Direct numerical simulation of H₂/air combustion with composition stratification in a constant volume enclosure relevant to HCCI engines

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Abstract

Two-dimensional direct numerical simulation (2-D DNS) is used to investigate the effect of turbulence intensity and composition stratification on H₂/air mixture auto-ignition in a constant volume enclosure relevant to homogeneous charge compression ignition (HCCI) engines. Different turbulence levels, composition fluctuations, EGR (Exhaust Gas Recirculation) ratios, initial pressure, domain lengths and energy spectra are simulated with detailed analysis in ten 2-D DNS cases. The results show that the ignition delay time tends to be prolonged and the heat release rate increased under higher turbulence intensity. Turbulence can affect the reaction zone, e.g., through wrinkling of reaction front and enhancement of mixing and heat transfer. Higher composition stratification can smoothen the overall heat release rate and shorten the ignition delay time. Budgets terms and Probability Density Function (PDF) of density weighted displacement speed show that in HCCI engines flame propagation can co-exist with volumetric auto-ignition. As expected, lower pressure leads to thicker flame thickness and longer ignition delay time. Increasing EGR ratio has a negative influence on the formation of OH reaction, resulting in a longer ignition delay time. Two energy spectra with respect to low and high Reynolds number are compared to show a discrepancy on ignition delay time due to different kinetic energy dissipation rates.

Keywords: 2-D DNS; HCCI engines; turbulent combustion; stratified mixture; EGR; energy spectrum

1. Introduction

Homogeneous charge compression ignition (HCCI) engine can be considered as a hybrid of spark ignition (SI) engine and compression ignition (CI) engine. It runs under a lean premixed condition, which is advantageous in suppressing NO_x and soot; combustion in HCCI engine is initiated by compression thereby it can be operated at a high compression ratio to achieve high engine efficiency. However, at low load the engine may suffer from misfire while at high load the combustion heat re-

lease rate may be very high causing high engine noise and deterioration of engine performance [1][2]. Various fuels have been used in HCCI engines to control the auto-ignition timing [3]-[6]. For example, hydrogen shows the potential for the future automotive application due to its wide range of flammability limits and absence of CO₂ and particular matters [7][10]. An amount of research has been focused on the usage of hydrogen as a fuel or fuel additive in HCCI engines [7]-[15].

It is well recognized that auto-ignition in HCCI engines is mainly controlled by chemical kinetics, such that in-cylinder pressure, temperature, and composition will determine the auto-ignition timings. Liu *et al.* [16] and Oh *et al.* [17] found that increasing intake pressure can advance auto-ignition timing and extend the operating range to lower and higher loads, such that, higher intake pressure is better to HCCI engines. For the effect of temperature, it is found that changing both intake and coolant temperatures, different temperature stratifications are formed and that can smooth pressure rise rate (PRR) [3]. Dec *et al.* [18] conducted experiments to show that first ignition site occurs in hotter mixtures with random distribution and then propagates to the colder mixtures due to the naturally temperature stratification. As to in-cylinder composition, exhaust gas recirculation (EGR) is an important factor to form charge composition stratification [19]-[21]. Ei-Asrag and Ju [22] found that NO in EGR enhances both low and intermediate temperature ignition delays by the rapid OH radical pool formation. Machrafi [21] further verified that the auto-ignition process is influenced by EGR chemical effects through species addition and also EGR increases temperature by thermal effect. Moreover, turbulence is shown to govern the thermal and composition field prior to ignition through mixing which can influence ignition delay time and the combustion process [14][23][24]. Using Direct numerical simulation (DNS), Yoo *et al.* [23] showed the ratio of turbulence turn-over time to ignition delay time (τ_t/τ_0) is an important parameter and the effect of u' on ignition delay depending on SACI or HCCI combustion. For the former, turbulence with higher u' (a fast τ_t) significantly enhances the overall combustion, while for HCCI combustion, higher turbulence intensity is able to retard the overall ignition, rendering the combustion similar to 0-D homogenous ignition due to the increased radical and heat loss [24]. Although an amount of work has presented the effect of in-cylinder conditions on HCCI combustion process, the detailed ignition mechanism by isolated variable (thermal or composition stratification, pressure, EGR, turbulence and so on) is still unknown.

