A Direct Numerical Simulation based comparison between conventional and MILD combustion processes of turbulent stratified mixtures

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1 Introduction

Moderate or Intense Low oxygen Dilution (MILD) combustion [1,2] can provide simultaneous emission reduction and improvement of thermal efficiency. A combustion process is considered to take place under MILD conditions when the inlet temperature (T_o) exceeds the mixture autoignition temperature (τ_{ign}) and the maximum temperature rise (ΔT) remains smaller than τ_{ign}[1]. Direct photography and Rayleigh thermometry of MILD combustion reveal a distributed combustion behaviour, whereas Planar Laser-Induced Fluorescence images of OH radicals (OH-PLIF) and Direct Numerical Simulations (DNS) indicate the existence of flame fronts [3-8]. Minamoto et al. [4] attributed the distributed flame fronts to the significant amount of reaction zone interactions. The current understanding of MILD combustion remains incomplete and further research is necessary. Several DNS studies [4-8] focused on fundamental physical understanding and assessment of different combustion modelling methodologies for MILD combustion. To date, most DNS of MILD combustion has been carried out for two conditions: (i) homogenous-mixture MILD combustion [4-6] and (ii) inhomogeneous-mixture MILD combustion [7,8]. In the former, there are no composition gradients, and the mixture is perfectly premixed. On the other hand, composition gradients exist in the latter and combustion is occurring over a wide range of mixture fractions (e.g., combustion is occurring in a stratified mixture). Several previous DNS studies [4,5] investigated the differences in combustion processes between homogenous-mixture MILD combustion with conventional turbulent premixed flames. For instance, Minamoto et al. [4] stated that flamelet-based models for premixed flames could be extended to homogenous-mixture MILD combustion. Moreover, Awad et al. [5] compared the reactive scalar gradient statistics between homogeneous mixture MILD combustion and conventional premixed flames and concluded that the models for turbulent premixed combustion could potentially be extended for homogenous-mixture MILD combustion with some adjustments. However, a comparison between inhomogeneous-mixture MILD combustion and conventional combustion of stratified mixtures is yet to be done in the literature. The current work aims to address this gap in the existing literature by analysing DNS datasets, conducted with a skeletal chemical mechanism of methane-air combustion, for turbulent stratified flames and inhomogeneous-mixture MILD combustion at the same global equivalence ratio $\langle \phi \rangle = 0.8$.

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2 Mathematical Background

The reaction progress variable c in stratified or inhomogeneous mixtures can be expressed in terms of fuel mass fraction Y_f according to the following relation [9,10]:

$$c = (\xi Y_{f\infty} - Y_f)/[\xi Y_{f\infty} - \max[0, (\xi - \xi_{st})/(1 - \xi_{st})]\, Y_{f\infty}] \quad (1)$$

where, ξ and ξ_{st} are the mixture fraction and the stoichiometric mixture fraction respectively, and $Y_{f\infty}$ is the mass fraction of fuel in the fuel stream. The mixture fraction can be specified in terms of the elemental mass fractions and atomic masses using the following relation [11]:

$$\xi = [2\, Z_C/W_C + 0.5\, Z_H/W_H + (Z_{O,2} - Z_O)/W_O]/[2\, Z_{C,1}/W_C + 0.5\, Z_{H,1}/W_H + Z_{O,2}/W_O] \quad (2)$$

$$\xi_{st} = Z_{O,2}/W_O/[2\, Z_{C,1}/W_C + 0.5\, Z_{H,1}/W_H + Z_{O,2}/W_O] \quad (3)$$

$$\phi = \xi(1 - \xi_{st})/[\xi_{st}(1 - \xi)] \quad (4)$$

where, W_j and Z_j are the elemental atomic masses and mass fractions of species j (i.e., $j =$oxygen, carbon, and nitrogen), and ϕ is the equivalence ratio. In Eq. 4, the subscript 1 indicates the fuel stream and subscript 2 refers to the oxidizer stream. In stratified mixtures, the reaction rate of the progress variable $\dot{\omega}_c$ is given by [10]:

$$\dot{\omega}_c = -\dot{\omega}_f/\xi Y_{f\infty} \text{ for } \xi \le \xi_{st}\, ; \dot{\omega}_c = -\dot{\omega}_f(1 - \xi_{st})/\xi_{st}(1 - \xi)Y_{f\infty} \text{ for } \xi > \xi_{st}\, ; \quad (5)$$

