

The effects of mixture fraction and its gradient on the localised ignition of turbulent mixing layers

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1 Introduction

Localised spark or laser ignition is common in igniting homogeneously mixed reactants. (i.e. gasoline engines). However, localised ignition of inhomogeneous mixtures has applications in high altitude gas turbine relight and Direct Injection engines and is less well-studied. Hilbert *et al.* [1] and Ray *et al.* [2] studied ignition phenomena in inhomogeneous mixtures in a turbulent environment using 2D Direct Numerical Simulation (DNS) with detailed chemistry and transport. Recently, Chakraborty *et al.* [3] analysed the flame structure following localised ignition of inhomogeneously mixed reactants using 3D DNS with simplified chemistry, and indicated that turbulence adversely affects the ignition performance and may even lead to extinction for high values of turbulent velocity fluctuation u' . DNS studies [1-3] reported a tribrachial flame structure, where two premixed flame branches are observed on fuel rich and lean sides and a diffusion flame is formed on the stoichiometric mixture fraction isosurface. Recent experimental data indicates the possibility of non-local effects of localised ignition of inhomogeneous mixtures [4]. The effects of ignitor location on the localised ignition of inhomogeneous reactants are yet to be analysed in detail using DNS. The main objectives of this study are to understand the effects of mixture fraction value and the magnitude of its gradient at the ignition location on the overall ignition performance using DNS.

2 Mathematical background and Numerical implementation

Most combustion DNS studies are done either in two-dimensions with detailed chemistry, or in three dimensions with simplified chemistry. In the present study the second approach is adopted and the chemical mechanism is described by a single step irreversible chemical reaction. The specific heats for all species are taken to be equal and independent of temperature for the sake of simplicity. The diffusion velocities of different species are accounted for by Fick's law of diffusion. Transport quantities such as viscosity μ , thermal conductivity λ and density weighted mass diffusivity (ρD) are assumed to be the same for all the species and are independent of temperature. Lewis number for all the species are taken to be unity. The localised ignition is accounted for by a Gaussian heat source in the energy conservation equation of the following form [5]: $q'''(r) = A \exp(-r^2/R^2)$ where r is the radial distance from the ignition centre, and R is the characteristic width of the ignitor (i.e. spark) which is taken to be $1.1l_f$ where $l_f = D_{ref}/S_L$, with D_{ref} being the reference diffusivity and S_L the laminar flame speed of the stoichiometric mixture. The constant A is determined by the following volume integration:

$$\dot{Q} = \int_V q''' dV \text{ and } \dot{Q} = a \rho_0 C_p \tau T_0 (4/3) \pi l_f^3 [H(t-t_1) - H(t-t_2)] / (t_2 - t_1) \quad (1)$$

where a is a parameter determining total energy input. Heaviside functions in the numerator ensures that the localised ignitor remains operational during $t_1 < t < t_2$. The time instants t_1 and t_2 determine the energy deposition duration $t_{sp} = (t_2 - t_1) = b t_F$ where b is a duration parameter and t_F is a chemical time scale given by: $t_F = l_f / S_L$. For

spark ignition, the optimum value of b varies from 0.2 to 0.4 [6] and b is taken here to be 0.2. The mixture fraction ξ profile is initialised by an error function profile with characteristic thickness $\delta_z = 1/\text{Max}(|\text{grad } \xi|)$. The fuel and oxidiser mass fractions are initialised by: $Y_F = Y_{F\infty}\xi$ and $Y_O = Y_{O\infty}(1-\xi)$ where $Y_{F\infty}$ and $Y_{O\infty}$ are fuel and oxidiser mass fractions in pure fuel and oxidiser. In the present case the values of $Y_{F\infty}$, $Y_{O\infty}$ and s are taken to represent methane-air mixture: $Y_{F\infty} = 1.0$ and $Y_{O\infty} = 0.233$, $s = 4.0$, where s is the mass of oxidiser consumed per unit mass of fuel consumption. These values are representative of methane/air mixtures. For the above values, the stoichiometric mass fraction of fuel is $Y_{Fst} = 0.055$. The heat release parameter τ and non-dimensional temperature T are given by: $T = (\tilde{T} - T_0)/(T_{ad} - T_0)$ and $\tau = (T_{ad} - T_0)/T_0$, where $\tilde{T}$ is the dimensional temperature and T_{ad} is the adiabatic flame temperature of stoichiometric mixture. The simulations have been carried out in a cubic domain where the boundaries in the direction of inhomogeneity are taken to be non-reflecting whereas the transverse direction boundaries are taken to be periodic. The velocity field is initialised by a pseudo-spectral method using Batchelor-Townsend spectrum. The spatial differentiation is carried out using a 10th order central difference scheme for internal grid points. The order of differentiation drops gradually to the 2nd of one-sided scheme near non-reflecting boundaries. The time-advancement is carried out using a low storage 3rd order Runge-Kutta scheme. All simulations have been carried out for 2 initial eddy turn over times which correspond to $7.35 t_{sp}$. The domain length $L = 21l_f$ and S_L are taken to be reference length and velocity scales respectively. The simulation parameters for the present DNS database are presented in Table 1.

