Post-doctoral position at IFP Energies nouvelles (IFPEN)
in *Mechanical engineering (Fluid mechanics and Energetic)*

Modelling hydrogen /air premixed flames in spark-ignition engines for low to high Karlovitz numbers

The environmental impact of cars, in the development process of an engine, is one of the most challenging problems. The reduction of greenhouse emissions, mainly carbon dioxide (CO_2) and nitrogen oxide (NOx) that are created through the combustion process, is a primary consideration for car manufacturers. The strong alternative to full electrification is the development of dihydrogen (H_2) as a renewable energy source, via a fuel cell of via its combustion in a spark-ignition engine. The use of hydrogen in internal combustion engines is a very promising solution to avoid CO_2 emissions. However, NOx emissions can be enhanced due to the high temperatures reached in the combustion process. In order to reduce the level of NOx, lean or ultra-lean combustion technologies must be adopted to lower temperatures and NOx emissions.

The use of diluted or ultra-lean mixtures yields smaller laminar flame speed S_L^0, which in turn leads to a decrease of the combustion speed and an increase in cycle-to-cycle variations of the in-cylinder pressure. To increase this combustion speed, manufacturers use combustion chambers that allow for increased aerodynamics, leading to a greater turbulent velocity fluctuation u' associated to the integral scale length of turbulence l_t. The reduction of S_L^0 and the increase in u' induce a sharp increase in the Karlovitz number defined by:

$$Ka = \left(\frac{\delta_L}{\eta}\right)^2 = \left(\frac{l_t}{\delta_L}\right)^{1/2}\left(\frac{u'}{S_L}\right)^{3/2} \approx \left(\frac{l_t}{\nu}\right)^{1/2}\frac{(u')^{3/2.}}{S_L}$$

As shown in the above expression, this Ka number compares the flame thickness δ_L to the smallest scale of the turbulence, the Kolmogorov scale η. The corrugated flamelet regime is defined by $Ka < 1$, which means that even the smallest scale of turbulence cannot penetrate the flame structure, so the flame can be assimilated to a locally laminar flame. In this situation, combustion models such as ECFM are valid. Conversely, in highly diluted engines, Ka becomes much larger than unity, and the combustion enters the so-called TRZ (Thickened Reaction Zone Regime) in which the flame structure is disturbed by the smaller turbulent scales. In this regime, the flamelet models are no longer valid because i/the flame speed is no longer necessarily that of a laminar flame, ii/the flame is strongly thickened by the turbulence, which strongly modifies its interaction with the turbulence.

In order to overcome this limitation of the flamelet models, IFPEN coordinated the ANR MACDIL project (2016-2020) in which Renault was involved. In this project, a premixed turbulent combustion modelling allowing to represent both the low Karlovitz combustion regime (flamelet regime) and the high Karlovitz, i.e. TRZ, was initiated. The initial model used was ECFM (Colin et Benkenida 2004; Richard et al. 2007) developed at IFPEN and used by Renault in the CONVERGE code for its engine studies. As this model is limited to the flamelet regime, the objective was to extend it to the TRZ regime by removing its limitations.

This project started with the creation of a database of three-dimensional direct numerical simulations (DNS) of turbulent flames at increasing Karlovitz for simplified and reduced iso-octane/air chemistries at stoichiometry and ambient conditions. Some resulting instantaneous reaction rate fields are illustrated in Figure 1. It can be seen that in case A the flame structure remains comparable to that of a laminar flame. In contrast, for cases B and E, the flame structure is strongly perturbed on the fresh gas side (left side of the flame front) and thickened. Moreover, if we neglect the effects of differential diffusion of iso-octane (Lewis=1 assumption), we obtain a disturbance of the flame front

(left column) that is much smaller than in reality (right column). These DNS therefore also show that the perturbation of the flame structure in the TRZ regime cannot be taken into account without taking into account the differential diffusion properties of the fuel, an aspect not taken into account by the ECFM reference approach.
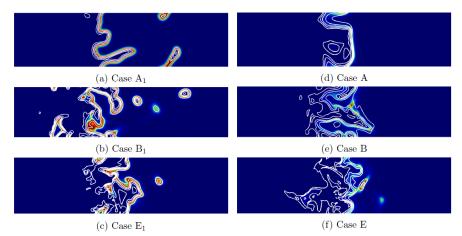

Fig. 1: instantaneous heat release rate fields on longitudinal cuts and contours of the progress variable (See (Suillaud et al. 2022) for details on legends and colorbar).

