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Direct Numerical Simulation of H2 Effect on Multistage Autoignition of DME/Air Mixture under HCCI Conditions

Tai Jin[1,2], Xujiang Wang[2], Kai Hong Luo[2*], Kun Luo[1], Jianren Fan[1]

[1]State Key Laboratory of Clean Energy Utilization, Zhejiang University

Hangzhou, 310027, China

[2]Department of Mechanical Engineering, University College London

London, WC1E 7JE , United Kingdom

Abstract

The effects of hydrogen addition on the multistage autoignition of a lean DME/Air mixture under elevated pressure are investigated by direct numerical simulations (DNSs). The results show that hydrogen addition has a negative effect in the DME low temperature ignition, leading to a declined maximum of the heat release rate (HRR) and a retarded ignition timing. The ignition at higher temperature is significantly delayed by hydrogen addition with increase of the maximum of heat release rate. DNS for thermally stratified turbulent ignitions shows an advanced first stage ignition, yet retarded with addition of hydrogen. The mean HRR in the turbulent cases is more spread out over time while its peak is significantly reduced. The mean HRR during the second and third stage ignition overlap in time, and therefore only a single peak is observed for the thermally stratified cases. And the overall pressure rise rate is smoothed. DNS of the ignition characteristics of uncorrelated and negatively correlated thermally- and compositionally- stratified mixtures is also briefly discussed.

1 Introduction

Homogeneous charge compression ignition (HCCI) engine is a viable new concept for next-generation internal combustion engines, with the potential to improve fuel-consumption economy relative to spark-ignition engines, to reduce particulate emissions relative to diesel engines and to reduce nitrogen oxides (NOx) relative to both spark-ignition and diesel engines[1]. Dimethyl ether (DME) as an alternative fuel for the engines has received extensive attentions and one of the most promising alternative fuels as the main fuel for HCCI engines due to its favorable chemical characteristics[2]. However, the ignition timing and combustion phase of DME in HCCI combustion process are hard to control because DME fuel is very easy to be self-ignited. An adjustment of the proportion of two kinds of fuels with different reactivities has been proposed as a common method for controlling the ignition timing in the HCCI combustion[3].

Hydrogen (H_2) has been used in DME HCCI engine to control the ignition timing and expand the operating range of the engines. A thorough understanding of the combustion properties of DEM/H_2 is crucial for developing advanced DME-based combustion engines and corresponding operating strategies. Pan et al.[4] conducted shock-tube experiments to measure the ignition delay of DME/H_2/air mixtures. It has been found that the ignition delay time of DME/H_2 binary fuel blends has complex dependence on the temperature. Yu et al.[5] measured the laminar flame speeds of DME/H_2/air flames at different temperatures, equivalence ratios, and fuel blending ratios. They found that the laminar flame speeds increased with an increase of H_2 fraction and initial temperature. It was also found that the chemical kinetic effects induced by H_2 addition played a dominant role in the increase of the laminar flame speed compared with thermal and diffusive effects. Simulations of the DME/H_2 flames are also conducted with detailed chemical reaction mechanisms. Liu et al.[6] simulated the effects of H_2 addition to the DME base flame. The results indicated that the reduction of CH_3OCH_3 mole fraction in the blend is the dominant factor for the reduction of CH_3OCH_3 and CO mole fractions in the flame. The H, O and OH radicals increased when H_2 was added, and these radicals promoted the combustion process. Hu et al.[7] simulated the autoignition characteristics of DME/H_2/Air blends in homogeneous charge compression ignition combustion engine. They found that the hydrogen addition can retard the autoignition timing of DME in HCCI combustion engine.

A key characteristic of all fuels in the HCCI context is their response of thermal stratification. Thermal stratification always occurs naturally in HCCI engines due to wall-heat transfer and imperfect mixing with residuals. It was found that thermal stratification had the potential to introduce a range of ignition delay times into the mixture, thus preventing the undesirable high pressure-rise rate (PRR) that would result from the simultaneous autoignition of the whole fuel charge[1]. Many computational studies of HCCI combustion using multidimensional direct numerical simulations (DNSs) have been conducted to elucidate the fundamental combustion characteristics of various fuel/air mixtures under HCCI conditions including hydrogen[8-10], dimethyl ether (DME)[11, 12], n-heptane[13], iso-octane[14], primary reference fuel (PRF)[15, 16], ethanol and biodiesel[17]. From these studies, the general characteristics of HCCI combustion have been elucidated: thermal stratification in an HCCI engine cylinder can spread out the PRR under high load conditions by changing the combustion mode of spontaneous auto-ignition into a mixed combustion mode of spontaneous auto-ignition and deflagration. Stratified-charge compression ignition combustion has been devised as another promising remedy for the problems in HCCI combustion. It has been found that fuel inhomogeneities may