Case	u'/S_L	L_{11}/l_f	a	b	δ_z/l_f	Ignitor location	l_f/η
A	4.0	3.36	3.6	0.2	2.3	$\xi = \xi_{st}$	2.87
B	4.0	3.36	3.6	0.2	1.5	$\xi = \xi_{st}$	2.87
C	4.0	3.36	3.6	0.2	4.6	$\xi = \xi_{st}$	2.87
D	4.0	3.36	3.6	0.2	2.3	$\xi = 1.33 \xi_{st}$	2.87
E	4.0	3.36	3.6	0.2	2.3	$\xi = 0.5 \xi_{st}$	2.87
F	-	-	3.6	0.2	2.3	$\xi = 0.5 \xi_{st}$	-
G	-	-	3.6	0.2	-	Premixed $Y_F = 0.5 Y_{Fst}$	-

Table 1: List of parameters for the DNS database. Ignitor location in x direction corresponds to the mixture fraction ξ value. The ignitor is located at $y/L = z/L = 0.5$.

3 Results & Discussion

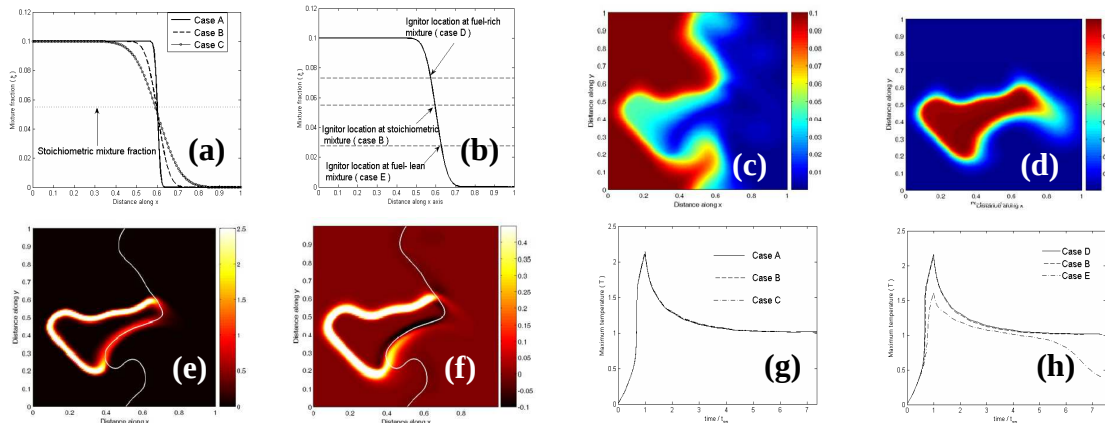


Fig. 1: Ignitor location in relation to initial profile of mixture fraction: (a) cases A-C, (b) cases B,D, and E; Important fields for case B at $t = 7.35t_{sp}$: (c) fuel mass fraction, (d) non-dimensional temperature, (e) fuel reaction rate magnitude, (f) cross-scalar dissipation rate. Temporal evolution of non-dimensional temperature: (g) cases A-C, (b) cases B,D, and E. Stoichiometric mixture fraction isosurface is shown by the white line in Figs. 1e and f.

