINST \( U_t \) PLACED ON X AXIS) [3, 6, 13-15]](image)

On the other hand, it is worth noticing that ANN model has one major drawback as well. Considering that our created network is fully connected, that means that neurons in each layer have to be multiplied with all neurons on next layer, due to the number of operations, makes our ANN model slower compared to simple expressions given by Bradley, Bray or Zimont [3, 4, 5]. This reduction in speed should be more noticeable.
considering that we use two networks and is undesirable in case we would want to use model for real-time predictions in CFD simulations. Yet, first network is used to simplify turbulent burning behavior for various mixtures which plausibly can be simplified up to simple correlation in future works, which would allow us to make predictions much faster. Another approach can be to use network which has high number of neurons and gives high accuracy predictions and feed data generated by such network to smaller ANN this way forcing learning. Yet, results of new model would be bounded by the performance of both networks. However, in general, with large database ANN would require less neurons to achieve similar results. These and similar tasks should be analyzed in future works in order to optimize model which would be able to work accurately and fast, this would be our next goal in the research.

4. CONCLUSION

Model for the prediction of turbulent burning velocity of Hydrogen-Air mixtures composed of two artificial neural networks was developed. Developed model predictions are adequate compared to Bradley correlation. Although, ANN performed better in terms of all 4 measures (MSE, MAE, R-Squared, MAPE) it cannot be stated yet that model performing better due to insufficient amount of hydrogen-air data. Therefore, further data gathering and testing is needed. Larger amount of data will most likely lead to the creation of more accurate and reliable model.

REFERENCES