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Corresponding author. Fax: +44-20-7679-3916
E-mail address: K.Luo@ucl.ac.uk

induce a sequential ignition event, leading to a prolonged combustion process.

The objectives of this paper are to investigate the combined effects of thermal stratifications and H_2 addition on autoignition and flame propagation in the NTC region for a lean DME/air mixture at high pressure. The initial turbulence and stratification length scales are chosen to mimic HCCI preignition conditions. The isentropic compression heating resulted from piston motion is also incorporated through inert density source terms in the governing equations.

2 Numerical methods and computational setup

The full compressible Navier-Stokes, species, and energy equations for a reacting gas mixture are solved with an in-house DNS code. A fourth-order explicit Runge-Kutta method for time integration and an eighth-order central differencing scheme for spatial discretization are used with a tenth-order filter for removing spurious high frequency fluctuations in the solution. The mixture is assumed to be a perfect gas and the mass diffusion of species is assumed to obey the Fickian law. CHEMKIN software libraries are linked to the current code to evaluate reaction rate, as well as thermodynamic and transport properties for both the individual species and the mixture-averaged. A reduced chemical mechanism for DME oxidation consisting of 30 chemical species is employed[12]. Detailed description of the DNS code is given in our previous studies[18, 19] .

The computation domain is a constant-volume enclosure. Periodic boundary conditions are employed at all boundaries. To mimic the pressure rise due to piston motion in practical engines, inert source terms are added to the respective mass, species, momentum and energy conservation equations. The density source terms is derived in [12], assuming that the compression process is locally isentropic. The engine parameters used to evaluate the change in volume for all cases are, as follows. The engine speed is 1200 rpm, the compression ratio is 18, and the ratio of connecting rod length to crank-shaft length is 3.2. The initial crank angle is set at 36 CAD before TDC.

Table 1: Simulations parameters for different cases

Case	n_{DME}: n_{H2}	u' (m/s)	T' (K)	ϕ'	L_{11} (mm)
1-a	1:0	0.5	25	0	0.5
3-a	1:1	0.5	25	0	0.5
3-b	1:1	0.5	25	0.05	0.5
3-c	1:1	0.5	25	0.05	0.5
5-a	1:2	0.5	25	0	0.5
5-b	1:2	0.5	15	0	0.5

The initial mean conditions for all the cases studied are set to be $\bar{T} = 677.73\text{K}$, $\bar{\phi} = 0.3$, $P = 10.834$ atm. The composition of the DME/H_2/Air mixtures investigated in this study varies with different blending ratio of hydrogen, in order to investigate the effect of hydrogen addition without changing the total equivalence ratio. The mole fraction ratio of H_2 and DME (n_{H2}:n_{DME}) is 0, 0.5,1,1.5,2.0 for Cases 1-5 respectively. Two dimensional simulations are conducted to study the turbulence, temperature stratification effects on the autoignition of the blending fuel. The mean flow is quiescent with isotropic turbulent velocity fluctuations prescribed by the Passot-Pouquet turbulent kinetic energy spectrum function. Random temperature field is superimposed on the mean temperature field, with a similar spectrum of the turbulence kinetic energy. The various turbulence parameters used for different cases are listed in Table 1. At the TDC prior to the main auto-ignition event, different $T - \phi$ correlations may exist due to such factors as fuel delivery strategy, injection timing, amount of EGR, intake charge heating, and wall heat loss. Two most-probable scenarios are examined here as negatively correlated $T - \phi$ fields (Case 3-b) and uncorrelated $T - \phi$ fields (Case 3-c). To understand different magnitude temperature fluctuations effects on the autoignition characteristics, Case 5-b with a smaller T'=15 K is simulated.

