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Numerical Investigation of Turbulent Mixing for Autoignition in Stratified Mixture and Temperature Inhomogeneity Relevant to HCCI Combustion

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***Abstract*— A Direct Numerical Simulation (DNS) have been performed for different values of turbulent intensity to study the turbulent mixing time scale. DNS data has been analysed for autoignition for both stratified mixture (methane/air binary mixture) and temperature inhomogeneity (using temperature fluctuation and Taylor micro-scale of temperature variation) under highly turbulent environments in order to understand the effects of turbulent mixing time on overall combustion. It has been found that higher number of ignition sites are present in the case with higher value of turbulent intensity. Furthermore detrimental effects of turbulence on flame kernel development and burned gas mass has been observed. The DNS findings show that temperature variation is not decaying over time, but rather increasing with time, suggesting turbulent mixing remains progressive during combustion and plays pivotal role in autoignition combustion. DNS results indicates that the turbulent mixing time decays after successful combustion and is settles into ≈ 50% of its initial value.**

***Keywords*—Direct Numerical Simulation, autoignition, stratified mixture, temperature inhomogeneity, flame kernel.**

I. INTRODUCTION

Among many low-temperature (LTC) and lean-mixture (LMC) combustion engines, homogeneous-charge compression ignition (HCCI) engines have emerged as one of the most probable alternatives to conventional gasoline and diesel engines. These HCCI engines are designed to operate under very low-temperature utilizing ultra-lean, highly-diluted, well mixed fuel/air (premixed) mixture with higher compression ratios. Therefore, these engines can provide high diesel-like thermal efficiency while avoiding excessive NOx and particulate emissions without the help of expensive after-treatment catalytic converters. LTC and HCCI is a viable new concept for next generation internal combustion (IC) engines to improve fuel efficiency and offers fuel flexible combustion. Moreover, the particular emission Nitric Oxide (NOx) creation rate increases as the temperature in the combustion chamber rises, especially over 1600K [1,2].

Due to depletion of fossil fuels and increased environmental problems, internal combustion (IC) engines must satisfy Governmentally imposed strongest emission standards for combustion products [3]. Despite their advantages of HCCI over the conventional IC engines, the development of practical HCCI engines remains challenging mainly due to: excessive pressure rise rate which may lead to engine knocking and unpredictable ignition-timing control. In HCCI engines, the fuel and air are well-premixed and auto-ignited with the help of compression. Moreover, the auto-ignition in the HCCI engine is primarily determined by the in-cylinder conditions such as overall pressure, temperature, mixture composition (i.e. equivalence ratio) and their fluctuations [4]. Therefore, the precise control of ignition timing of HCCI combustion should be achieved from a well-designed mixture composition (i.e. mixture stratification) and amount of exhaust gas recirculation (EGR) (i.e. temperature inhomogeneity).

Many combustion systems used for transportation and power generation operate in regimes where reactants are neither homogeneously mixed (i.e. premixed flame) nor segregated on two sides of a contiguous (i.e. diffusion flame). These modes offers their own particular advantages and disadvantages [3]. Stratified combustion, in which flame propagates through non-uniformly mixed reactants, is common in practical systems and in model combustors that have been designed to study relevant phenomena at atmospheric pressure [5]. Stratified combustion has found to result in reduced burned gas temperature, and therefore offers in reduction of NOx emissions [6,7]. The premixed combustion has cleaner burnt products but it has a smaller range of operating conditions, making this mode of flame difficult to control [8]. On the divergent, having a wider operating range, a non-premixed combustion is easier to control [6,7,9]. Stratified combustion combines advantages of both premixed and non-premixed combustion modes [8].