The ignitor location for cases A-E is shown in Figs. 1a and b. It is apparent from Fig.1a that, for cases A-C, the mixing layer thickness is modified but the ignitor is placed at the stoichiometric mixture fraction location. On the other hand, in cases D and E, the ignitor is placed in fuel-rich and fuel-lean locations respectively. The fuel

mass fraction, temperature and reaction rate field for case B are shown in Figs. 1c,d and e respectively for time $t = 7.35t_{sp}$. It is evident that reaction rate magnitude $\dot{w}_F$ assumes significant values for both fuel-rich and lean sides and for stoichiometric mixtures. In order to understand the flame structure, it is instructive to look into cross-scalar dissipation rate ($\chi_c = 2D \text{grad } Y_F \cdot \text{grad } Y_O$), which is positive for premixed flames and negative for diffusion flames. The cross-scalar dissipation rate field for case B at $t = 7.35t_{sp}$ is shown in Fig. 1f where it is evident that premixed flames are formed on both fuel-rich and lean sides and a diffusion flame is stabilised on the stoichiometric mixture fraction isosurface. The temporal evolutions of the maximum non-dimensional temperature T for cases A-E are shown in Figs. 1g and h. For all cases the maximum temperature increases with time during the energy deposition time ($t \leq t_{sp}$). Once the non-dimensional temperature reaches a value in the order of $T_c = 1 - 1/\beta$, a small change in temperature leads to a large change in fuel reaction rate which rapidly increases the maximum temperature. Once the energy deposition is completed, the maximum temperature drops and, for the cases of self-sustained combustion, settles close to the adiabatic flame temperature ($T \approx 1$). It is evident from Fig. 1h that, for case E, the ignitor was successful in igniting the mixture but eventually the flame extinguishes. This behaviour may be explained by the reaction zone structure. The scatter of reaction rate magnitude with mixture fraction is shown in Fig. 2a, which shows that high values of reaction rate are attained for fuel-rich mixtures due to the simultaneous presence of high temperature and fuel concentration. The maximum value of temperature decreases with time, thus the maximum value of chemical reaction rate (heat release) also decreases with time. Finally when the maximum temperature settles close to the adiabatic flame temperature, if the heat release due to chemical reaction overcomes heat transfer from the hot gas kernel, the flame survives and self-sustained combustion ensues. In case E, the ignition kernel encloses a smaller amount of fuel-rich mixture in comparison to other cases. As a result, the heat transfer from the kernel eventually overcomes the heat release and leads to flame extinction. The amount of reaction is characterised by a reaction progress variable given by: $c = (\xi Y_{F\infty} - Y_F) / [\xi Y_{F\infty} - \max[0, (\xi - \xi_{st}) / (1 - \xi_{st})] Y_{F\infty}]$ (2)

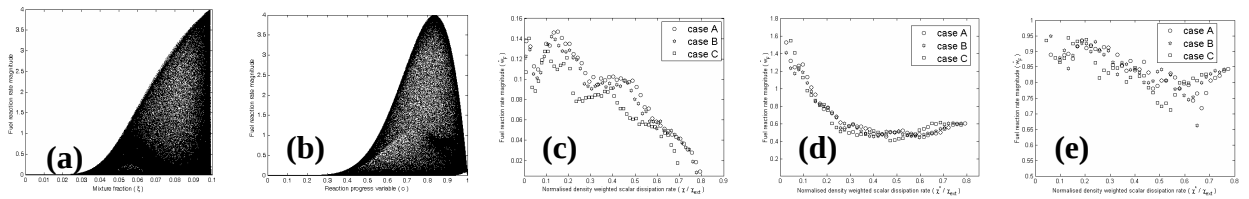


Fig. 2: (a) Scatter of fuel reaction rate magnitude (a) with mixture fraction, (b) with reaction progress variable, (c) Variation of mean fuel reaction rate magnitude conditional on normalised density weighted scalar dissipation rate χ^*/χ_{ext} , (d) Variation of mean fuel reaction rate magnitude conditional on χ^*/χ_{ext} in the most reactive region $0.7 < c < 0.9$, (e) Variation of mean fuel reaction rate magnitude conditional on χ^*/χ_{ext} in the region $0.5 < c < 0.9$ on the stoichiometric mixture fraction isosurface.