The relative alignment of $\nabla\xi$ and ∇c plays a key role in the combustion of stratified mixtures, which can be quantified using the following relation [10,12]:

$$cos\theta_{c\xi} = \nabla c . \nabla\xi/|\nabla c||\nabla\xi| \quad (6)$$

Here, $cos\theta_{c\xi} > 0$ ($cos\theta_{c\xi} < 0$) indicates a back (front) supported mode of flame propagation. Moreover, combustion in inhomogeneous mixtures can give rise to the coexistence of different modes of combustion, which can be characterized by the Flame index (FI) [13]:

$$FI = \frac{\xi - \xi_{st}}{2|\xi - \xi_{st}|}\left(1 + \frac{\nabla Y_{CH_4} . \nabla Y_{O_2}}{|\nabla Y_{CH_4}||\nabla Y_{O_2}|}\right) \quad (7)$$

According to Eq. 7, FI takes a value close to -1.0 and 1.0 for lean and rich premixed modes of combustion, respectively, whereas a value of zero is indicative of pure non-premixed mode of burning. Doan et al. [7] described a mixed mode for $0.1 \le |FI| \le 0.8$. MILD combustion exhibits the coexistence of ignition, flame-front interaction and flame propagation modes [6] and these aspects can be characterized by considering the balance between the convection, diffusion, and reaction terms in the c transport equation. The reaction progress variable c transport equation is given as [6]:

$$\rho\, \partial c/\partial t + \underbrace{\rho u_j\, \partial c/\partial x_j}_{C:convection} = \underbrace{\partial\left(\rho D_c\, \partial c/\partial x_j\right)/\partial x_j}_{D:Diffusion} + \underbrace{\dot{\omega}_c}_{R:reaction} \quad (8)$$

Here, $\beta = |C - D| - |R| > 0$ represents a situation where flame propagation is dominant, whereas $\beta < 0$ occurss where the chemical reaction and flame surface interactions dominate [6].