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As mentioned before, one of the key challenges in HCCI engines is to control the start of combustion (i.e. ignition timing) and to ensure smooth heat generation during the cycle under various load conditions. Therefore, accurate predictive simulations of the ignition and subsequent combustion process in a HCCI-like environment plays vital role in development of HCCI engines. The combustion mode in HCCI engines can be both volumetric and front-like, which is not well investigated to date [10]. Another major challenge for using HCCI method of combustion is to control the heat release rate, as it is required to spread out over several crank angle degrees, suppressing the occurrence of rapid rate of pressure rise [11,12]. By introducing temperature inhomogeneity and mixture stratification in order to produce the desired heat release rate can be the possible control strategy [13,14]. However, incomplete turbulent mixing and temperature inhomogeneity between bulk gases can cylinder wall can lead to a range of combustion modes, which are distinct from HCCI autoignition [11,12]. Number of previous both experimental [16,17] and numerical [11,12,15,18,19] investigations concentrate on effects of temperature inhomogeneity under HCCI conditions with fixed mean and root-mean square (RMS) values of temperature field. The effects of turbulence and importance of turbulent mixing time subjected to different RMS of turbulence fluctuations have received limited attention [11,12,20] in spite of its practical relevance. This gap has been addressed here by analysing the influences of turbulence and turbulent mixing time for autoignition in stratified mixture and temperature inhomogeneity relevant to HCCI combustion using Direct Numerical Simulations.

II. Direct Numerical Simulation Setup

A single step chemical mechanism ($\text{Fuel} + s \cdot \text{Oxidizer} \rightarrow (1+s)\,\text{Products}$) has been considered here for the purpose of computational economy [21], where s represents the mass of oxidizer consumed per unit mass of fuel consumption under stoichiometric conditions. The activation energy and heat of combustion are taken to be function of equivalence ratio (ϕ) following [21] so that a realistic equivalence ratio dependence of the laminar burning velocity ($S_{b(\phi)}$) can be obtained. The equivalence ratio ϕ can be expressed as: $\phi = AFR_{st}/AFR$, where AFR_{st} and AFR are the stoichiometric and actual air-fuel ratio respectively. The properties here are representative of the stoichiometric methane/air binary mixtures (i.e. $s = 4$ and $AFR_{st} = 17.16$) and considered in here in this study. The mixture fraction is defined as:

$$\xi = \left[Y_F - \frac{Y_O}{s} + \frac{Y_{O\infty}}{s}\right] \Big/ \left[Y_{F\infty} + \frac{Y_{O\infty}}{s}\right] \qquad (1)$$

where Y_F and Y_O are the local fuel and oxidizer mass fractions respectively, and the $Y_{F\infty}$ and $Y_{O\infty}$ fuel mass fraction in pure fuel and in air stream respectively.

TABLE I
DNS Simulation Parameters

$\frac{u'}{S_{b(\phi)}}$	Case	Stratified Mixture	Thermal Inhomogeneity	$\frac{L_{11}}{l_F}$
4.0	[A]	$\langle\phi\rangle = 0.4$ $\phi' = 0.2$ $\frac{l_\phi}{l_F} = 3.4$	$\langle T\rangle = 0.4$ $T' = 0.2$ $\frac{l_T}{l_F} = 4.6$	10
6.0	[B]			
7.5	[C]			
9.8	[D]			

The stoichiometric mixture fraction is defined as:

$$\xi_{st} = Y_{O\infty} \Big/ \left[sY_{F\infty} + \frac{Y_{O\infty}}{s}\right] \qquad (2)$$

Based on this, the equivalence ratio is given as:

$$\phi = (1-\xi_{st})\xi/(1-\xi)\xi_{st} \qquad (3)$$

The extent of the completion of the chemical reaction is quantified using a reaction progress variable as:

$$c = (\xi Y_{F\infty} - Y_F) \Big/ \left(\xi Y_{F\infty} - \max\left[0, \frac{\xi-\xi_{st}}{1-\xi_{st}}\right] Y_{F\infty}\right) \qquad (4)$$