3 Results and discussion

3.1 H2 effects on homogeneous autoignition

Prior to examining the turbulent cases, simulations of the HCCI combustion of DME/H_2/Air mixtures are conducted using the single-zone, time-dependent volume, adiabatic, and zero-dimensional reactor in CHEMKIN pro package with SENKIN approach. These results can provide a baseline reference for the 2-D turbulent simulations, and also provide a chemical description of DME/H_2/Air mixtures autoignition without the additional complexities of molecular and turbulent transport.

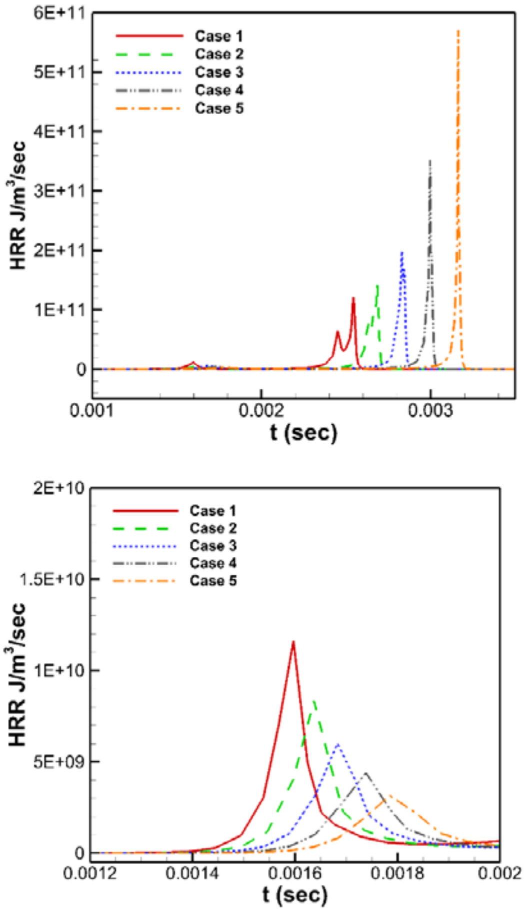
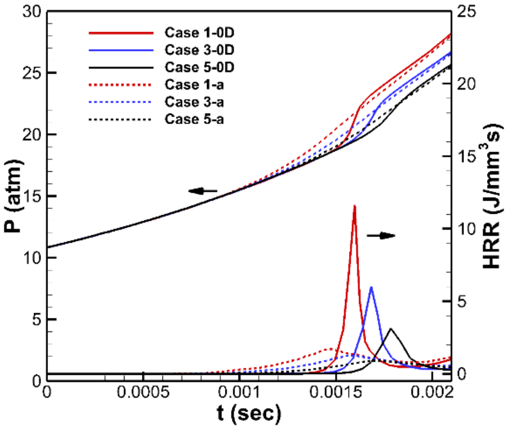


Figure 1: Heat release rate evolution for mixtures with different hydrogen blending ratios

The time evolution of heat release rate during the HCCI combustion process for mixtures with different hydrogen blending ratios are demonstrated in Fig.1. It can be observed that DME and all the blends calculated exhibit a typical multi-stage heat release. For DME only Case 1, it presents two maximum of heat release rate at the high temperature reaction (HTR), which means three-stage ignition. With the increase of the hydrogen blending ratio, the two peaks of heat release rate at HTR would overlap and the “three-stage” heat release phenomenon disappears. It also can be found that both the low temperature reaction (LTR) and the high temperature reaction (HTR) are delayed with the increase of the hydrogen blending ratio. The peak value of the heat release rate of low temperature reaction decreases monotonously with the increase of the hydrogen blending ratio. The declined maximum of the heat release rate and the retarded ignition timing at LTR indicate that the addition of hydrogen has a negative effect in the DME low temperature ignition. This is mainly because that hydrogen acts as competitor with DME during the LTR process through consuming OH radicals (CH_3OCH_3+OH=CH_3OCH_2+H_2O, H_2+OH=H_2O+H). The ignition at higher temperature are significantly delayed by hydrogen addition, however, the maximum of heat release rate increases a lot for higher hydrogen blending ratio. It indicates that the hydrogen addition promote the HTR by making the burning process more intense. This is due to the oxidation of H_2 which provides OH radicals during the HTR process[7].