DNS is a viable approach to elucidate the complicated chemical and physical processes in HCCI engines due to the resolution of fine details in terms of flow and chemistry over a wide spectrum of spatial and temporal scales. Extensive numerical studies on thermal [12]-[14][23]-[27] or composition stratification [28][29] and also both of the stratifications [30][31] have been performed using single stage ignition fuel hydrogen [12]-[14][32]-[34], iso-octane [23] and two-staged ignition fuel [22][24][28][30][31][35]. Effects of thermal stratification on the auto-ignition and the subse-

quent heat release in a homogeneous hydrogen/air mixture were studied by Hawkes *et al.* [14]. It was found that the presence of hot gas results in an earlier ignition delay and longer burning duration. Both deflagration front and spontaneous ignition wave-like propagation were predicted. The results also revealed that temperature stratification is of primary importance on combustion phasing control. In a real engine, it is more reasonable to have simultaneous thermal and composition stratifications. Therefore, Bansal and Im [32][33] conducted two-dimensional (2-D) DNS under positive and negative correlated temperature-composition ($T-\phi$) distribution. With positive relationship flame propagation dominates, otherwise volumetric spontaneous ignition prevails. Recently, Luong *et al.* [27] used a reduced n-heptane/air mechanism to study temperature and composition inhomogeneities relevant to HCCI combustion. The prior work suggests that an appropriate $T-\phi$ stratification together with a well-prepared $T-\phi$ correlation can control combustion timing and alleviate high pressure rise rate. These previous DNS work focuses on thermal stratification ($T' = 0, 15 \text{ K}, 60 \text{ K}$) or small composition stratification ($\phi' = 0.01-0.1$) under relatively low pressure ($P = 40 \text{ bar}$), low load ($\phi = 0.1, 0.45$) conditions. The current work extends the prior HCCI studies to a wider range of composition stratification at a higher pressure condition and study more parameters such as turbulence, EGR and pressure effects.

The sequential question is how the combustion looks like in HCCI engines, whether the reaction front propagates as a flame or as an ignition wave, which has been studied by various authors in 2-D DNS [14][22][23][32]. Hawkes *et al.* [14] proposed a density weighted displacement speed to account for transport and chemical reaction rates of hydrogen species and found that both ignition front and normal deflagration flame front simultaneously exist in HCCI engines. Gu *et al.* [36] used initial temperature gradients to identify five reaction front characterizations. These results suggest that different combustion modes depend on initial conditions dramatically and more cases need to be studied for comparison.

In the current work, 2-D DNS of H_2/air auto-ignition in a constant volume enclosure relevant to HCCI engines is studied. First, some key parameters such as initial pressure, temperature, EGR and equivalence ratio are studied using Senkin package. The following is a series of 2-D DNS cases, which use detailed transport properties together with a detailed hydrogen mechanism. The effects of turbulence intensity, composition stratification, pressure, EGR ratio, domain length and energy spectrum on the first ignition site and the subsequent combustion process are examined. The correlation of temperature, equivalence ratio and major species is used to identify the most flammable site. Two combustion modes: deflagration and spontaneous ignition front propagation are distinguished based on budget terms and density weighted displacement speed. Two different initial turbulent energy spectra are compared to show the discrepancy in 2-D DNS cases.

2. Numerical methods

Turbulent reacting flows in HCCI engines are governed by the continuity equation, Navier-Stokes equation and transport equations for species and energy. Since the flow velocity is relatively low, we have adopted the low Mach number assumption. With this assumption, the physical pressure can be decomposed into a spatially constant thermodynamic part, $P(t)$, which only changes over time and a hydrodynamic part, $p(x,t)$, which is used in computing the pressure gradient in the momentum equations. The body force, Soret/Dufout effects and radiation heat transfer are neglected. The mixture is assumed to be a perfect gas, and the mass diffusion of species is given by Fickian law. Note that, the compression process is not considered because the ignition process is very short about 0.05 ms, corresponding to 0.33 CAD at the condition of engine speed 1100 rpm, such that the previous DNS studies in HCCI engine related conditions also neglect compression process [14][33][37]. To properly simulate the ignition process, a detailed chemical kinetic mechanism of hydrogen which has been validated in a wide range of experimental conditions (298-3000 K, 0.3-87 atm, $\phi = 0.25$ -5.0) [38] and detailed transport properties are considered in the simulations.

The governing equations are numerically solved using a high order method based on a stiff chemistry solver [39]. The temporal integration is performed using 2nd order symmetrical Strang splitting algorithm for a convection-diffusion-reaction (CDR) problem [40]; the integration of one full time step of the stiff reaction rates is placed in between two half-step integrations of diffusion and convection terms. A strategy of 2nd order Adam-Bashforth (AB2) scheme starting from a 2nd order Runge-Kutta (RK2) scheme (RK2+AB2) is adopted due to its simplicity. A variable coefficient Poisson equation for hydrodynamic pressure is solved using high efficient Multigrid method [41]. A 5th order weighted essentially non-oscillatory (WENO) scheme is used for the convective terms in the species mass and energy equations to avoid wiggles in species transport process, whereas all other spatial discretization is made using a 6th order central difference scheme. The spatial discretization of governing equations is based on a staggered rectangular Cartesian grid on which the velocity is defined on the cell surfaces while all scalars are defined on the cell center. The spatial/temporal accuracy of the numerical scheme has been verified with grid/time-step dependency tests and the code was used to study different combustion processes [35][42]. Detailed description of the numerical method is given in Ref. [39].