According to above Equation (4), the reaction progress variable c rises from 0 in the fully unburned reactants to 1.0 in the fully burnt products [8]. Here, the length scale of stratified mixture (i.e. l_ϕ) and temperature inhomogeneity (i.e. l_T) is taken as the Taylor micro-scale of the equivalence ratio and temperature variation and is defined as (Eswaran and Pope, 1988):

$$l_\Psi = \sqrt{\frac{6\langle[\Psi - \langle\Psi\rangle]^2\rangle}{\langle\nabla[\Psi - \langle\Psi\rangle]\cdot\nabla[\Psi - \langle\Psi\rangle]\rangle}} \qquad (5)$$

where the $\langle\cdots\rangle$ indicates the global mean evaluated over the whole computational domain and Ψ represents the passive scalar. In this study the ϕ variation is initiated using a random distribution of ϕ following a Bi-modal distribution for specified values of mean global equivalence ratio (i.e. $\langle\phi\rangle = 1.0$) and equivalence ratio variance (i.e. $\phi' = 0.2$). In practical, when fuel is introduced in the liquid phase, the probability density function (PDF) of the ϕ distribution is likely to be Bi-modal as a result of localized liquid fuel evaporation during the early stage of mixing.

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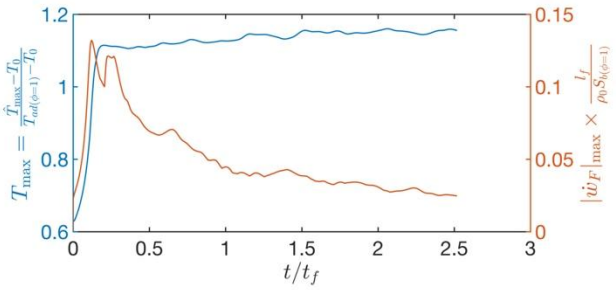
The fuel-air mixture is likelt to be fuel rich close to the evaporation sites and fuel-lean far away from the droplets.

The temperature inhomogeneity has been accounted for by a random Gaussian distribution of non-dimensional temperature for specified values of global mean temperature (i.e. $\langle T \rangle$), temperature fluctuation (i.e. T') and length scale of thermal inhomogeneity (i.e. l_T/l_F) [23]. Here l_F is the Zel'dovich flame thickness and can be defined as $l_F = D_0/S_{b(\phi)}$, where D_0 is the mass diffusivity of unburned reactants and $S_{b(\phi)}$ is the unstrained laminar burning velocity of given equivalence ratio (ϕ) mixture. For all cases, the mean temperature is taken as $\langle T \rangle = 0.4$, and the amplitude of T' is modulated, where $T = 1.0$ being an adiabatic flame temperature. Initial values RMS values of turbulence intensity are taken following previous studies [8,11,12,23,24].

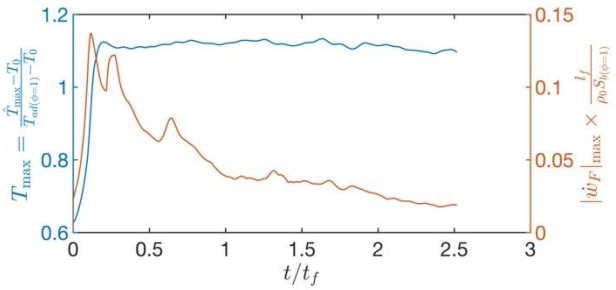
A fully compressible three-dimensional DNS code SENGA [25] was used to carry out all the simulations under decaying isotropic turbulence in a cubic domain of size $51l_F \times 51l_F \times l_F$, which further discretised by a Cartesian grid size of $310 \times 310 \times 310$ with uniform grid spacing ensuring at least 10 grid points within the thermal flame thickness:

$$\delta_{\mathrm{th}(\phi=1)} = \frac{T_{ad}(\phi) - T_0}{\max|\widetilde{\nabla}\hat{T}|_L} \qquad (6)$$