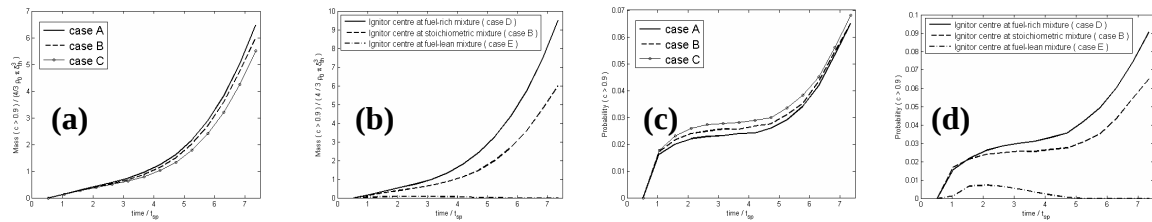


Fig. 3: Temporal evolution of the mass with $c \geq 0.9$: (a) cases A-C, (b) cases B,D, and E. Temporal evolution of the probability of finding $c \geq 0.9$ on the stoichiometric mixture fraction isosurface: (c) cases A-C, (d) cases B, D, and E. The mass of the burned region is normalised by the mass of the sphere with fresh gas density ρ_0 and with radius equal to the thermal flame thickness of a stoichiometric premixed flame δ_{th} .

The variation of fuel reaction rate magnitude with reaction progress variable is shown in Fig. 2b, which shows that peak value of reaction rate is attained close to $c = 0.8$. The large scatter in Fig. 2b is due to the variation of equivalence ratio of the mixture. The variation of reaction rate conditional on density-weighted scalar dissipation rate ($\chi^* = \rho \chi / \rho_0$) is shown in Fig. 2c, which shows a predominant negative correlating branch and a positive correlation branch. As ρD is assumed to be constant, χ^* becomes $\chi^* = 2D_{ref}(\text{grad } \xi)^2$ and χ^* is normalised in Fig. 2c with respect to extinction scalar dissipation rate $\chi_{ext} = \xi^2 \cdot (1 - \xi)^2 / t_f$ [7]. The reaction rate and χ^* are negatively correlated in the most reacting zone $0.7 < c < 0.9$. This indicates that most of the heat release takes place in the premixed combustion mode. The variation of mean reaction rate conditional on χ^* values on stoichiometric

mixture fraction isosurface is shown in Fig. 2e, which shows both positive and negative correlation trends. The negative correlation trend is consistent with previous autoignition studies, and the positive correlation trend originates from the non-premixed mode of combustion [3]. Among these two trends the negative correlation trend dominates over the other.

In order to assess the overall ignition performance the temporal evolution of the mass of the region $c \geq 0.9$ is shown in Figs. 3a and b. It can be seen that for the ignition at the stoichiometric location, the thinner mixing layer encloses greater amount of fuel-rich mixture in the hot gas kernel. As the reaction rate is high in the fuel-rich mixture, and since χ^* assumes small values, the overall rate of burning increases with the decrease in mixing layer thickness. Among cases A-C, the mass of the burned region with $c \geq 0.9$ is the highest in case A and the lowest in case C. As the localised ignition in case D encloses more fuel-rich mixture, the mass of $c \geq 0.9$ is the highest among cases B,D, and E, and the lowest in case E where the ignitor was placed in the fuel-lean location. The overall edge flame propagation on the stoichiometric mixture fraction isosurface can be characterised by the probability of finding $c \geq 0.9$ on the $\xi = \xi_{st}$ isosurface. The temporal evolution of the probability of finding $c \geq 0.9$ for cases A-E are shown in Figs. 3c and d. As high values of reaction rate are associated with small values of χ^* on most locations on the $\xi = \xi_{st}$ isosurface, the reaction front spreading on $\xi = \xi_{st}$ isosurface is the highest for case C and the lowest in case A among cases A-C. The heat received from the rich premixed flame augments the chemical reaction on $\xi = \xi_{st}$ isosurface, so the probability of finding burned fluid on $\xi = \xi_{st}$ isosurface is the highest for the fuel-rich ignition (case D) and the lowest for the fuel-lean ignition (case E). In the present case, the maximum heat release takes place in the rich premixed flame branch, which increases the temperature at the triple point of the tribrachial flame as a result of heat transfer, which in turn leads to the greater propagation the reaction front in case D compared to cases B and E.