3 Numerical Implementation

The standard governing equations for mass, momentum, energy and species mass fractions for compressible reacting flows have been solved using the compressible DNS code SENGA2 [4-8]. In SENGA2, the thermophysical properties are estimated as a function of temperature. The spatial derivatives for the internal grid points are approximated using 10th order central difference scheme. However, near the non-periodic boundaries, the accuracy of the spatial derivatives decreases gradually to a one-sided 4th order scheme. An explicit 4th order Runge-Kutta time integration method has been adopted for time advancement. A skeletal methane-air chemical mechanism [14] consisting of 16 species and 25 reactions has been used in the current study. A cube (rectangular cuboid) of size $10\text{mm} \times 10\text{mm} \times 10\text{mm}$ ($20\text{mm} \times 10\text{mm} \times 10$ mm) discretized by a uniform cartesian grid of 252×252×252 (504×252×252) has been used for the MILD combustion (stratified flames) simulations. The domain discretization for both MILD combustion and stratified flames simulations ensures that there are at least 12 grid points for resolving the thermal flame thickness $\delta_{th} = (T_{ad} - T_0)/max|\nabla T|_L$ of the mixture corresponding to the global mean equivalence ratio of $\langle \phi \rangle = 0.8$ with T, T_{ad} and T_0 being the instantaneous, adiabatic flame and reactant temperatures, respectively for $\phi = 0.8$ and the subscript 'L' refers to the values in the corresponding 1D unstretched premixed flame. Moreover, the domain discretization also ensures that the Kolmogorov length scales remain greater than the grid spacing. The same boundary conditions have been imposed for both MILD combustion and stratified flames. The boundary condition at the left x-direction has been assigned a turbulent inflow with specified density, velocity and species mass fractions, whereas the right x-direction boundary has been considered to be partially non-reflecting outflow. The remaining boundaries (i.e., transvers boundaries) have been considered to be periodic. The initial fields have been generated following the methodology previously used by Minamoto et al. [4] and Doan et al. [7]. The stratified and MILD combustion cases have been simulated at the same global mean equivalence ratio $\langle \phi \rangle = 0.8$ at two turbulence intensities u'/S_L= 4.0 and 8.0 for the same integral length scale ratio l/δ_{th} =2.5 where S_L is the unstrained laminar burning velocity corresponding to $\phi = 0.8$. The thermochemical conditions in terms of mole fractions in the oxidizer stream (i.e., of O_2, CO_2 and H_2O), the unstrained laminar burning velocity corresponding to $\phi = 0.8$, and unburned gas temperature T_0 and the initialization conditions in terms of root-mean-square values of equivalence ratio ϕ' and the normalized length scale of equivalence ratio variation are listed in Table 1 for both MILD and conventional stratified mixture combustion conditions. The ϕ varies between 0.3-1.3 in MILD combustion, whereas it varies between 0.6-1.0 in stratified flames as stratified mixture combustion in most engineering applications occurs at lean conditions. The MILD combustion cases have been conducted for about 2.5 flow-through time (i.e., $2.5L_x/U_{in}$ where $U_{in} = 20\ m/s$ is the mean inlet velocity and L_x is the domain length in the x-direction), which amounts to $11.0\ l/u'$ and $22.0\ l/u'$ for cases with initial $u'/S_L = 4.0$ and 8.0, respectively. The stratified flames were continued for about 1.0 chemical time scale, which amounts to $1.6\ l/u'$ and $3.2\ l/u'$ for cases with initial $u'/S_L =$ 4.0 and 8.0, respectively. These simulation times remain comparable to several previous analyses [4-8].

Table 1: DNS initial conditions for MILD combustion

Case	X_{O_2}	X_{CO_2}	X_{H_2O}	$S_L(m/s)$	$T_0(K)$	$\langle \phi \rangle$	ϕ'	l_ϕ/l
MILD	0.048	0.061	0.121	3.20	1500	0.8	0.5	1.42
Stratified	0.21	0.0	0.0	0.28	300	0.8	0.2	1.25

4 Results and Discussion

Figure 1 shows the distributions of normalized mixture fraction ξ/ξ_{st} and non-dimensional temperature $\theta = (T - T_0)/(T_{ad} - T_0)$ in the central $x - y$ midplane for both the stratified flame and inhomogeneous-mixture MILD combustion cases for initial u'/S_L= 8.0. It can be seen from Fig. 1 that combustion occurs over a wide range of mixture fractions for both conventional stratified mixture and MILD combustion cases. Moreover, the level of mixture inhomogeneity decreases towards the burned gas side for both cases, but this effect is more prominent in the conventional stratified flames than in the MILD combustion cases. The molecular diffusivity increases significantly in the burned gas due to a marked increase in temperature in the case of conventional stratified mixture combustion, which acts to enhance mixing and reduces the mixture inhomogeneity in the burned gas. As the temperature rise remains smaller in MILD combustion cases compared to stratified flame cases, the reduction in ξ variation towards the burned gas side is more prominent for stratified flames than in MILD combustion.

Figure 2 shows the normalized turbulent burning velocity $S_T/S_L = (\rho_0 A_p S_L)^{-1} \int_V \dot{\omega}_c dV$ (where ρ_0 is the unburned gas density and A_p is the projected area in the direction of mean flame propagation) and the flame surface area $A_T = \int_V |\nabla c| dV$ normalized by its corresponding values (shown with subscript L) attained from the 1D unstretched $\phi = 0.8$ laminar premixed flame solution for all cases investigated. It can be seen from Fig. 2 that $S_T/S_L > A_T/A_L$ is obtained for MILD combustion cases. However, S_T/S_L and A_T/A_L remain comparable for stratified flames with A_T/A_L being slightly higher than S_T/S_L. It is also evident from Fig. 2 that S_T/S_L increases with increasing u'/S_L for both stratified flames and MILD combustion cases. However, an increase in the turbulence intensity results in a slight decrease (increase) in A_T/A_L in the inhomogeneous-mixture MILD combustion (conventional stratified mixture) cases.

