Machine Learning for the Modeling of Hydrogen Combustion

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Hydrogen, with its rising prominence in combustion applications, presents real challenges in combustion modeling. The stretch response of hydrogen flames significantly alters its structure, leading to pronounced local consumption rates, especially under turbulent and lean conditions. The aim of this project is to study the possibility of using **Machine Learning (ML) to model the hydrogen flame dynamics** on coarse meshes. This is a hot topic mixing **decarbonized combustion** (hydrogen) and **artificial intelligence**.

The complexity of the project will be gradual. First, a model will be trained on resolved stretched laminar premixed one-dimensional flames. Then, we will try to apply the model to under-resolved flames. Then, the validity of the approach will be assessed and the model can be corrected if necessary. Next, time permitting, a model can be trained on two-dimensional turbulent flames. We will then try to apply the model to Large Eddy Simulation (LES), where what happens at the sub-grid scale level needs to be modeled. The last step is a bonus, if all goes well and time permits.

Ideally, the candidate would have studied topics related to **Machine Learning (ML)**, **thermochemistry** and turbulent combustion. The following skills are required:

- hands-on knowledge on Machine Learning (ML), Deep Learning (DL), Convolutional Neural Network (CNN)
- knowledge in thermochemistry;
- know how to work in a Linux environment and in a terminal;
- know how to use python, write useful scripts;
- be motivated, and autonomous when needed.

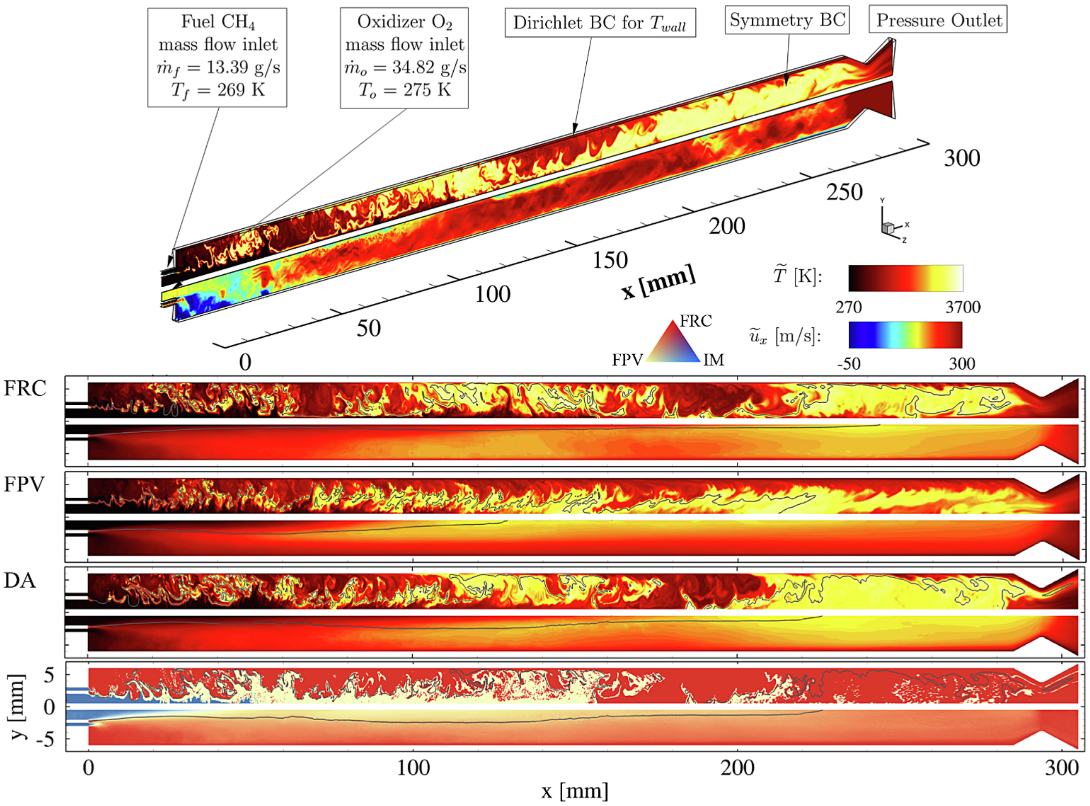

Figure 1: Simulation of a rocket combustor, comparing instantaneous and time-averaged flow fields from monolithic finite-rate chemistry (FRC) simulation, a two-scalar flamelet/progress variable (FPV) model, and data-assisted (DA) LES, with DA-combustion submodel assignment at the bottom. From Ref. [1].

References

[1] W. T. Chung, A. A. Mishra, N. Perakis, and M. Ihme, "Data-assisted combustion simulations with dynamic submodel assignment using random forests," *Combustion and Flame*, vol. 227, pp. 172–185, 2021.