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Effects of turbulence and strain rate on hydrogen-enriched high Karlovitz number lean premixed methane flames

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ABSTRACT

Effects of hydrogen addition at constant heat release, with the influence of turbulence and strain for lean methane-air turbulent counterflow premixed flames in the distributed regime (high Karlovitz number), are investigated using large eddy simulation (LES). Fuel mixtures of up to 60% of hydrogen in volume are considered, and sub-filter turbulence/chemistry interaction is modelled using the finite rate chemistry partially stirred reactor (PaSR) approach combined with detailed kinetics of a skeletal mechanism based on GRI-MECH3.0. Local flame structure and species formation are examined at different turbulence conditions. With constant heat release, hydrogen addition shows its benefits as species emission decreases with a more stable flame. By increasing integral length scale of turbulent structures, global strain rate of the flame is more significant, leading to an increase in flame thickness and reduction in the formation of intermediate species, pollutant NO and heat release. At higher strain rate, ratio of turbulent to laminar flame speed increases faster with increased hydrogen content of fuel, and the flame structure displays more wrinkling and is shorter as a consequence of faster mixing. It is also found that flame and heat release are less influenced by stretch when hydrogen is present within the fuel mixture, indicating the potential of hydrogen substitution for reaching a defined power output while reducing pollutant emissions.

1. Introduction

Among all fossil fuels, natural gas mostly composed of methane (CH_4) leads to the lowest global warming emissions [1]. Each year, regulations concerning pollutant emissions become stricter for internal combustion engine and gas turbine manufacturers, requiring cleaner combustion. Hydrogen-enrichment is a solution to enhance stability and to reduce pollutant emissions of lean methane-air premixed flames [2–5]. It has been pointed out that hydrogen-enriched flames exhibit greater laminar flame speeds [6] and increased resistance to strain [7]. Hydrogen-natural gas mixtures have successfully been used in internal combustion engines [8] and gas turbines [9]. By operating in lean mode, a compromise is set between emitting less pollutant and releasing less power. A solution is to operate the burner in the thin/broken reaction regime [10], where Karlovitz number $Ka > 100$. This number Ka corresponds to the smallest eddies of the flow (Kolmogorov scale η), defined as the ratio of the chemical time scale τ_c to the Kolmogorov time scale τ_η, and is one of the relevant non-dimensional numbers for characterization of different turbulent premixed regimes [11],

$$Ka = \frac{1}{Da(\eta)} = \frac{\tau_c}{\tau_\eta} = \frac{u'(\eta)/\eta}{s_u/\delta_u} = \left(\frac{\delta_u}{\eta}\right)^2, \quad (1)$$

where u' corresponds to the turbulent fluctuation velocity, s_u is the stretched laminar flame speed, δ_u is the stretched laminar flame thickness and Da is the turbulent Damkhüler number. δ_u can be defined as $\delta_u = \frac{T_f - T_u}{\left(\frac{dT}{dx}\right)_{max}}$, where T_f is the adiabatic flame temperature, T_u the temperature of unburned gases and $(dT/dx)_{max}$ the highest temperature gradient. High Karlovitz number Ka flames have gained more attention due to their capability to operate at higher power [12] without increasing pollutant emissions. With difficulties of experiments at high Karlovitz number, computational simulation has recently gained more interest especially in the field of direct numerical simulation (DNS) [13–18]. These studies have led to understanding the complexity of flame structure, and the process of local quenching and reignition at high Ka. Despite being still computationally expensive DNS are progressively implemented for practical combustion devices [19–21]. An alternative is to use the LES approach, which captures larger structures of the turbulent flow and is applicable to real devices. Accuracy of LES depends on the quality of sub-grid modelling to represent the effect of sub-filter scales. However, very few studies have been conducted at

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high Karlovitz number by LES [22–24]. The studies of Duwig et al. [23,24] notably shown that finite rate chemistry approach with detailed chemistry is suitable to describe this type of flow, as it is essential to track all the species present in a mechanism.