where $\hat{T}$ is the instantaneous temperature. The domain size and grid spacing for this DNS study is sufficient to capture smallest length scale of turbulence (i.e. Kolmogorov length scale). The boundary conditions in the all directions are taken to be periodic in nature [26]. A standard pseudo-spectral method [27] is used to initialize the turbulent velocity fluctuations and to bring about the different values of u'. A high order finite difference scheme is used for spatial differentiation and third-order low storage Runge-Kutta scheme is used for explicit time-advancement [28]. All simulations have been carried out for $t = 2.52\, t_f$ and this simulation time has been found to be sufficient in order determine self-sustained combustion, where t_f is the characteristic chemical time scale [8]. All the simulation parameters for this study are presented in Table 1.



Case [A]



Case [D]

Fig 1: Temporal evolution of temperature and corresponding reaction rate profile for selected cased from Table 1.

III. Results And Discussions

A. Temperature and Reaction Rate Profile

The temporal evolution of maximum values of non-dimensional temperature within the domain i.e.

$$T_{\max} = \frac{\hat{T}_{\max} - T_0}{T_{ad(\phi)} - T_0} \qquad (6)$$

And corresponding normalised fuel reaction rate magnitude:

$$\left(\dot{\Omega}_F\right)_{\max} = |\dot{w}_F| \times \frac{l_F}{\rho_0 S_{b(\phi)}} \qquad (6)$$

are shown in Figure 1. For the sake of brevity only cases [A] and [D] are shown here in Figure 1. The $T_{\max}$ and $\left(\dot{\Omega}_F\right)_{\max}$ both rises with time during $0 \leq t \leq 0.5t_F$ showing rapid increases in flame kernel development and initiation of autoignition mode of combustion.

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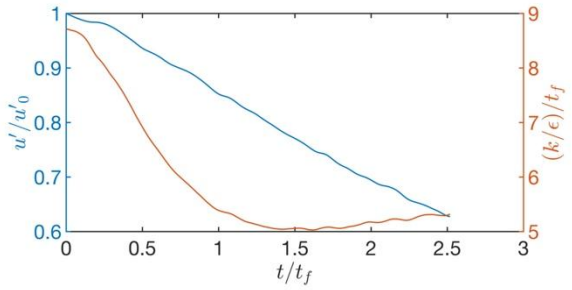
The high thermal gradient between hot gas kernels and surrounding unburned reactant gives rise to high rate of heat transfer from hot flame kernel and therefore $\left(\dot{\Omega}_F\right)_{\max}$ decreases with time. The $T_{\max}$ eventually fluctuates around the non-dimensional adiabatic flame temperature of stratified mixture (i.e. $T \approx 1.0$) and $\left(\dot{\Omega}_F\right)_{\max}$ settles to much smaller non-zero value showing self-sustained combustion has been achieved for all cases considered here. Due to stratified mixture and temperature inhomogeneity available in the domain, the value of $T_{\max}$ continue to rise for case [A], which indicates the flame kernel growth is still originating from multiple sites and is progressive in nature. The higher value of u' provides additional driving effects on increasing $\left(\dot{\Omega}_F\right)_{\max}$ (see case [D] and compare it with case [A]) and this is due to high energetic turbulent eddies supports great level of mixing between fresh reactants and burnt products. Another important observation is that the self-sustained combustion is possible for chosen cases (i.e. modifying mixture composition by stratified combustion and introducing temperature inhomogeneity) even with ultra-lean methane/air mixture (i.e. $\langle\phi\rangle = 0.4$ and $\phi' = 0.2$). Furthermore it can be concluded that high value of temperature during combustion can be avoided for all present values of u', which ultimately reduces the thermal NOx emission and still provides self-sustained combustion. It can be seen that value of $\langle\phi\rangle$, $\langle T\rangle$, ϕ', T' and u' plays an important role in auto-ignition and subsequent combustion process.

