PhD Thesis at PPRIME Institute UPR3346 CNRS – ENSMA (Poitiers, France)

Duration: 36 months Gross salary: 2050 euros per month Recruitment period : open from now and until the end of the first semester 2023 Desired level of education: Engineer and/or Master of Science Knowledge and know-how: Fluid mechanics, Turbulence, Combustion, Fortran and Python programming, Cantera The PhD Thesis work will be done at ENSMA Poitiers, a French Engineering School of the ISAE group.

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PhD Thesis Title

"Benchmarking turbulent combustion models in conditions relevant to aero-engines fed by hydrogen or hydrogenhydrocarbon mixtures"

PhD Thesis Framework

The Thesis will be done within the framework of the HESTIA (HydrogEn combuSTion In Aero engines) research program funded by European HORIZON Action Grant, a program that does involve 23 international partners from Deutschland, France, Italy, Poland, and UK with both academic and industrial partners (SAFRAN, Rolls-Royce, General Electric, and MTU).

PhD Thesis Description

Carbon dioxide is considered as the most influential greenhouse gas: it is indeed estimated that the increase in atmospheric carbon dioxide concentration is responsible for about two-thirds of the total energy imbalance that is causing the rise of the Earth's temperature. As a consequence, partial decarbonization of energy conversion systems does not only appear as a technological challenge but also as a priority to fight against climate changes and global warming. Thus, hydrogen or hydrogen addition has been early identified as a possible solution to reduce emissions issued from conventional fossil fuels combustion. However, its use in existing combustion devices poses severe challenges and only a few studies have been concerned with the analysis of the effects resulting from the use of hydrogen (or its addition) in relevant conditions. For instance, studies devoted to the influence of hydrogen on flame dynamics and stabilization (blow-off or flashback) remain relatively scarce.

The proposed work aims at contributing to strengthen our current state of knowledge on hydrogen mixture combustion by (i) analysing the behaviour of computational models that are currently used to describe turbulent combustion in aero-engines, e.g., thickened flame model (TFM) or any others, when applied to hydrogen combustion. It also aims at (ii) discussing their possible extensions and/or generalization if required (and possible), and finally (iii) introducing – if necessary – other alternative modelling proposals.

The above-mentioned turbulent combustion models (TCM), which are used to describe lean-premixed pre-vaporized (LPP) or combustion in aero-engines in general, have been developed on the basis of the asymptotic fully-premixed combustion limit. This idealized regime was chosen because the associated combustion physics is sufficiently well understood to be cast in a framework that accounts for how turbulence and chemistry interact and the corresponding models were customized to be applied to partially premixed conditions [1]. The corresponding partially premixed regimes, which may involve transitions between premixed and non-premixed behaviour are however not very well understood and the relevance of these models remains questionable. This issue becomes even more critical for hydrogen or hydrogen/hydrocarbon mixtures. Indeed, hydrogen has a much higher diffusivity than standard fuels. It features also a higher flame speed S_L and much wider flammability limits than kerosene. Thus, hydrogen mixtures combustion is expected to display an increased tendency for flame flashback [2], i.e., core flow flashback or boundary layer flashback in the inlet flow. In addition to this, possible departures from the lean premixed pre-vaporized (LPP) regimes may be expected.

The proposed study will be conducted on the basis of high-fidelity simulations (DNS/LES) conducted with the CREAMS computational solver [3-17]. The performance of the solver has been assessed on massively parallel architectures. It is coupled to the CVODE solver and to the EGLIB library [18]. Based on an original combination of direct and ghost point forcing schemes [11,15], an immersed boundary method allows to handle typical geometries.

Different conditions will be considered. The first one is the geometry of reference to analyse boundary layer flashback in premixed systems: it corresponds to a premixed flame stabilized downstream of the sudden expansion of a turbulent planar channel flow. The possible influence of equivalence ratio stratification will be studied in another distinct – but similar – geometry featuring two separated inlets. These inlets will be fed with reactive mixtures that are characterized by two distinct equivalence ratio values Φ_1 and Φ_2 . The influence of increasing equivalence ratio gradient will be studied by increasing the difference between Φ_1 and Φ_2 . Finally, because the presence of swirl in the combustion system is expected to produce a marked change in their boundary layer flashback behaviour, the last test case will correspond to a turbulent channel flow with a wall-normal pressure gradient [19]. The corresponding effects will be introduced through a body force along the wall-normal direction leading to a wall-normal acceleration g_y with its intensity evaluated from a reduced gravity $g_y(\rho_u - \rho_b)/\rho_u$ or Froude number $S_L/\sqrt{g_y\delta(\rho_u - \rho_b)/\rho_u}$ where δ characterizes the channel height and $(\rho_u - \rho_b)/\rho_u$ is the normalized density gradient. The ability of the turbulent combustion models to reproduce the DNS results will be studied from a priori analyses of the DNS data. Since largeeddy simulation closures are already available in the CREAMS solver, the research proposal could also be readily extended to a posteriori analyses conducted for various levels of computational resolution. This may provide some very interesting and original information on the behaviour of the turbulent combustion models as the computational resolution is decreased up to levels similar to those retained in practical simulations of aero-engines.