In this paper, the PaSR model [25–27] is used to handle complex chemistry. Opposed jet geometries have been used extensively under laminar and turbulent conditions to investigate premixed and non-premixed combustion. From an experimental point of view, studies of premixed turbulent counterflow flames (TCF) started in the early 1990's with the work of Kostiuk et al. [28–30] and has evolved as a benchmark case for the assessment of turbulence/chemistry interaction [31–33]. From a numerical point of view, LES simulations based on mixture fraction formulation have been conducted on this particular geometry [31,34,35], and recently using probability density functions (PDF) [36]. The counterflow configuration present several advantages that have been partially reviewed by Bray et al. [37]. These include simplicity of the experimental setup, flame stabilization occurring in a stagnation plane requiring no particular anchoring method, compact domain suitable for experiments or numerical simulations, and the ability to study the effect of strain and heat losses. Furthermore, as boundary conditions are simple and dynamics of the flame mainly depends on aerothermochemistry, TCF configuration constitutes an appealing test case for the evaluation of fuel effects.

Turbulence effects have been investigated experimentally by Coriton et al. [38] and Goh et al. [33], leading to a better understanding of production of turbulence with the use of fractal grids. The influence of hydrogen addition on flame structure and pollutant emission of high Karlovitz TCF at fixed equivalence ratio was presented in an earlier paper of the authors [39], where the LES procedure using OpenFOAM [40] was validated by comparison with DNS data from Carlsson et al. [41] on a freely propagating flame at high Karlovitz number. In industry, burners and furnaces are usually designed for a specific power output (MW). Hydrogen addition allows the combustor to operate at lower temperatures and to reduce pollutant emissions while keeping flame speed almost constant. In this paper, different CH_4-H_2-air mixtures, in terms of volume fraction of hydrogen are then considered with the same laminar heat release. The influence of hydrogen addition on flame structure and pollutant emissions is presented.

2. Governing equations and numerical procedure

In this paper, compressible Navier-Stokes equations with energy and species transport are used with a low mach number approach. We consider a mixture of N species considered as perfect gases which evolves in space $\mathbf{x}$ and time t. LES equations of reacting flows are obtained by both Favre and implicit filtering operations as

$$\begin{cases} \frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0 \\ \frac{\partial}{\partial t}(\overline{\rho}\widetilde{u}_i) + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}[\overline{\tau_{ij}} - \overline{\rho}(\widetilde{u}_i\widetilde{u}_j - \widetilde{u}_i\widetilde{u}_j)] \\ \frac{\partial}{\partial t}(\overline{\rho}\widetilde{Y_k}) + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{Y_k}) = -\frac{\partial}{\partial x_i}[\overline{V_{k,i}Y_k} + \overline{\rho}(\widetilde{u_iY_k} - \widetilde{u}_i\widetilde{Y_k})] + \overline{\dot{\omega}_k} \quad ; k \\ \qquad\qquad = 1,.,N, \\ \frac{\partial}{\partial t}(\overline{\rho}\widetilde{h^s}) + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{h^s}) = \frac{\partial}{\partial x_i}\left[\overline{\lambda\frac{\partial T}{\partial x_i}} - \overline{\rho}(\widetilde{u_ih^s} - \widetilde{u}_i\widetilde{h^s})\right] - \sum_{k=1}^{N} h_k^o\overline{\omega_k}, \end{cases} \tag{2}$$

where usual symbols are used. The open source code OpenFOAM (Open Field Operation and Manipulation) [40] is used in this study. For the convective and diffusive terms, 2nd order accuracy is achieved in space using central difference with linear interpolation, along with a normalised variable diagram (NVD) scheme (Gamma difference scheme). The Pressure Implicit with Splitting Operators (PISO) algorithm is chosen to solve the unsteady Navier-Stokes equations by the Rhie and Chow procedure [42], requiring no under-relaxation when the corrector step of momentum is recalled more than once. The PISO procedure follows 3 pressure and momentum corrections (1 outer and 3 inner iterations) with a residuals criterion of 10^{-10}. Time integration is carried out using an implicit quadratic backward approximation, corresponding to 2nd order accuracy. The pressure equation is solved using a generalised geometric-algebraic multi-grid (GAMG) solver along with a Gauss-Seidel smoother. Concerning the velocity field and other scalar fields, the code uses a preconditioned bi-conjugate gradient (PBiCG) solver for skew-symmetric matrices with the diagonal incomplete LU (DILU) matrix as preconditioner.