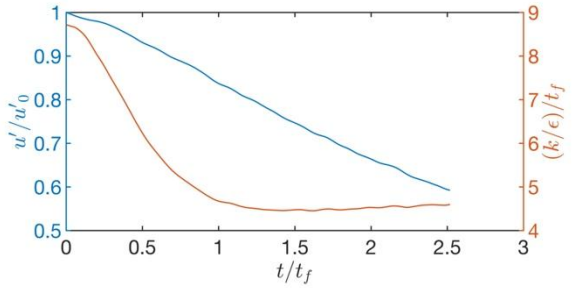
B. Turbulence Decay and Corresponding Mixing Time Scale profile

Figure 2 shows the temporal evolution of turbulence decay profile and corresponding turbulent mixing time scale for cases [B] and [C] from Table 1. Again for the sake of brevity only two cases are shown in Figure 2. The turbulence decay profile has been normalised with its original values for respective cases and turbulent mixing time is represented as: $\tau = (k/\epsilon)/t_f$, where k and ϵ are the turbulent kinetic energy and turbulence energy dissipation rate. It can be seen from Figure 2 that turbulence decay is faster for case [C] compare to case [B]. The faster rate of turbulence decay profile corresponds to higher value of u', where energetic turbulent eddies along with mixture stratification support great level of mixing. Furthermore Figure 2 shows that the turbulent mixing time decays over time until $t \approx 1.5\, t_f$ and then picks up its momentum, suggesting turbulence mixing remain progressive throughout the combustion process.

It can be seen that initial value of temperature inhomogeneity, mixture stratification, turbulence intensity and turbulent mixing time scale plays an important role in auto-ignition combustion process and contributes to extent of burned gas mass.

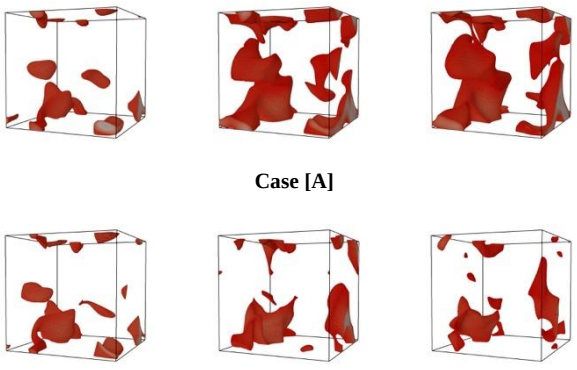


Case [B]



Case [C]

Fig 2: Temporal evolution of turbulence decay profile and corresponding mixing time scale for selected cased from Table 1.



Case [A]

Case [D]

@ 0.53 t_f **@ 1.58 t_f** **@ 2.52 t_f**

Fig 3: Volume rendered contours of $T \approx 1.0$ at three different time intervals for selected cases from Table 1.

International Journal of Emerging Technology and Advanced Engineering
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C. Flame Kernel Development

The volume rendered contours of $T \approx 1.0$ is shown in Figure 3 at different time intervals for cases [A] and [D] from Table 1. It is evident from Figure 3 that in both cases [A] and [D] the multiple site of flame kernel initiation are present at $t = 0.53\ t_f$ and these sites merges and new site originates as flame kernel develops and autoignition take place with time. Despite, higher number of ignition sites presents in case [D], the overall flame kernel volume is larger for case [A] (compare case [A] with case [D] at $t = 2.52 t_f$ in Figure 3). It is worth noting that contours of T depends on the magnitude of the reaction rate at the local mixture composition and flame stretch induced by the background fluid motion due to turbulence intensity for specific case. The results in Figure 3 shows that higher values of u' has detrimental effects of flame kernel development and burned gas volume was found to decrease with increasing turbulence intensity.

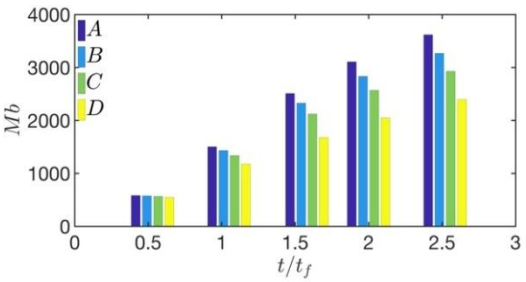

Fig 4: Burned gas mass for all the cases from Table 1.