3. Homogeneous ignition results

First, zero-dimensional (0-D) cases are performed using Senkin package to show the relationship between P , T , EGR, ϕ and τ_0 . Figure 1a shows the maximum adiabatic temperature ($T_{\max}$) and ignition delay time τ_0 as a function of EGR ratio. Here, τ_0 is defined as the time at which the maximum time derivative of PRR is obtained. EGR is composed of complete H_2 /air combustion products:

H₂O, N₂ and O₂. EGR ratio is defined as the ratio of mass of EGR to mass of inlet fuel air mixture. As expected $T_{\max}$ decreases and τ_0 increases with higher EGR ratio. Figures 1b-1d further show that higher initial temperature, pressure and ϕ reduce ignition delay time in both 50% EGR cases and no EGR cases. These results will be compared with 2-D DNS in the following section.

Figure 2 shows the heat release (HR) rate and pressure as a function of time in 0-D DNS case at the condition of 1175 K, 80 bar and 50% EGR, which uses the same code as that of 2-D DNS. Consistent with Senkin result, 0-D DNS case in Fig. 2 shows the same ignition delay time (0.211 ms) and validates the accuracy of 0-D DNS code.

5. 2-D non-homogeneous DNS results

5.1 Problem definition and initial conditions

In 2-D DNS the computational domain is a 2.5 mm×2.5 mm constant-volume enclosure. Periodic conditions are employed at all boundaries. A uniform grids of 2048² is used, resulting in a grid resolution of 1.2 μm in high pressure cases 1-4. The grid points decreases in lower pressure cases 7-9, leading to a grid resolution four times larger than cases 1-4. The initial turbulent flow is assumed to be isotropic and prescribed by a turbulent kinetic energy spectrum [43][44] using a synthetic method [45][46]. The initial mean flow velocity is assumed to be zero. Initial random temperature and composition fields are superimposed on the mean temperature and mean composition field. It is noted that two-dimensional turbulence is suitable for HCCI engines under current conditions because the simulation is prescribed at the time very close to the top dead center and the mixing time is short. Also, 2-D and 3-D DNS comparisons showed a similar ignition process [34].

In this paper two spectra (E_1 and E_2) are used in Fig.6. E_1 [43][44] (also called Passot-Pouquet spectrum) is a simple spectrum for turbulence at low-Reynolds number often used in theoretical studies, which reads in 2D:

$$E_1(k; u', l_0) = \frac{32}{3} \sqrt{\frac{2}{\pi}} \left(\frac{k}{k_0} \right)^4 \exp \left(-2 \left(\frac{k}{k_0} \right)^2 \right) \quad (1)$$

where $k_0=2\pi/l_0$ and l_0 is the integral scale, and u' is turbulent intensity, known as the root-mean-square (rms) velocity. $u'=(2 K/3)^{0.5}$ in 3D and $u'=K^{0.5}$ in 2-D, where K is the turbulent kinetic energy. The second spectrum E_2 is a more general one, covering a range of Reynolds number (cf. Pope [43]), which is written as:

$$E(k) = C \left(\frac{u'^3}{l_0} \right)^{2/3} k^{-5/3} \left(\frac{kL}{(K^2 L^2 + c_L)^{1/2}} \right)^{5/3+p_0} \exp \left(-\beta \left(\left(k^4 (l_0 \text{Re}_{l_0}^{-2/4})^4 + c_\eta^4 \right)^{1/4} - c_\eta \right) \right) \quad (2)$$

where Re_{l_0} is the Reynolds number based on the integral scale. The constants are set as $C=1.5$, $p_0=2$, $c_L=6.78$, $\beta=5.2$, $c_\eta=0.4$. In Fig.3, it shows the energy in E_1 spectrum dissipates quickly at high wave numbers while it gains higher energy at low wave numbers. For E_2 , the energy spectrum spans from large energy containing scale to the small energy dissipation scale. In between, the slop of E_2 spectrum at the universal inertial sub-range is about $-5/3$, which can be representative of a whole energy spectrum and is adopted to initialize a homogeneous isotropic turbulent field.