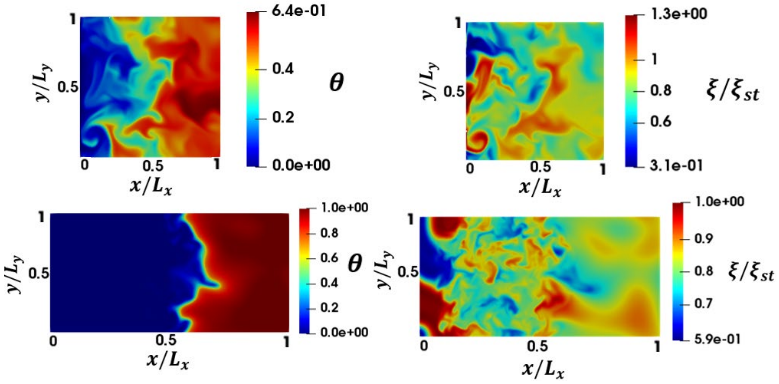

Figure. 1: Distribution of ξ/ξ_{st} (right) and $\theta = (T - T_0)/(T_{ad} - T_0)$ (left) at $x - y$ midplane: MILD combustion (top) and conventional stratified flame (bottom) cases corresponding to initial u'/S_L= 8.0.

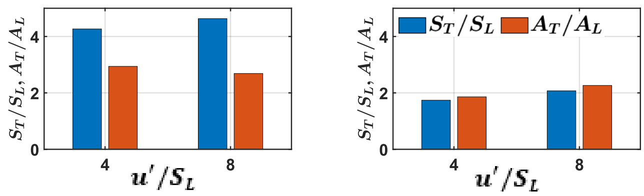

Figure 2: Values A_T/A_L and S_T/S_L for MILD combustion (left) and stratified flames (right).

The analysis of different combustion modes can be quantified using the FI and by investigating the balance between different terms in the reaction progress variable c transport (i.e., β). The percentages of heat release rate arising from different combustion modes, distinguished by FI, as a percentage of the total heat release rate $HR_{Total} = \int_V HR\ dV$ for all cases investigated here are presented in Fig. 3 where the heat release rate is defined as: $HR = -\sum_{k=1}^{N} h_{f,i}^0 \dot{\omega}_i$ with $h_{f,i}^0$ being the enthalpy of formation for species i. Figure 3 shows that lean premixed mode (LP) remains the dominant heat release contributor for both MILD combustion and stratified flames. It can further be seen from Fig. 3 that there are non-negligible heat release contributions from the rich premixed mode (RP), non-premixed mode (NP) and mixed mode (MIX) in the MILD combustion cases, which is consistent with previous DNS analysis [7] involving inhomogeneous-mixture MILD combustion. However, the contributions of RP, NP, and MIX remain negligible for stratified flames. The heat release rate (HR) contributions from different combustion modes based on the β are shown in Fig. 4. It is evident from Fig. 4 that the HR contribution arising from flame propagation-dominated (FD) regions dominates over reaction-dominated (RD) regions for both inhomogeneous-mixture MILD combustion and conventional stratified flame cases. Moreover, the percentage of HR arising from the RD regions remains slightly higher for the MILD combustion cases compared to the stratified flame cases. Figure 4 also shows that more that 80% of the domain experiences FD regions for both inhomogeneous-mixture MILD combustion and stratified flame cases. However, that behaviour is found to be more prominent in the latter. Moreover, it can be observed that the effect of RD zones on the HR is more significant for the stratified flames especially at high turbulence intensities (i.e., 7% of the domain results in about 25% of HR for the stratified flames, whereas 18% of the domain results in about 30% of HR for MILD combustion cases).