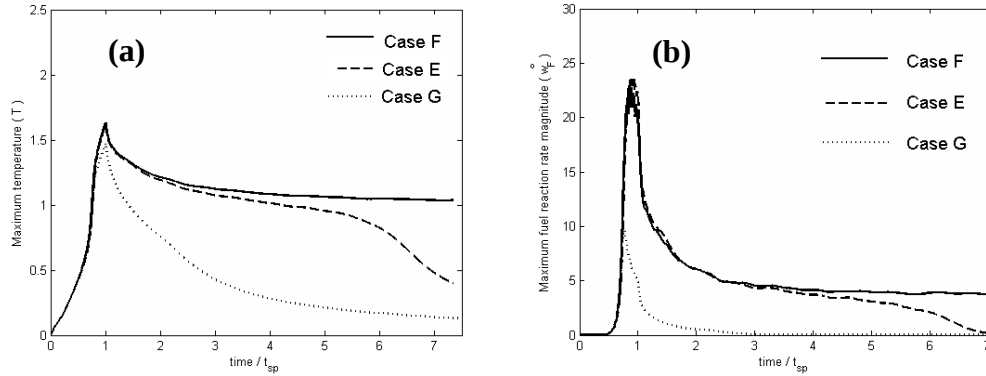


Fig. 4: (a) Temporal evolution of maximum non-dimensional temperature T for cases E-G; (b) Temporal evolution of maximum fuel reaction rate magnitude $\dot{w}_F$ for cases E-G.

From the above discussion it is evident suggest that the local mixture fraction gradient can have a large impact on the rate of flame spreading following the energy deposition by the ignitor. The statistics of the scalar dissipation at the mixing layer will also play a role in the overall combustion behaviour. Since in a turbulent flow both ξ and $|\nabla \xi|$ involve large variations, a large variation in flame evolution between different realisations of the localised forced ignition can be expected, with flame quenching a distinct possibility. This flame quenching can occur either at the very early stages of energy deposition (e.g. when u' is very high [3]), or immediately following the kernel initiation even at low u' as in Case E in the present study. It has already been demonstrated that heat transport also affects ignition characteristics, which points to the fact that the success of forced ignition of inhomogeneous mixtures cannot simply be understood by the presence or not of nominally flammable mixture at the ignitor location. The present findings are consistent with the conjectures of Ahmed *et al.* [4] that local and non-local fluid mechanical effects can contribute to a discrepancy between the ignition probability and the probability of finding flammable mixture at the spark.

In order to demonstrate further the non-local effects on ignition, two simulations (cases F and G) have been carried out. In case F, the ignitor was placed in the same location of the mixing layer as that in case E, but the background turbulence is absent. Case G corresponds to a quiescent homogeneous mixture with fuel mass fraction $Y_F = 0.5Y_{Fst}$ which is the value of the fuel mass fraction at the centre of the spark in case E. The temporal evolutions of the maximum values of non-dimensional temperature T and fuel reaction rate magnitude $\dot{w}_F$ for

cases E-G are shown in Figs. 4a and 4b respectively. It is evident from Figs. 4a and 4b that, for the same energy input, the quiescent homogeneous mixture does not give rise to a self-sustained combustion process. In case G the maximum temperature and reaction rate increase during the energy deposition period ($t \leq t_{sp}$) and temperature becomes high enough to autoignite the homogeneous mixture, but eventually the heat transfer from the hot gas kernel overcomes the chemical heat release and leads to flame extinction. In contrast, ignition of the inhomogeneous mixture in case F leads to a self-sustained combustion process where both T and $\dot{w}_F$ increases with energy deposition. The reaction rate increases rapidly when the temperature is high enough to auto-ignite the fuel-air mixture. After the energy deposition period ($t > t_{sp}$) the maximum values of both T and $\dot{w}_F$ decrease with time and the maximum value of T settles close to adiabatic flame temperature ($T \approx 1$) and the maximum value of $\dot{w}_F$ settles to a value which does not change appreciably with time. The temporal evolutions of the maximum values of T and $\dot{w}_F$ for case E indicates ignition of the inhomogeneous mixture by the assistance of the ignitor but the combustion process was not sustained under turbulent environment for the same input energy as that of in case F.