Table 1 lists the 2-D DNS computational cases. In all cases, the mean temperature is 1175 K with a stratification of 15 K. The mean equivalence ratio ($\bar{\phi}$) is 0.67, with 50% EGR for cases 1-8 and 30% EGR for case 9. The initial pressure is 80 bar for cases 1-6 and 40 bar for cases 7-9. The initial turbulence velocity (u') varies from 0.2 to 2 m/s and the equivalence ratio stratification (ϕ') varies from 0.05 to 0.3. Note that, the composition fluctuation such as 0.3 is too large to be found for HCCI combustion but for a fundamental study it is still valuable to perform the cases with such high composition fluctuations and also it can exist in PCCI (partially-premixed charge compression ignition) engines. The Reynolds number (Re) based on the integral scale of turbulence varies from 126 to 1260. The number of integral length scale (L/l_0) in all cases is set to be 2, where L is the domain length and l_0 is the integral length scale. Cases 5 and 6 are in a smaller square domain of 0.8 mm×0.8 mm, the corresponding mesh size (h) is 1.56 μ m. The Kolmogorov length scale (η) varies from 4.35 μ m to 33 μ m. In all cases E_2 spectrum is used to generate initial isotropic turbulence except case 8 which adopts E_1 spectrum. The ignition delay time for 2-D DNS case is τ_{2D} . The turbulence eddy turnover time τ_t is defined as (l_0/u') . The turbulence timescale in real HCCI engines is the order of 1 ms such that the turbulence timescale in the present DNS study is representative of HCCI engines [27]. It also should note that in practical HCCI engines the combustor size is 2-3 orders of magnitude larger than the DNS domain [14][37][47]. On one hand, due to the limited CPU hours, 2-D DNSs are often used for parametric study and reveal the knowledge about the spatial and temporal detailed combustion process, including the reaction zone structure, budget terms of diffusion and reaction, density weighted displacement speed, which is still valuable to optimized HCCI combustion. A typical simulation case took 10752 CPU core-hours with a Cray XE6 cluster.

5.2 Composition stratification and turbulence effect on auto-ignition

Figure 4 shows the spatial distribution of temperature in the computational domain during the combustion process in cases 1-4 (from left to right). One can see that there are more hot spots appearing at the onset of ignition (0.161 ms) in the higher charge stratification case (case 2) than that in case 1. The same trend is found in cases 3 and 4. The figure is not present for brevity. It appears that due to a stronger composition fluctuation of $\phi'=0.3$, the local equivalence ratio spreads out over a wider range (e.g. 0.2-1.3 in cases 2 and 4, 0.58-0.78 in cases 1 and 3), which provides more ignitable

locations. This is coincident with homogeneous case in Fig.1, showing that the higher equivalence ratio leads to a shorter ignition delay at the same temperature.

It is known that stronger turbulence intensity leads to a higher Reynolds number and smaller Kolmogorov scales; hence, thinner and more wrinkled reaction fronts can be seen at 0.19 ms in Fig. 4 for cases 1 and 2 (as compared with those in cases 3 and 4). Turbulence is shown to prolong the ignition delay time τ_{2D} , cf., Table 1. Previous studies of HCCI combustion showed that ignition delay time is longer under high turbulence intensity in the homogeneous mixture [23], which is consistent with the present case. Care should be taken because it also shows that the condition of $\tau_t/\tau_0 \leq 1$ plays an important role; otherwise the turbulence effect is very small. In non-premixed configurations [48] the results showed that turbulence can track and accumulate heat in some spots as a reduction of ignition delay time followed by a sequential combustion process. However, it concluded that the shortest ignition site is more correlated with a lower scalar dissipation rate and the most reactive mixture fraction. For the current cases, it is found that the first ignition site advances regardless the value of τ_t/τ_0 with the same composition and thermal stratifications. On the other hand, the charge stratification is induced to promote ignition so that the overall effect of ignition delay time can be shortened.

To illustrate the composition stratification effect on auto-ignition of HCCI combustion, Fig. 5 shows instantaneous snapshots of key species H_2 , H_2O_2 , OH mass fraction and reaction HR at 0.171 ms for case 2 (upper) and case 4 (lower) with large composition stratification of $\phi'=0.3$. It is seen that the highest heat release is in a rather thin sheet layer indicating the reaction zone, embracing the presence of OH mass fraction which represents the high temperature in the post flame zone. At 0.171 ms hydrogen mass fraction is depleted inside the reaction layer, where H_2O_2 is also consumed completely through the induction phase of ignition. However, intermediate species i.e. OH can be observed at this time because it is formed through H_2O_2 dissociation indicating high temperature combustion.

