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Tabulation of thermochemical states in reactive flows via machine learning algorithms

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During the numerical simulation of combustion, the computation of thermochemical sources is expensive if the direct ODE solvers are used to compute the stiff equations. Traditionally, reduced chemistry approaches or tabulation methods such as intrinsic low-dimensional manifold (ILDM) were used to simplify the chemistry in the system and to accelerate the simulation. In the context of reduced chemistry, ODE solvers are still needed, and the computational cost remains prohibitive if pollutants are to be predicted. The main drawback of traditional tabulation methods is that they require a large quantity of disk memory to store the tables. More recently, the tabulation of chemistry using deep learning methods such as artificial neural networks (ANN) has been proposed [1][2][3]. While promising results have been obtained for simple fuels such as H_2, tackling more complex hydrocarbon fuels is a more challenging task. Some techniques have been suggested in the literature, for instance predicting the high-dimensional chemical state using multiple neural networks [3][4].

The aim of this paper is to develop an appropriate robust learning model to improve the performance of machine learning based tabulations. Our simulation case is 0D combustion simulation for ethylene (C_2H_4), which is a complex combustible that yields high-dimensional dynamics with around thirty chemical species. To achieve this goal, we investigate the impact of the trajectory sampling, the pre-processing of the training datasets as well as the separation of chemical species. We propose to leverage the time step adaptation of standard numerical schemes such as the ones implemented in the CVODE solver to generate a database that is well balanced between the various combustion phases. Besides, we compare various methods to pre-process the data and deal with the difference in scales of the various chemical species. We propose to use different transformations depending on the nature of the species, comparing the performance of power and log laws. Finally, we investigate the relevance of training different models for each category of chemical species.

REFERENCES

[1] L.L.C. Franke , A.K. Chatzopoulos , S. Rigopoulos , Tabulation of combustion chemistry via artificial neural networks (ANNs): methodology and application to LES-PDF simulation of sydney flame l, Combust. Flame 185 (2017) 245–260 .
[2] K. Wan , C. Barnaud , L. Vervisch , P. Domingo , Chemistry reduction using machine learning trained from non-premixed micro-mixing modeling: application to DNS of a syngas turbulent oxy-flame with side-wall effects, Combust. Flame 220 (2020) 119–129 .
[3] T. Ding , T. Readshaw, S. Rigopoulos, W.P. Jones, Machine learning tabulation of thermochemistry in turbulent combustion: An approach based on hybrid flamlet/random data and multiple multilayer perceptrons, Combustion. Flame 231 (2021) 111-493

[4] T. Readshaw , T. Ding , S. Rigopoulos , W.P. Jones , Modeling of turbulent flames with the Large Eddy Simulation-probability density function (LES-PDF) approach, stochastic fields, and artificial neural networks, Phys. Fluids 33 (3) (2021) 035154 .