Pprime Institute UPR 3346 CNRS ISAE-ENSMA and University of Poitiers

Ph.D. Proposal

Scalar dissipation rates and flame regime index models for Large Eddy Simulation of multi-regime turbulent combustion

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General context

The development of clean energy technology is of paramount importance to meet net zero carbon emissions in power generation and propulsion. Alternative fuels are candidates for combustion applications, with hydrogen, ammonia, or carbon-neutral fuels (SAF, biofuels) gaining attention worldwide. Efforts are being made to understand combustion using these fuels in complex turbulent reacting flow scenarios. Combustion models primarily designed for hydrocarbon fuel combustion must be revisited and adapted to alternative fuels. Indeed, practical application often introduces multi-regime combustion, this is, when multiple fuel-mixture burning regimes coexist: premixed, nonpremixed, and partially premixed. Multiphase flows or highly recirculating flows typically allow for multi-regime combustion. These could incorporate undesired effects such as low combustion efficiency and pollutant formation, making combustion chamber design very challenging so further modeling efforts are needed.

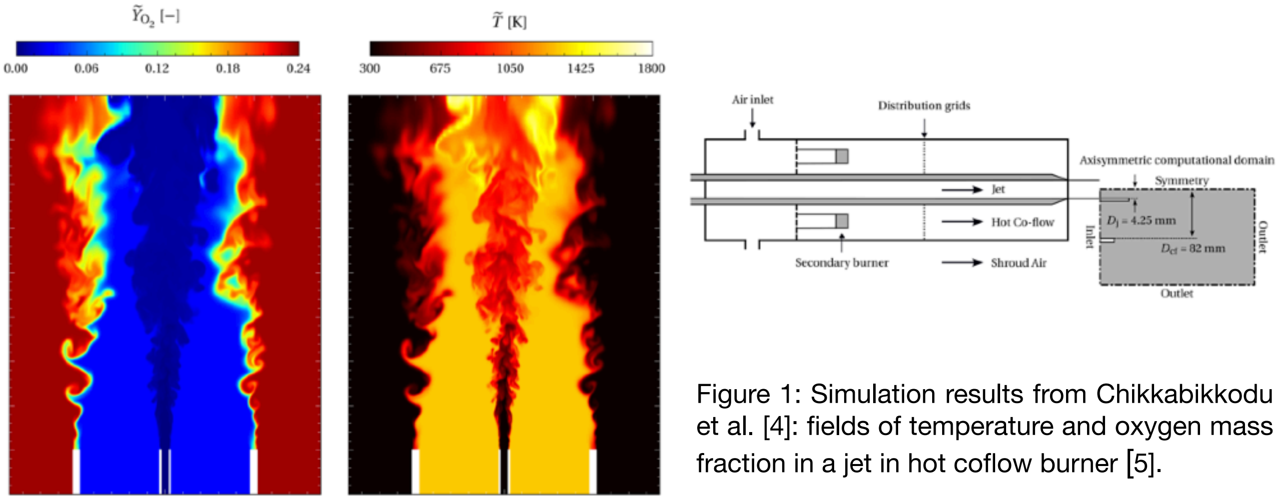

Figure 1: Simulation results from Chikkabikkodu et al. [4]: fields of temperature and oxygen mass fraction in a jet in hot coflow burner [5].

Description of the proposal

Research on turbulent combustion in partially premixed burning regimes is a recurrent topic at Pprime Institute [1–4] (see Fig. 1). In turbulent combustion modeling, two variables are strictly necessary to describe the local thermochemical state in partially premixed (adiabatic) systems [6], which relies on passive (mixture fraction) and reactive (progress variable) scalars formulation. Two-dimensional manifold-based models have been presented in different opportunities [7–9], making it attractive to reduce the computational cost of simulations. Moreover, closures for the scalar dissipation rates based on the variance and crossed scalar variance budgets has been proposed [1], which could allow for fine and *practical* description of partially premixed turbulent combustion at the flamelet regime using Large Eddy Simulation (LES). Moreover, a proper indicator of the reaction progress is needed in these situations, which should be able to capture the interchangeability between modes [3,10]. In the context of hydrogen (or ammonia) combustion, additional challenges are identified since disparate diffusive properties of key chemical species within the flame reactive region is observed. These challenging conditions motivate the derivation of fast and accurate models that are *viable* for LES of multi-regime turbulent combustion.

The objectives of the PhD thesis are: (i) to investigate the contribution of passive and reactive scalar dissipation rates contributions in multi-regime turbulent combustion at the LES subfilter scale including differential diffusion effects, (ii) to derive a dynamic turbulent flame regime index model accordingly. The PhD candidate will focus on both physics-based and data-driven modeling of turbulent reacting flows, including manifold-based modeling [11] and statistical approaches for turbulence-chemistry interactions [12,13] in LES. A *practical* metric for the dynamic flame index will be proposed, which would allow for LES that are both accurate and computationally efficient, especially for industrial applications. The PhD candidate will implement models on and use high-end computational tools for full- and high-fidelity simulations. Also, the PhD candidate will have the opportunity to interact with the experimentalists of the laboratory working on partially premixed turbulent hydrogen combustion, which will beneficial for further model validation.

Resources

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References

[1] A. Mura, V. Robin, M. Champion, Combust. Flame 149 (2007), 217-224

[2] P. D. Nguyen, P. Bruel, S. Reichstadt, Flow Turbul. Combust. 82 (2009)155–183

[3] E. Illana, D. Mira, A. Mura, Combust. Theory Model. 25 (2021), 121–157

[4] U. Chikkabikkodu, G. Boyer, F. Richard, A. Mura, Combust. Flame (2025) *Accepted*

[5] B. B. Dally, A. N. Karpetis, R. S. Barlow, Proc. Combust. Inst. 161 (2002) 1147–1154.

[6] P. A. Libby, F. A. Williams, Combust. Sci. Technol. 161 (2000) 351–390.

[7] P. D. Nguyen, L. Vervisch, V. Subramanian, P. Domingo, Combust. Flame 157 (2010) , 43–61

[8] E. Knudsen, Shashank, H. Pitsch, Combust. Flame 162 (2015) 159–180

[9] M. E. Mueller, Combust. Flame 214 (2020) 287–305

[10] A. G. Novoselov, B. A. Perry, M. E. Mueller, Combust. Flame 231 (2021), 111475

[11] H. Maldonado Colmán, M. E. Mueller, Combust. Flame (2025) *Accepted*

[12] H. Maldonado Colmán, A. Attili, M. E. Mueller, Combust. Flame 258 (2023) 112602

[13] H. Maldonado Colmán, D. Veynante, N. Darabiha, B. Fiorina, Combust. Flame 247 (2023) 112496