Combustion and Flame

Application of machine learning for filtered density function closure in MILD combustion --Manuscript Draft--

Manuscript Number:	CNF-D-20-00762R1
Article Type:	Full Length Article
Keywords:	Machine learning; Deep neural networks; Filtered density function; MILD combustion; Subgrid scale modelling
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Abstract:	<p>A machine learning algorithm, the deep neural network (DNN) ^{{The DNN code and a sample training dataset are available for public access at \url { https :// github . com / cz5224043 / ml-mild-combustion}.}}, is trained using a comprehensive direct numerical simulation (DNS) dataset to predict joint filtered density functions (FDFs) of mixture fraction and reaction progress variable in Moderate or Intense Low-oxygen Dilution (MILD) combustion. The important features of the DNS cases include mixture fraction variations, turbulent mixing lengths, exhaust gas recirculation (EGR) dilution levels, etc ., posing a great challenge for data-driven modelling. The DNN architecture is built and optimised with extreme care to achieve high robustness and accuracy, resorting to dimensionality reduction techniques such as principal component analysis (PCA) to identify and remove the outliers in the training data. To better interpret the predictive ability of the DNN , two analytical joint FDF models respectively using two independent β and copula distributions, are also employed for a detailed comparison with the DNS data.</p> <p>The FDFs in MILD combustion behave differently compared to those in conventional flames because the reaction zones are more distributed. They generally exhibit non-regular (neither Gaussian nor bi-modal) distributions and strong cross correlations, which cannot be captured adequately by the analytical models. However, the DNN is well suited for this physico -chemically complex problem and its predictions are in excellent agreement with the DNS data for a broad range of mixture conditions and filter sizes. Furthermore, a priori assessment is conducted for filtered reaction rate closure. It is found that the DNN model significantly outperforms the analytical models for all cases showing very good predictions for the filtered reaction rate for a range of filter sizes. The DNN prediction improves as the filter size becomes larger than the characteristic reaction zone thickness while the analytical models works relatively better for smaller filter sizes. This is a clear advantage for the DNN to be used in practical LES applications.</p>