For the overall combustion process, Figs. 6a and 6b show the time history of the volume averaged heat release rate and pressure for cases 1-6. With increasing composition stratification, i.e. cases 2, 4 and 6 the onset of ignition is advanced, the peak HR is lower, and the combustion duration is longer compared with cases 1, 3 and 5, respectively. In detail, the ignition delay time is 0.201 ms, 0.194 ms, 0.193 ms and 0.185 ms for cases 1-4 respectively shown in Table 1. It is found that the overall effect of both turbulence and composition stratification on the ignition delay time is small but the combustion process is rather different. The earlier ignition for cases 2, 4 and 6 is owing to the initial wide composition distribution which increases the possibility of reaching the most reactive mixture condition. Subsequently, a sequential equivalence ratio leads to a successive combustion process indicated by the longer combustion duration. As shown in Table 1, the higher turbulence intensity cases with $\tau_t/\tau_0 > 1$ (cases 1 and 2) have longer ignition delays and stronger heat release compared

with cases 3 and 4, which is consistent with previous conclusion that stronger turbulence intensity may increase heat and radical losses from the ignition pool and thus the prolonged ignition delay [23]. For smaller domain cases 5 and 6, the number of integral length scale of both thermal and composition fluctuation is kept the same as 2 and thus the turbulence turnover time is decreased by the same factor as the length scale. As a result, a smaller domain length corresponds to an increase in scalar dissipation rate ($\chi=2D|\nabla Z||\nabla Z|$), where D is the diffusion coefficient and Z is the mixture fraction, which will lead to a longer ignition delay time and higher PRR. This observation is consistent with the result of Hawkes *et al.* [14].

5.3 The first ignition site

Figure 7 shows the probability density function (PDF) of temperature and equivalence ratio at four instants of time for case 2. The PDF is obtained based on the total grid points in the domain. The local equivalence ratio is defined as: $\phi = (Y_H/Y_O)/(W_H/W_O)$, where Y_H and Y_O are the mass fractions of element H and O in the local mixture, respectively. It is seen that at 0.0134 ms, equivalence ratio spans a wide range from 0.3 to 1.1 due to initial stronger mixture stratification ($\phi'=0.3$). Most of the points reside in an equivalence ratio of 0.67 and temperature of 1200 K owing to the initial prescribed condition. As combustion proceeds to 0.151 ms, local pockets of mixture at the higher equivalence ratio regions prefer to ignite first instead of the leaner side of the fuel mixture. At 0.171 ms, more favourable ignition sites start to ignite and show a trend that is fuel richer regions growing to ignite earlier. The peak temperature is at stoichiometric condition. After the fuel is depleted, i.e. 0.227 ms, the overall temperature is almost above 2000 K, which may imply thermal NO_x cannot be avoided.

In the present work, HO₂ mass fraction is introduced to identify the first ignition site. Using hydrogen fuel, Bansal and Im also use HO₂ radical as ignition kernel indicator [32]. Figure 8 shows the HO₂ mass fraction contour in temperature and equivalence ratio space at the first ignition time: 0.153, 0.151, 0.122, 0.11 ms for cases 1-4, respectively. It is found that higher temperature region positively correlates with the accumulation of HO₂ mass fraction but the first ignition site can be at different equivalence ratios rather than the highest one especially for the weak composition stratification cases 1 and 3. The random ignition sites maybe result from locally relatively higher temperature which is uncorrelated with the equivalence ratio. However, in larger composition stratification cases 2 and 4, an amount of HO₂ forms first at fuel richer regions such that the first ignition site takes place accordingly, which indicates composition stratification plays an important role on the first ignition site.

Figure 9 shows a zoomed region colored with heat release rate for case 1 at 0.173 ms. It is seen that the heat is released intensively in a rather thin layer which is resolved by at least six grids. Four white lines A, B, C and D in Fig. 9 are extracted normal to the propagation front to discuss the dif-

ferent combustion modes on the reaction front based on the four lines in detail in the following section.

5.4 Flame propagation versus ignition wave propagation

A crucial question is, when temperature and mixture stratifications are introduced, whether the reaction fronts propagate as a flame or as an ignition wave. For the former, the flame propagation speed is low and local molecular transport time scale and chemical reaction time scale can be balanced and there is enough time for species diffusion. Additionally, the temperature gradient in the flame front is large enough. For the latter, the reaction front is chemical kinetically controlled such that the molecular transport effect is negligible and the spontaneous ignition speed is high. Using 2-D DNS, the identification of two ignition regimes, namely, flame propagation and spontaneous ignition front propagation, has been studied by various authors and different fuels are involved.