D. Extent of Burning

Once the flame kernel or multiple flame kernels are successfully starts to propagate towards the unburned reactants, the extent of burning can be characterised by the burned gas mass m_b with reaction progress variable $c \geq 0.9$.

$$M_b = \frac{m_b(c \geq 0.9)}{(4/3)\pi \rho_0 l_F^3} \qquad (7)$$

The burned gas mass in Equation (7) is normalised with the mass of unburned gas sphere with radius equals to Zel'dovich flame thickness l_F. It is important to note that the accuracy of M_b depends on the choice of $c \geq 0.9$ and not on $\int_V \rho\, c\ dV$, as this provides the measure of total burned gas mass but it is not accurately captures the extent of burning. Initial sites of autoignition flame kernels are important and also influences the subsequent combustion including the extent of burning.

It can be seen from Figure 4 that the extent of burning is strongest for lowest value of turbulence intensity (i.e. Case [A] – also refer to Figure 2). The probability of finding high values of reaction progress variable with $c \geq 0.9$ decreases with increasing value of RMS of turbulence intensity (i.e. u'). The higher values of u' enhances the heat transfer rate from the multiple sites of hot gas kernels in autoignition. The mean heat flux from the hot gas kernel can be expressed as function of both molecular and eddy thermal diffusivities. Furthermore the eddy thermal diffusivity can be scale as $D_t \sim u' L_{11}$ [8] and according to this increase in u' leads to increase in eddy thermal diffusivity for given value of L_{11} considered here. This further implies and leads to a greater amount of heat loss from the hot gas kernel from high values of turbulence intensity. The detrimental effects of turbulent intensity and reduction in burning rate for high values of u' in stratified mixture is consistent with previous experimental [29,30] and computational [10,11,12,18] findings.

It is well-known that the combustion succeeds only for some realisations, even when the turbulent flow statistics are the same [31,32,33]. Pera *et al.* [34] investigated the effects of residual burnt gas heterogeneity on premixed early flame propagation on cycle-to-cycle variation observed in IC engines. DNS results from Pera *et al.* [34] suggested that the effect of residual burnt gas heterogeneity on heat release fluctuation is due to fluctuations of local mixture conditions in the case of engine's cycle-to-cycle variation. This aspect is particularly dominant in the cylinder of IC engines in autoignition due to cycle-to-cycle variations, therefore analysis for more realisation of initial mixture stratification and temperature inhomogeneity will be necessary, which will form the basis for future investigation.

IV. Conclusions

A numerical investigation using Direct Numerical Simulations have been performed to study the effects of turbulence and turbulent mixing time scale on autoignition relevant to HCCI combustion. DNS data has been analysed for both stratified methane/air binary mixtures and temperature inhomogeneity under different turbulence intensity values. It has been shown that higher number of ignition sites are present associated with higher values of turbulence intensity u'. Furthermore higher values of u' has detrimental effects on flame kernel development and burned gas mass.

The above findings demonstrates that favourable conditions in terms of initial turbulence intensity, mixture composition stratification (i.e. $\langle\phi\rangle$, ϕ' and l_ϕ/l_F), temperature inhomogeneity (i.e. $\langle T\rangle$, T' and l_T/l_F), and turbulent mixing timescale (τ) are required in order to achieve self-sustained combustion subsequent to successful autoignition even in ultra-lean mixtures. The DNS findings suggests that the viscous term, i.e. turbulent energy dissipation rate ϵ plays pivotal role for turbulent mixing timescale and remains progressive throughout the autoignition combustion process. The DNS results indicates that the decay of turbulent mixing time scale τ settles into almost $\sim 50\%$ of its initial value and promotes enhanced mixing during combustion process.

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