It has already been shown that the reaction rate attains high values towards the fuel rich side (see Fig. 2). This indicates that a homogeneous fuel-rich mixture with a composition $Y_F = 1.33Y_{Fst}$ and same turbulence parameters as that of case B, will burn in a self-sustained manner. This is because the heat release from the fuel-rich mixture in a kernel of the same size as case B is going to be greater than the total heat release in the hot gas kernel in case B. Moreover, with turbulence the heat transfer from the hot gas kernel gets augmented which decreases the rate of burning and may lead to extinction in the case of very high turbulent velocity fluctuation u' [3]. This essentially indicates a quiescent homogeneous case with $Y_F = 1.33Y_{Fst}$ will also give rise to self-sustained combustion for the same input energy.

A successful ignition and self-sustained combustion in case F and a failed ignition in case G, clearly substantiates non-local effects of localised forced ignition in inhomogeneous mixtures. This further indicates that the critical energy for inhomogeneous mixture may sometimes be smaller than the homogeneous mixture at the average mixture composition. It might also happen that the homogeneous mixture is impossible to burn in a self-sustained manner, but if the ignitor is placed at that composition, the inhomogeneous mixture can burn in a self-sustained manner because the input energy will be transported to stoichiometric and fuel-rich mixtures by advection and diffusion. If the energy is high enough to autoignite the stoichiometric and fuel-rich mixtures the heat release in the inhomogeneous mixture (e.g. case F) will be greater than the fuel-lean homogeneous mixture (e.g. case G). Therefore the finite size of the ignitor and heat transport from the ignition centre imply that at least some energy reaches to the stoichiometric mixture, which may assist in igniting inhomogeneous mixtures. This is consistent with the laminar non-premixed flame simulation results of Richardson and Mastorakos [8] where the critical strain rate for ignition was found to be a function of spark location. It is evident from Fig. 4 that combustion takes place in self-sustained manner in quiescent environment in case F but for $u'/S_L = 4$ the flame extinguishes in case E. This is due to the enhanced heat transfer from the kernel due to turbulence as observed earlier by Chakraborty *et al.* [3]. However, it is to be noted that in cases B and D self-sustained combustion have been obtained for the same turbulence level and input energy. This is consistent with the expectation that the critical turbulent velocity fluctuation u' at which flame extinction takes place is smaller in fuel-lean ignition in comparison to stoichiometric or fuel-rich ignitions.

4 Conclusions

Compressible 3D DNS simulations based on simplified chemistry have been carried out in order to understand the effects of mixture fraction and the magnitude of its gradient at the ignition centre on the localised ignition of turbulent mixing layers. The ignitor is represented by a Gaussian power source in the energy equation. The important conclusions of the present study are as follows: (a) The flame shows tribrachial structure following successful localised ignition, (b) The reaction rate and the scalar dissipation rate are found to be negatively correlated in the burning fluid, (c) Increasing the mixture fraction gradient leads to slowing down of the reaction front propagation on $\xi = \xi_{st}$ isosurface due to the negative correlation between the fuel consumption and mixture fraction gradient. By contrast, for a given size of hot gas kernel, more fuel-rich mixture is engulfed for the thinner mixing layer, which leads to a greater amount of burning because of the increased contribution of the

high reaction rate in the rich premixed branch of the tribrachial flame, (d) For a given energy input, an ignitor located in fuel-rich and stoichiometric mixtures may give rise to successful self-sustained flame propagation, whereas the flame initiated by igniting at a fuel-lean region may not survive. This indicates that successful self-sustained flame propagation for an ignition at fuel-lean regions requires a large amount of input energy, (e) The critical u' at which misfire takes place in the case of localised forced ignition of inhomogeneous mixture is smaller for fuel-lean ignition than the critical u' values for stoichiometric and fuel-rich ignitions, (f) Mixture inhomogeneity may help in assisting self-sustained combustion in fuel-lean localised forced ignitions. However, a self-sustained combustion process may not ensue if the ignitor with same input energy is placed at same fuel-lean composition in a homogeneous mixture. This is because in inhomogeneous mixtures the energy deposited by the ignitor at a given fuel-lean location eventually gets transported to stoichiometric and fuel-rich mixtures. The higher rate of heat release from stoichiometric and fuel-rich combustion may lead to a self-sustained combustion process if it overcomes the heat transfer from the hot gas kernel.

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