One criterion to distinguish the two ignition regimes is to use density weighted displacement speed, which is defined to account for both species transport and chemical reaction rates as follows:

$$S_d^* = \frac{1}{\rho_u |\nabla Y_k|} \left[\dot{\omega}_k - \frac{\partial}{\partial x_i} (\rho Y_k V_{k,j}) \right] \quad (3)$$

where ρ_u is a representative density of assumed unburned reactants and S_d^* is based on the iso-surface of a chosen value of species k . Here, H_2 mass fraction ($Y_{H_2}=0.0005$) is adopted. While the first term in the square bracket $\dot{\omega}_k$ denotes the net reaction rate of H_2 and the other term represents diffusion such that the two budget terms measure the importance of radical reactivity and molecular diffusivity. In order to delineate the two ignition modes quantitatively, a Damköhler number, Da , is further defined:

$$Da = \dot{\omega}_k / \left| - \frac{\partial}{\partial x_i} (\rho Y_k V_{k,j}) \right| \quad (4)$$

From a 1-D laminar simulation at the same thermal dynamic condition as that in the 2-D DNS case, it is found that the diffusive limit Da is about 2 such that it less than 2 represents deflagration wave. Correspondingly, the laminar flame speed (S_L) is about 0.7 m/s and if $S_d^* > 3S_L$, it is ignition wave, otherwise the flame propagation. It should note that for the current cases, the chemical reaction can be a little larger than the corresponding diffusion term and S_d^* is larger than S_L due to the high temperature in the unburnt region to increase fuel reactivity so that we choose $3S_L$ as the limit.

To investigate the propagation front it is useful to plot the spatial distribution of the budget terms from diffusion and chemical reactions in Eq. (3). Figure 10 shows the spatial profiles of two budget terms and density weighted displacement speed along the lines A, B, C and D. It is seen that along the lines C and D, reaction rate term is almost two times larger than the diffusion term ($Da > 2$) whereas along the lines A and B the reaction rate budget term is almost balanced by the diffusion

term. Furthermore, in Fig. 10 S_d^* is relatively lower (below 2.5 m/s) along the lines A and B but it increases to around 5 m/s along the lines C and D. Therefore, it indicates that the reaction front propagates as a deflagration wave at A, B and as an ignition wave at C, D. It also implies in the early stage of auto-ignition and highly curved kernels (C and D), it accumulates hydrogen in the curved region due to differential diffusion effect which favors chemical reactions. The result is consistent with previous studies on the ignition of a thermally stratified premixed hydrogen-air mixture [11].

Figure 11 shows temporal evolution of density weighted displacement speed S_d^* for cases 1 and 2 in the whole combustion process. It is seen that all S_d^* curves are of the “U-shape” which represent a stabilized low speed front propagation. The result correlates well with previous DNS studies [14][34]. In case 1, the unbound speed at 0.151 ms denoting the occurrence of the first ignition site and the other unbound speed at 0.208 ms represents the final stage of fuel consumption, both of which occur at spatial locations with zero fuel gradient. In total, S_d^* is a little higher in case 1 than that in case 3, which is due to the stronger turbulence intensity, leading to a more homogeneous volumetric ignition event. The same trend can be found in cases 2 and 4.

Figure 12 shows the PDF of density weighted displacement speed S_d^* for cases 1 and 3. In case 3 (the right plot), it is seen that the peak of S_d^* decreases as combustion proceeds. At 0.134 ms, S_d^* is always larger than 2 m/s. After 0.183 ms, most of S_d^* is around 1.5 m/s or higher, whereas there is a certain probability of S_d^* less than 1 m/s, which is close to the corresponding laminar flame speed. This indicates that at a later time there could be flame front propagation co-existing with ignition wave propagation. The interplay of different reaction fronts propagation determines the heat release rate and PRR, and as such the performance of the engine. For comparison, four time instants of S_d^* in case 1 is shown. At the first ignition time (around 0.153 ms) the peak of S_d^* is around 5 m/s which is larger than that in case 3 at 0.134 ms owing to the initial stronger turbulence intensity and more wrinkled reaction kernels. Later, the peak of S_d^* decreases dramatically but increases a little at 0.19 ms due to the final fuel consumption. Similar observations can be found for the other two cases. The present results provide insightful information for development of controllable HCCI engines.

5.5 EGR and pressure effect in 2-D non-homogeneous DNS cases

In order to clarify the influence of pressure and EGR addition on combustion process under stratified mixtures, Fig. 13a presents ignition delay time, reaction layer thickness and (b,c) time evolution of key species in 2-D DNS case 3(80 bar, 50%EGR), case 7(40 bar, 50%EGR), case 9(40 bar, 30%EGR) and case 10(40 bar, 60%EGR). The detailed initial conditions can be found in Table 1. From the figure, some conclusions can be summarized as follows:

1. Decreasing initial pressure leads to a longer ignition delay time which is consistent with the corresponding homogeneous 0-D case as seen in Fig.1 and a thicker reaction layer thickness.

