LES MODELS FOR TURBULENT HYDROGEN FLAMES WITH CONVOLUTIONAL NEURAL NETWORKS

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Abstract

Lean hydrogen flames are prone to thermodiffusive instabilities, which have a strong effect on the structure and dynamics of the flame and can enhance flame speed by several times. Conventional combustion models perform poorly for unstable hydrogen flames and often fail in capturing the effects of thermodiffusive instabilities. In this work, the capability of Convolutional Neural Networks (CNN) to model the unclosed reaction rate term in Large Eddy Simulations (LES) of turbulent hydrogen premixed flames is investigated using high-fidelity data from a large-scale Direct Numerical Simulation (DNS). It is shown that the CNN model can accurately reproduce the filtered reaction rate over a large range of filter sizes. Traditional models usually require at least two scalars, e.g., two progress variables or a progress variable and a mixture fraction, to capture the local fluctuations of equivalence ratio caused by thermodiffusive effects; remarkably, the CNN-based model requires only a single progress variable, due to its ability to consider the topology of the three-dimensional progress variable field, which embeds the information regarding the fluctuations of equivalence ratio. Finally, the capability of the CNN to generalize to different filter sizes and filter kernels is investigated.

Introduction

Recent developments in Machine Learning (ML) have granted remarkable success in several challenging tasks and sparked interest into the possibility to use ML in turbulence and combustion modelling. ML models are often based on the idea of training a Neural Network (NN) using high-fidelity data of turbulent (reactive) flows, which result from Direct Numerical Simulations (DNS) or sophisticated experiments. In Large Eddy Simulation (LES) of turbulent premixed flames, the filtered non-linear reaction rate needs to be modelled in terms of the resolved fields. Convolutional Neural Networks (CNN) have been shown to perform remarkably well in approximating the filtered reaction rate [1] and the subgrid flame wrinkling

[2,3]. However, it has been observed in many applications, ranging from speech recognition to medical diagnosis, that ML-based approaches might perform poorly when applied to data that are different from those employed for training. In this work, we investigate the application of CNN-based models for the computation of the filtered reaction rate in hydrogen flames. In addition, we perform a systematic analysis of the effect of the filter size used to filter the data for the training of the Neural Network. This is important in applications, since the filter size in an actual LES is typically strongly inhomogeneous due for example to grid refinement and most likely unknown a-priori since it results from a complex interaction of grid spacing, numerical accuracy, and modelling assumptions.

DNS database

A large-scale DNS of a lean hydrogen flame of Berger *et al.* [4] is used to train the CNN-based models and to verify their performance. The DNS features a jet Reynolds number of Re = 11000 and a Karlovitz number of Ka ≈ 15. The simulation is performed using detailed finite-rate chemistry, non-unity Lewis numbers, and including the Soret effect. A slot turbulent premixed jet flame with equivalence ratio φ=0.4, a temperature of T_u = 298 K and a pressure of 1 bar, surrounded by a coflow of burnt gases, is considered.

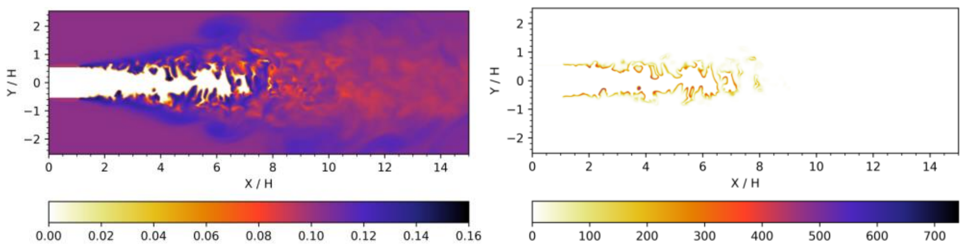

Figure 1. H_2O mass fraction (left) and H_2O reaction rate (right) in the DNS of Berger *et al.* [4] for a turbulent hydrogen flame in a two-dimensional cut of the three-dimensional simulation domain.

Impact of thermodiffusive instabilities and related modelling challenges

Figure [1] shows the mass fraction of water and its reaction rate. The flame is strongly affected by the thermodiffusive instability [4], which causes the typical overshoots of product mass fraction visible in the H_2O mass fraction plot. The thermodiffusive instability is even more evident in the reaction rate, which is very large in regions where the flame surface has positive curvature (convex towards the unburned gas), while the reaction rate is smaller, or even zero, where the curvature is negative. Because of differential diffusion, hydrogen tends to diffuse preferentially towards positive-curvature regions, increasing the local equivalence ratio, which enhances the local reactivity and flame speed for a globally lean flame. A remarkable fact, observed by Aspden *et al.* [5,6] and Berger *et al.* [4], is that turbulence does not cancel-out the impact of thermodiffusive effects, except for the case of very large

Karlovitz numbers [5,6], but turbulence and instability interact synergistically with thermodiffusive effects being even stronger in the turbulent regime than in laminar flames [4]. As shown in Fig. 2, for a methane at similar conditions, [7] the reaction rate is always very close to the one dimensional unstretched laminar flame (flamelet), while there is very large scatter in the hydrogen case.