In order to ensure that simulations are stable, the maximum CFL number allowed in the simulations is 0.2. Complex kinetic mechanisms are employed in the simulations for detailed chemistry investigations. Thermophysical properties of the species k are calculated using JANAF tables. The unresolved Reynolds stress tensor $(\widehat{u_iu_j} - \widetilde{u}_i\widetilde{u}_j)$ is modelled using the dynamic Smagorinsky model of Lilly [43]. The unsolved species flux $(\widehat{u_iY_k} - \widetilde{u}_i\widetilde{Y_k})$ and enthalpy flux $(\widehat{u_ih^s} - \widetilde{u}_i\widetilde{h^s})$ are described using a simple gradient assumption such that $(\widehat{u_iY_k} - \widetilde{u}_i\widetilde{Y_k}) = -\frac{\nu_{sgs}}{Sc_t}\frac{\partial \widetilde{Y_k}}{\partial x_i}$ and $(\widehat{u_ih^s} - \widetilde{u}_i\widetilde{h^s}) = -\frac{\nu_{sgs}}{Pr_t}\frac{\partial \widetilde{h^s}}{\partial x_i}$, where the subscript "sgs" corresponds to subgrid scale. The filtered mass and heat diffusion fluxes are also specified using a simple gradient hypothesis leading to $\overline{V_{k,i}Y_k} = -\overline{\rho}\overline{D_k}\frac{\partial \widetilde{Y_k}}{\partial x_i}$ and $\overline{\lambda\frac{\partial T}{\partial x_i}} = \overline{\lambda}\frac{\partial \widetilde{T}}{\partial x_i}$. The diffusion coefficients D_k of different species k are considered as constant for each of the species, obtained on a one dimensional laminar freely propagating flame using the open source solver CANTERA [44], and are defined considering the median of Schmidt numbers Sc_k [45] such as $D_k = \nu/Sc_k$.

Although counter-gradient has been proven to exist in turbulent flames, its importance still remains controversial. Performing 2D and 3D DNS, Veynante et al. [46] have described when each type of turbulent diffusion is more prone to occur. Counter-gradient diffusion exists if the flowfield near the flame is rather controlled by thermal dilatation than chemical reaction whereas gradient diffusion becomes more important when turbulent motions of the flow dominate the flame. Turbulence levels then dictate the type of turbulent transport. Indeed, when turbulence levels are low, the flame is able to impose its own dynamics to the flowfield (by thermal expansion as a consequence of heat release) and counter-gradient turbulent diffusion occurs. On the other hand, when turbulence levels are high enough, gradient type of turbulence transport is expected as the flame is no longer able to prescribe its own behaviour to the flow. Veynante et al. [46] then proposed a "Bray number" N_B to assess which type of turbulent diffusion occurs inside the flame as

$$N_B = \frac{\varsigma s_u}{2\sigma u'}, \tag{3}$$

where ς corresponds to the heat release factor and σ is a function of order unity to consider the restricted capacity of small vortices to wrinkle the flame front. σ decreases with the length scale ratio l_I/δ_u. Counter-gradient (gradient) turbulent diffusion is fostered by low (high) values of u'/s_u and high (low) values of ς, equivalent to $N_B \geqslant 1$ ($N_B \leqslant 1$). Experimental results from Kalt [47] corroborate this criterion's definition. Considering that the heat release factor ς usually varies from 5 to 7 in premixed flames and with the use of Eq. 3, counter-gradient turbulent transport is then expected when $u'/s_u \leqslant 3$, which never occurs in any case of study in this paper.

Detailed description of the LES modelling and numerical procedure are reported in the authors' previous paper [39]. However, the modelling of the **filtered reaction rate** of species k is reminded in the section below, with addition of some more information.

2.1. Combustion modelling

Finite rate chemistry with the partially stirred reactor (PaSR) approach derived by Karlsson [48] is considered for modelling the filtered reaction rate of species k,$\overline{\dot{\omega}_k}$, along with the skeletal mechanism of Karalus [49] to handle CH_4-H_2 mixtures. Mathematically, for all species k, the PaSR model can be formulated by