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Data-driven modelling of filtered reaction rates with optimized progress variables for ammonia/hydrogen/air premixed flames

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In the context of a tabulated chemistry framework it is essential to construct tables that capture the fundamental behaviour of all the quantities that are needed at runtime, for example diffusion and chemical source terms of the transported quantities. When using a data-driven approach the table-building method consists in choosing a representative enough dataset from which we want to construct our tables, then define a series of transported (or control) variables, and finally construct a model that links those variables to the ones that we need at runtime [1]. That model may be for example an analytic function built with an interpolator or a conditional average of the quantity with respect to the chosen control variables. The control variables can instead be defined by expert choice, or by using other techniques such as PCA or autoencoders [2]. Regardless of the choices made, the terms that are tipically more difficult to properly tabulate are the chemical source terms, since they span very diverse orders of magnitude. This generally results in a crude tradeoff between accuracy at low orders of magnitude (which are very important for the ignition behaviour of a flame) and high orders of magnitude.
In this work, starting from the DNS simulation of an ammonia/hydrogen/Air premixed flame, we propose a combination of data pre-processing and dataset sampling that allows for a good reconstruction accuracy for the source terms, at all orders of magnitude. The dataset is pre-processed through a combination of range scaling and yeo-johnson transformation. Then a weighted sampling procedure, tailored to capture more information on the flame front, is applied to the dataset, prior to the model building step. Results are presented as errors between the reconstructed and true values. A comparison between results obtained with and without the application of our technique is offered.

References

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