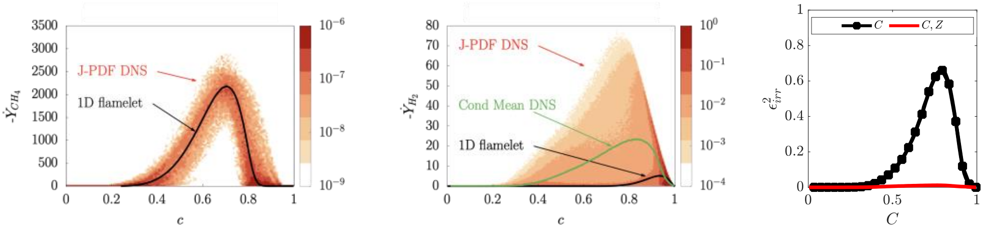

Figure 2. Statistics of the fuel reaction rate for a methane [7] (left) and a hydrogen [4] (center) turbulent flame DNS, compared with a flamelet (one dimensional unstretched laminar flame). Irreducible error for two different parametrizations of the reaction rate in a turbulent hydrogen flame [8].

A direct consequence is that reaction rates in hydrogen flames cannot be parametrized by the progress variable only [8] as usually more than adequate for methane flames [7]. A second variable, such an additional progress variable, a mixture fraction, or curvature, is therefore required to parametrize the local reaction rate. This is quantitatively assessed in Fig. 2, where the irreducible error for the parametrization with only the progress variable C and with the progress variable and mixture fraction Z is also shown.

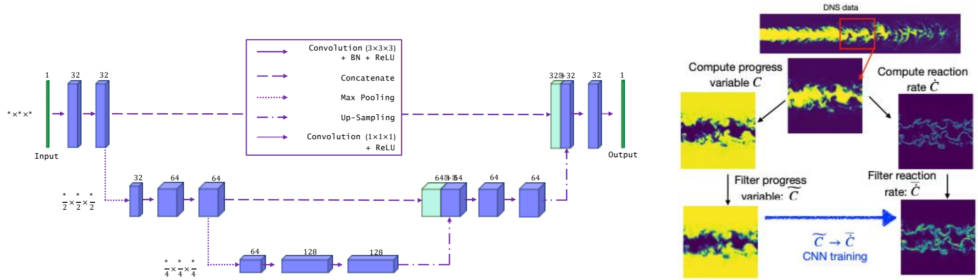

Figure 3. Architecture of the UNET CNN (left) and pipeline to extract and process DNS data and CNN training (right).

CNN-based models

An alternative approach to traditional closures of the filtered reaction rate in LES, is the use of neural networks (NNs). Specifically relevant in the present context are the Convolutional Neural Networks (CNN) employed in approximating the filtered reaction rate by Seltz *et al*. [1] and the subgrid flame wrinkling by Lapeyre *et al*. [2] and Attili *et al*. [3]. A neural network is trained to learn the relation between an input field, in this case the filtered progress variable, and the desired output, the reaction rate. The data for the NN training need to be obtained from high-fidelity databases, which in the present case are the DNS of the turbulent hydrogen flame. The CNN architecture employed here is shown in Fig 3. A Convolutional Neural Network (CNN) derived from a U-net architecture has been designed to consider (multiple) three- dimensional (3D) input fields, e.g., $\bar{C}$ and $\bar{Z}$, and provide 3D fields as output, i.e., the filtered reaction rate.

Results

Traditional models for hydrogen flames require to account for the fluctuations of local equivalence ratio. It has been shown that the fluctuations of equivalence ratio correlate with the topology of the progress variable field [4], opening to the possibility to parametrize the reaction rate by adding non-local information of the progress variable field. Being able to learn the relation between 3D fields (filtered or not), CNN-based models could be employed for that. A comparison of two CNN models which employ as input *i)* only the progress variable and *ii)* progress variable plus mixture fraction is shown in Fig. 4. The performance is extremely good in both cases. It is worth noting that the results for the joint probability density function J-PDF are shown in log scale to highlight the very small difference. The accuracy for both models in Fig. 4 are comparable to those shown in Fig. 2 when progress variable and mixture fractions are used and both are largely superior to a local parametrization with only the progress variable. We conclude that a CNN with only the progress variable can be used for the reaction rate in lean hydrogen flames.

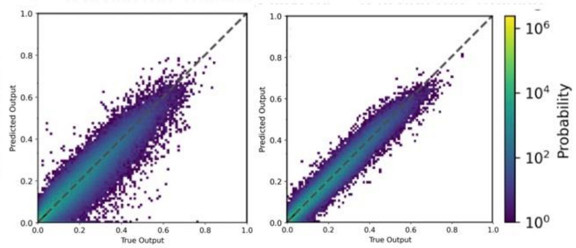

Figure 4. J-PDF of true filtered reaction rate from DNS and predicted values by the CNN models using only the progress variable (left) and the progress variable and mixture fraction (right) as inputs of the CNN. The result is shown for a filter size of $\Delta_{train} = \Delta_{test} = 8\,\Delta$, where Δ is the DNS grid cell size.