The PhD Thesis will address several challenging issues relevant to the description of finite-rate chemistry effects and pollutant formation, multicomponent molecular transport (non-unity Lewis number) and its possible footprints (e.g., thermo-diffusive instability) in turbulent flow conditions, multi-regime combustion and departures from premixed conditions : partially-premixed and stratified conditions, characterization of the propensity to flashback with hydrogen mixtures, a priori analyses of TCM with emphasis placed on the turbulence resolution scale dependence.

Bibliography

[1] H. Knudsen, H. Pitsch, Large-eddy simulation for combustion systems: modeling approaches for partially premixed flows, **The Open Thermodynamics Journal**, 4 (2010) 76-85

[2] A.C. Benim, K.J. Syed, Flashback mechanisms in lean premixed gas turbine combustion, Academic Press, 2015

[3] P. J. Martínez Ferrer, R. Buttay, G. Lehnasch, A. Mura, A detailed verification procedure for compressible reactive multicomponent Navier-Stokes solvers, **Computers & Fluids** 89 (2014) 88–110.

[4] P. J. Martínez Ferrer, G. Lehnasch, A. Mura, Compressibility and heat release effects in high-speed reactive mixing layers: growth rates and turbulence characteristics, **Combustion and Flame** 180 (2017) 284–303.

[5] P. J. Martínez Ferrer, G. Lehnasch, A. Mura, Compressibility and heat release effects in high-speed reactive mixing layers: structure of the stabilization zone and modeling issues relevant to turbulent combustion in supersonic flows, **Combustion and Flame** 180 (2017) 304–320.

[6] R. Buttay, G. Lehnasch, A. Mura, Analysis of small-scale scalar mixing processes in highly under-expanded jets, Shock Waves 26 (2016) 93

[7] R. Buttay, L. Gomet, G. Lehnasch, A. Mura, Highly resolved numerical simulation of combustion downstream of a rocket engine igniter, **Shock Waves** 27 (2017) 655–674.

[8] R. Boukharfane, Z. Bouali, A. Mura, Evolution of scalar and velocity dynamics in planar shock-turbulence interaction, **Shock Waves** 28 (2018) 1117–1141.

[9] A. Techer, Y. Moule, G. Lehnasch, A. Mura, Mixing of fuel jet in supersonic crossflow, AIAA Journal 56 (2018) 465–481.

[10] R. Buttay, G. Lehnasch, A. Mura, Turbulent mixing and molecular transport in highly under-expanded hydrogen jets, **Int. J. Hyd. Energy** 43 (2018) 8488–8505.

[11] R. Boukharfane, F. H. E. Ribeiro, Z. Bouali, A. Mura, A combined ghost-point-forcing / direct-forcing immersed boundary method (IBM) for compressible flow simulations, **Computers & Fluids** 162 (2018) 91–112.

[12] D. Martínez-Ruiz, C. Huete, P. J. Martínez Ferrer, D. Mira, Irregular self-similar configurations of shock-wave impingement on shear layers, Journal of Fluid Mechanics 872 (2019) 889–927.

[13] R. Boukharfane, P. J. Martínez Ferrer, A. Mura, V. Giovangigli, On the role of bulk viscosity in compressible reactive shear layer developments, **European Journal of Mechanics B/Fluids** 77 (2019) 32–47.

[14] J. Ciesko, M. F. P. J., R. Penacoba Veigas, X. Teruel, V. Beltran, HDOT – an approach towards productive programming of hybrid applications, Journal od Parallel and Distributed Computing 137 (2020) 104–118.

[15] F. H. E. Ribeiro, R. Boukharfane, A. Mura, Highly-resolved large-eddy simulations of combustion stabilization in a scramjet engine model with cavity flameholder, **Computers & Fluids** 197 (2020) 104344.

[16] D. Martínez-Ruiz, C. Huete, P. J. Martínez Ferrer, D. Mira, Specific heat effects in two-dimensional shock refractions, **Shock Waves** (2021) 31 (2021) 1–17.

[17] A. Mura, A. Techer, G. Lehnasch, Analysis of high-speed combustion regimes of hydrogen jet, Combust. Flame (2022)

[18] A. Ern, V. Giovangigli, Fast and accurate multicomponent transport property evaluation, J. Comput. Phys. 120 (1) (1995) 105-116.

[19] J.R. Bailey, E.S. Richardson, DNS analysis of boundary layer flashback in turbulent flow with wall-normal pressure gradient, **Proceedings of the Combustion Institute**, 38 (2021) 2791-2799