2. Increasing EGR ratio will enhance ignition delay time which is the same as that in 0-D case, c.f. Fig. 1a and increase reaction layer thickness, however, the thickness depends on the time and local conditions because the filamentary and highly strained regions often cause thinner reaction thickness.

3. The EGR ratio has a minor impact on HO_2 and H_2O_2 mass fraction, whereas it decreases OH and H mass fraction dramatically with increasing EGR. The reason will be illustrated by sensitivity analysis in the following.

Figure 14 shows sensitivity analysis of the hydrogen/air mechanism in 2-D DNS cases for 0%, 30% and 50% EGR ratios at the first ignition delay time to identify the important and dominant reactions. The normalized sensitivity coefficient and ROP (rate of production) are defined as the normalized variation of each reaction pre-exponential factor with respect to temperature and rate of OH production, respectively. The positive coefficient indicates exothermic reaction, where increasing reaction production rate leads to the production of temperature and OH by chemical heat release. Correspondingly, negative sensitivity coefficients will reduce ignition strength by reducing the temperature and by consumption of OH. From Fig. 14a, it is seen that increasing EGR ratio significantly reduces the sensitivity of almost all the above reactions except the last two termination reactions, and hence, reactivity is decreased. In Fig. 14b, all the important chemical pathways contribute to OH reduction via EGR addition and the predominant reactions represented by OH through the most important reaction path way: $\text{H} + \text{O}_2 \longrightarrow \text{O} + \text{OH}$ which is responsible for OH production and thermal explosion. As EGR ratio increases, this reaction decreases dramatically resulting in a prolonged ignition delay. The same sensitivity analysis is performed for the production and consumption rate of H, HO_2 and H_2O_2 . The results show that increasing EGR ratio leads to a reduction of H formation and has a small overall effect on HO_2 and H_2O_2 which is consistent with Fig.13b and 13c. The figure with respect to normalized ROP of HO_2 , H_2O_2 and H are not present for brevity, see the supplementary file.

5.6 E_1 and E_2 spectra comparison in 2-D non-homogeneous DNS cases

Indeed, almost all the DNS of HCCI combustion use E_1 the low Reynolds number spectrum (case 8) to prescribe initial synthetic homogeneous isotropic turbulence field [14][23]-[27][30]-[35]. However, as Fig. 15 shows, the Passot-Pouquet spectrum E_1 loses energy at small turbulent eddies, and the high Reynolds number spectrum E_2 (case 7) represent the energy in a wider range of wave numbers. Therefore, it is needed to know the impact of initial spectrum on the results. First, Fig. 15a presents the time history of overall ensemble averaged pressure and heat release rate in cases 7 and 8. The ignition delay time is shorter with low Reynolds number spectrum E_1 in case 8 and the combustion duration is longer which reduces peak heat release rate dramatically.

The observation is consistent with the temporal evolution of turbulence intensity and displacement speed in Fig. 15b and 15c, respectively. The time both for turbulence intensity starting to increase instead of decaying and for a steadily propagating displacement speed is shorter in case 8. Since the mean kinetic energy dissipation rate scaling with the mean strain rate, is denoted by $\varepsilon \equiv 2\nu \langle S_{ij}^2 \rangle$ under homogenous turbulence, where ν is kinematic viscosity. The mean strain rate in case 7 (E_2) is much larger than that in case 8 (E_1), resulting in a smaller energy dissipation rate in the latter and thus the shorter ignition delay. The figure is shown in the supplementary file. The spatial 2-D distribution of temperature and key species are not shown for brevity but it is observed that there are fewer and larger hot spots during the whole combustion process in case 8 with E_1 spectrum. It is interesting to notice that the minimum value of S_d^* during reaction front propagation process in both cases are almost the same.