When employing ML models for subgrid closure, a critical factor to consider is their ability to extrapolate and generalize. ML models should be able to perform well when the fields used for training are different from the fields on which the model is applied. A requirement is the capability to extrapolate at higher Reynolds number since DNS data used for training cannot be generated at the high Reynolds number that is typical of applications. This aspect is discussed by Attili *et al.* [3] and it is shown that CNN models are capable to extrapolate at higher Reynolds numbers if the Reynolds number of the training data is high enough and the ratio between the filter size and the Kolmogorov scale of turbulence is properly considered. In this work, we investigate an important aspect related to the size of the filter size. In Fig. 4, the filter size used for training is the same as that used in the model test. In actual LES applications, the filter size can change significantly in the simulation domain, for example due to local grid refinement. Even more importantly, the actual filter size in LES is not known, since it results from a complex combination of grid size, numerical accuracy, and the formulation of the LES model itself. Therefore, it is important to assess how the CNN model performs when the filter size used in training Δ_{train} is not the same as that used when the model is tested Δ_{test}. A summary of this systematic analysis is shown in Fig 5. The model performs extremely well when the training and test filters are the same $\Delta_{train} = \Delta_{test}$, while a large bias is observed otherwise. This challenge is expected, and it must be addressed; otherwise, the model would have limited use in a practical LES setting.

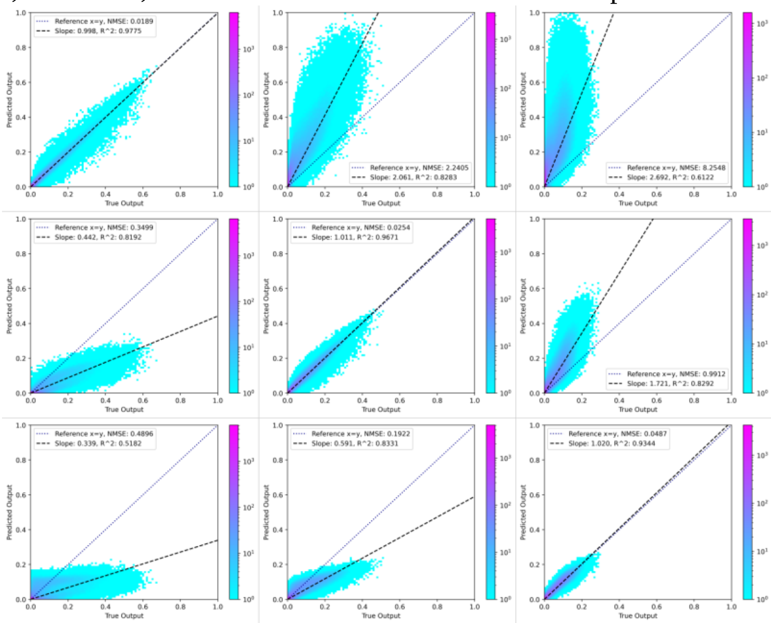

Figure 5. J-PDF of true and predicted values for different combinations of the raining and testing filter sizes. Top to bottom: $\Delta_{train} = 4$, $\Delta_{train} = 8$, $\Delta_{train} = 16$; left to right: $\Delta_{test} = 4$, $\Delta_{test} = 8$, $\Delta_{test} = 16$.

The idea considered here is to train with a collection of fields obtained by filtering DNS data with multiple filter sizes, up to the limit of including data obtained with all possible filter sizes in a certain range. An assessment of this approach is summarized in Fig. 6, where the error for several different models (each line represents a CNN model), obtained by training with different set of data, is shown. When all the possible filter sizes are used for training (blue line in the right graph) the model performs extremely well for all sizes of the filter used in the testing data. As certain filter sizes are progressively removed from the training set, the performance degrades in the range of Δ_{test} that have not been covered by the training. We conclude that, using multiple filter sizes in training is a viable option to build a model that works for a wide range of filter sizes, and that the model obtained in this way is as good as the model trained with a single filter size and applied to test data with the same filter used for training.

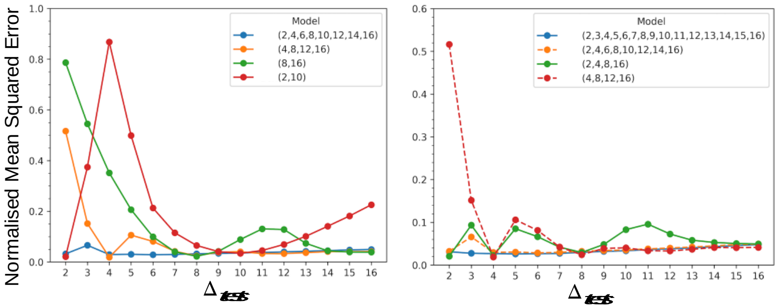

Figure 6. Error for models trained with different combinations of filter sizes and tested for filter sizes ranging from $\Delta_{test} = 2$ to 16. Each line represents a model trained with a collection of data obtained with the set of filters shown in the legend.

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