A first formulation of a model, henceforth called CFM-HK, was then proposed during the PhD thesis of Edouard Suillaud[1][2] and compared to the results of these DNS simulations by carrying out one-dimensional RANS calculations (Suillaud et al. 2022). This model simultaneously takes into account the flamelet and TRZ regimes as well as the differential diffusion effect (for fuel Lewis numbers greater than one) through the Markstein length L of the fuel, tabulated as a function of pressure, temperature, equivalence ratio and dilution. A posteriori LES simulations showed some limitations of this approach. First, the displacement velocity Sd modelled in Suillaud's model depends strongly on the filtered progress variable, but in the ignition phase this progress variable does not only reflect the position in the flame front but also the under-resolution of the flame kernel. As a result, this displacement speed is not suitable in the ignition phase and requires a specific correction. Furthermore, in the TRZ regime, the displacement speed can become negative on the unburned gas side (i.e. low values of the filtered progress variable), which is numerically a problem as this displacement speed enters the progress variable source term. A second PhD thesis has begun in 2021 to propose an improved version of CFM-HK. In particular, it focuses on the modelling of a consumption speed, which remains positive, instead of the displacement speed. Besides, an analysis of laminar and turbulent fluxes trough the flame front is conducted at Karlovitz numbers to improve the modeling of the turbulent Markstein length introduced in Suillaud's PhD.

The use of hydrogen implies being able to simulate at high Karlovitz numbers gasoline/H_2 blends with a high fraction of H_2 or even pure H_2 in the case of direct H_2 injection. In these situations, the Lewis can become less than unity (Huang et al. 2006) leading to a negative Markstein length (L<0). Although the CFM-HK approach takes into account the Markstein length, only the case of iso-octane was considered in Suillaud's PhD, corresponding to a Lewis of the order of 2 and a strongly positive Markstein length. A very different flame behaviour is then expected for H_2 since the positive curvature of the flame will this time accelerate and not slow down the flame (Trouvé et Poinsot 1994) leading to a self-sustained instability. The model of the displacement speed proposed in Suillaud's PhD is therefore not valid in this case.

High Karlovitz combustion has been the subject of numerous publications over the last ten years (Bruno Savard et Guillaume Blanquart 2014; Lapointe, Savard et Blanquart 2015; Savard et

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[1] https://www.youtube.com/watch?v=ffVbquDF0Q8
[2] https://www.ifpenergiesnouvelles.fr/article/modelisation-combustion-karlovitz-les-moteurs-allumage-commande

Blanquart 2015; Savard, Bobbitt et Blanquart 2015; Aspden, Day et Bell 2019; GÜLDER 2007), but most of them are mainly concerned with the analysis of this regime from DNS or experiments. A few publications propose closures of some source terms for the flame surface density equation (Hawkes et Chen 2005; Katragadda, Malkeson et Chakraborty 2014; Bruno Savard et Guillaume Blanquart 2014) or the G-equation (PETERS 1999), but no complete model that can be used in practice. A few others propose to apply already existing LES models, only validated in the flame regime, to academic high Karlovitz cases, with a correct predictivity often due to the very good resolution of the turbulence (Han et al. 2019).

The CFM-HK approach initiated in Suillaud's PhD is thus one of the few attempts to propose a model for the high Karlovitz regime, remaining otherwise valid in the flamelet regime. The post-doctoral study proposed here is therefore a continuation of this modelling effort aiming at developing a fully exploitable model for engine applications.

The planned research strategy is the following:

M1-M12 The DNS database will be extended to mixtures with a negative Markstein length (pure H_2). In addition, temperature, pressure and dilution conditions closer to the engine will also be considered in order to validate the fact that the analyses carried out under ambient conditions remain valid under engine conditions. This DNS database will then be exploited according to the same strategy adopted in the PhD study. The aim will be to propose a revised formulation of CFM-HK allowing to reproduce the DNS results in both the L>0 and L<0 cases.

M12-M18: Engine calculations on an experimental IFPEN database will be carried out with the improved version of CFM-HK to evaluate the gain in predictivity brought by the developments of this thesis compared with the standard CFM.

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Duration and start date	12 months with possible 6 months extension, as soon as possible
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Academic requirements	PhD Fluid mechanics and/or Energetic
Language requirements	Fluency in French or English, willingness to learn French
Other requirements	Turbulent combustion, Computational fluid mechanics, programming (Python), interest in the field of new energy technologies

For more information or to submit an application, contact the IFPEN supervisors.

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