6. Conclusions

Two-dimensional detailed numerical simulations are performed to study the effect of turbulence and composition stratification on ignition delay time, heat release rate and the characteristics of different combustion regimes in a lean hydrogen/air mixture under HCCI engine related conditions. Several key parameters: turbulence level, composition stratification, EGR ratio, initial pressure, energy spectrum and the domain length are examined in ten 2-D DNSs. The corresponding 0-D homogeneous cases from Senkin and DNS code are performed for validation and comparison. The heat release rate profile in 2-D non-homogeneous DNS case shows an apparent staged combustion with a slower rate of overall heat release than that in the 0-D case due to stratified mixture and turbulence involved. It further shows that higher turbulence intensity will retard ignition delay time and shorten the combustion duration. In addition, increasing composition stratification leads to an earlier onset of ignition and prolonged combustion duration. The statistics of local displacement speed of the reaction front shows the peak of S_d^* decreases as the combustion proceeds. It also implies that both deflagration wave and spontaneous ignition wave co-exist. As expected, lower pressure leads to a thicker flame thickness and a longer ignition delay of the mixture. Increasing EGR ratio has a negative influence on the formation of OH reaction primarily through chain branching reaction $H+O_2 \rightarrow O+OH$, and then ignition delay time is short. The low Reynolds number energy spectrum E_1 shows a relatively shorter ignition time of the mixture due to lower kinetic energy dissipation rate, but both E_1 and E_2 energy spectra yield qualitatively similar results.

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Table 1
2D Simulation cases and initial conditions

Case	Re	u' [m/s]	ϕ'	l_0 [mm]	η [μm]	h [μm]	L [mm]	τ_t/τ_0	τ_{2D} [ms]	P[bar]	EGR%
1	1260	2	0.05	1.25	5.9	1.2	2.5	2.96	0.201	80	50
2	1260	2	0.3	1.25	5.9	1.2	2.5	2.96	0.194	80	50
3	126	0.2	0.05	1.25	33	1.2	2.5	29.6	0.193	80	50
4	126	0.2	0.3	1.25	33	1.2	2.5	29.6	0.185	80	50
5	415	2	0.05	0.4	4.35	1.56	0.8	0.95	0.208	80	50
6	415	2	0.3	0.4	4.35	1.56	0.8	0.95	0.202	80	50
7	260	0.2	0.05	1.25	19	4.8	2.5	26	0.254	40	50
8	E_1	0.2	0.05	1.25	19	4.8	2.5	26	0.236	40	50
9	260	0.2	0.05	1.25	19	4.8	2.5	35	0.18	40	30
10	260	0.2	0.05	1.25	19	4.8	2.5	20	0.311	40	60

FIGURE 1

(a)

(b)

(c)

(d)

FIGURE 2

FIGURE 3

FIGURE 4

FIGURE 5

FIGURE 6

(a)

(b)

FIGURE 7

FIGURE 8

FIGURE 9

FIGURE 10

FIGURE 11

FIGURE 12

FIGURE 13

FIGURE 14

FIGURE 15

FIGURE CAPTION

Fig. 1 Homogeneous case calculation using Senkin package for (a) Maximum temperature and ignition delay time as a function of EGR ratios; (b) ignition delay time for different initial temperatures; (c) ignition delay time as a function of equivalence ratios with 50% EGR; (d) ignition delay time as a function of equivalence ratios without EGR.

Fig. 2 Temporal evolution of heat release rate and pressure in 0D DNS case at the condition of 1175 K, 80 bar and 50% EGR.

Fig. 3 Energy spectra as function of wave number.

Fig. 4 Temperature distribution for cases 1-4 from left to right. Upper row: at the instance of time of first ignition site; lower row: at the instance of time of highest PRR. The domain length is 2.5mm.

Fig. 5 2D distribution of HR, H_2 , H_2O_2 and OH mass fraction at 0.171 ms from left to right in case 2 (upper) and case 4 (lower). The domain length is 2.5 mm.

Fig. 6 Temporal evolution of heat release rate (a) and pressure (b) for cases 1-6.

Fig. 7 PDF of equivalence ratio and temperature distribution at 0.0134 ms, 0.151 ms, 0.171 ms and 0.227 ms for case 2.

Fig. 8 HO_2 mass fraction contour in temperature and equivalence ratio space at the first ignition time 0.153 ms, 0.151 ms, 0.122 ms, 0.11 ms for cases 1-4, respectively.

Fig. 9 Instantaneous heat release rate in a zoomed region. The A-D white lines are normal to the reaction front.

Fig. 10 Profiles of budget terms and density weighted displacement speed along the lines A, B, C and D for case 1 in a zoomed region shown in Fig. 7.

Fig. 11 Temporal evolution of density weighted displacement speed for cases 1 and 2.

Fig. 12 PDF of density weighted displacement speed at four different time instants for cases 1 and 3.

Fig. 13 (a) Ignition delay time and inner flame thickness for cases 3, 7, 9, 10; (b) time evolution of OH and HO₂ mass fraction; (c) time evolution of H₂O₂ and H mass fraction for different EGR ratios.

Fig. 14 (a) Temperature sensitivity analysis and (b) normalized rate of OH production at the first ignition delay time.

Fig. 15 Time evolution of (a) overall pressure and volume-averaged heat release; (b) turbulence intensity; (c) density weighted displacement speed for cases 7 and 8.