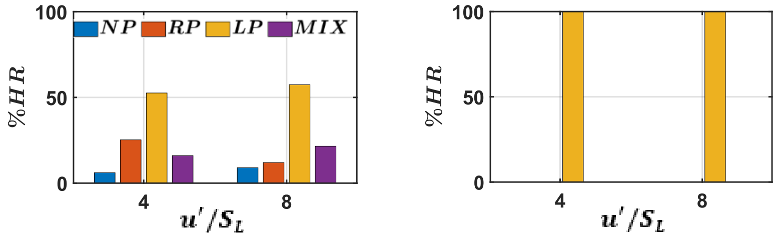

Figure 3: Percentages of HR for different combustion modes based on FI: MILD combustion (left) and stratified flames (right).

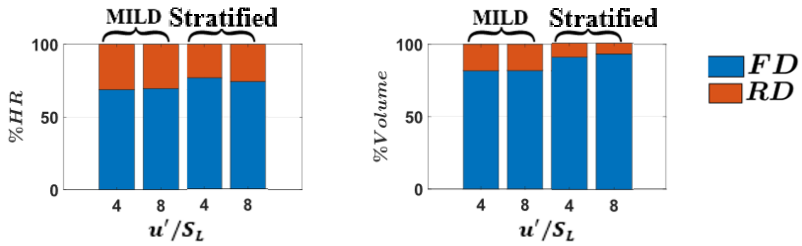

Figure 4: Percentages of HR and volume for different combustion modes based on β.

Figure 5 shows the heat release and volume percentage arising from back- and front-supported flame propagation modes for both MILD and conventional stratified flame cases. It can be seen from Fig. 5 that more than 80% of the total heat release rate originates from back-supported stratification in stratified flame cases. By contrast, the front-supported heat release contribution assumes higher values compared to back-supported heat release contribution for MILD combustion. However, unlike stratified flame cases where HR predominantly comes from the back-supported mode and the front-supported contribution remains insignificant, both front- and back-supported HR contributions are of equal importance in MILD combustion cases. Figure 5 further shows that, the back-supported HR contribution increases (mildly decreases) and front-supported HR contribution decreases (mildly increases) for MILD combustion (stratified flame) cases with increasing u'/S_L. However, that effect of u'/S_L is more prominent for the MILD combustion cases than the stratified flames cases.

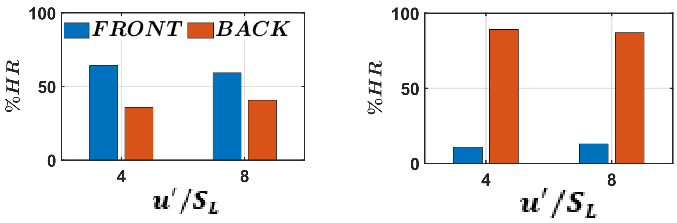

Figure 5: Percentages of HR form front/back-supported mode: MILD combustion (left) and stratified flames (right).

4 Conclusions

The qualitative differences between conventional and MILD stratified mixture combustion at a global equivalence ratio of $\langle \phi \rangle = 0.8$ have been investigated using three-dimensional DNS. Significant differences between A_T/A_L and S_T/S_L have been found for MILD combustion, whereas these values are comparable for the conventional stratified flames considered here. Moreover, it has been observed that lean premixed mode remains the dominant heat release contributor for all cases considered here but rich-premixed and diffusion modes of combustion play more significant roles in MILD combustion cases than in conventional stratified flames. Furthermore, for both MILD combustion and stratified flame cases, most of the heat release arises from the flame propagation dominated regions. It has been found that most of the heat release originates from back supported flame propagation in stratified flame cases considered here, whereas, both front and back supported heat release contributions are of equal importance in the MILD combustion cases.

Acknowledgements

The authors are grateful for the financial and computational supports from the Engineering and Physical Sciences Research Council, UK (Grant: EP/S025154/1 and EP/R029369/1).

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