3.2 Stratification effects on autoignition

To highlight the stratification effect on autoignition, Figure 2 shows the temporal evolution of volume averaged pressure and mean heat release rate (HRR) for the turbulent cases with temperature inhomogeneities together with the corresponding 0-D homogeneous ignitions simulations. It can be found that the mean HRR in the turbulent cases is more spread out over time while its peak is significantly reduced compared to the corresponding values of 0-D autoignition. And the combustion duration is longer. The ignition occurs sooner for the first stage in the turbulent cases than the 0-D ignition. This is due to the temperature inhomogeneities, leading to higher temperature in some locations and shorter ignition delay. The first stage ignition is found to be retarded with addition of hydrogen. It is also noted that the mean heat release rate during the second and third stage ignition overlap in time for the Cases 1-a and 3-a, and therefore only a single peak is observed, where two maximum of heat release rate can be observed during the HTR for the 0-D ignition. Two significant rising of pressure can be found for the 0-D ignition, which correspond to the LTR and HTR. The pressures after the LTR and HTR are both decreased with the addition of hydrogen. For the turbulent cases, the overall pressure rise rate is smoothed.



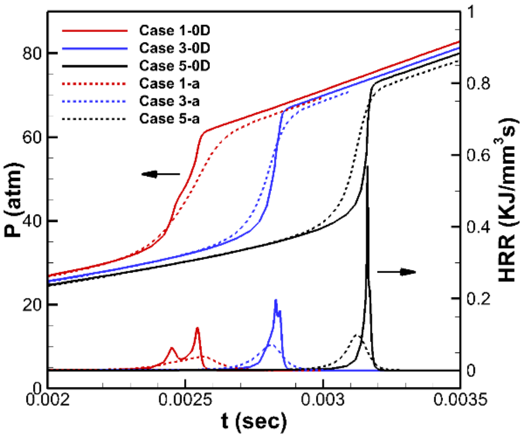


Figure 2: Time evolutions of mean Heat release rate for mixtures with different hydrogen blending ratios

Figure 3 shows the isocontours of heat release field for the three cases at times corresponding to the onset of ignition, the peak first stage ignition and second stage ignition. The onset of ignition correspond to the high temperature locations. It is significantly retarded for Cases 3-a&5-a with hydrogen addition. For the peak first stage ignition, the HRR is much higher for the Case 1-a with DME only than cases with hydrogen blends. It can be observed that the first stage heat release occurs in thin reaction fronts for all three cases. For the peak second stage ignition, the HRR is much higher for the Case 5-a than the other two cases. Heat release occur in thicker reaction fronts for Cases 3-a&5-a than that in Case 1-a.

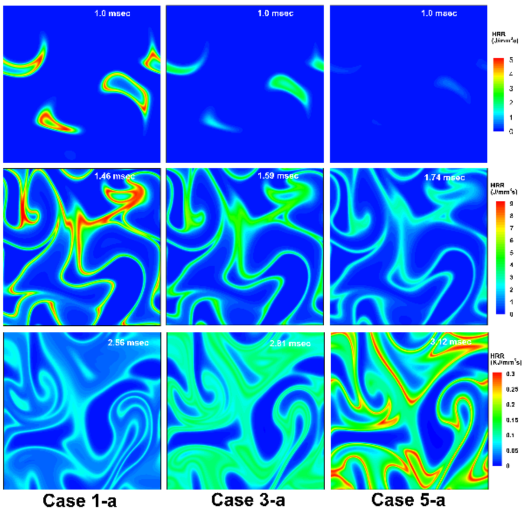


Figure 3: Isocontours of heat release rate at times of the onset of ignition (first row), peak first stage ignition (middle row) and peak second stage ignition (last row)

To understand the effect of two different $T-\phi$ correlations on the ignition of the mixture, the temporal evolution of the mean pressure and HRR for the negatively-correlated (Case 3-b) and uncorrelated (Case 3-c) cases is shown in Fig.4. It can be found that for the three turbulent cases, the heat release rate profile is quite similar, with sooner first stage ignition and reduced maximum of HRR during the low temperature reaction. However, the HRR profiles appear quite different at the high temperature reaction. For Case 3-c with uncorrelated $T-\phi$ fields, the second stage reaction has been advanced significantly, with a reduced maximum HRR. For Case 3-b with negatively correlated $T-\phi$ fields, the volume averaged pressure and heat release rate appear to be consistent with the 0-D ignition, with a high maximum HRR at the high temperature reaction.

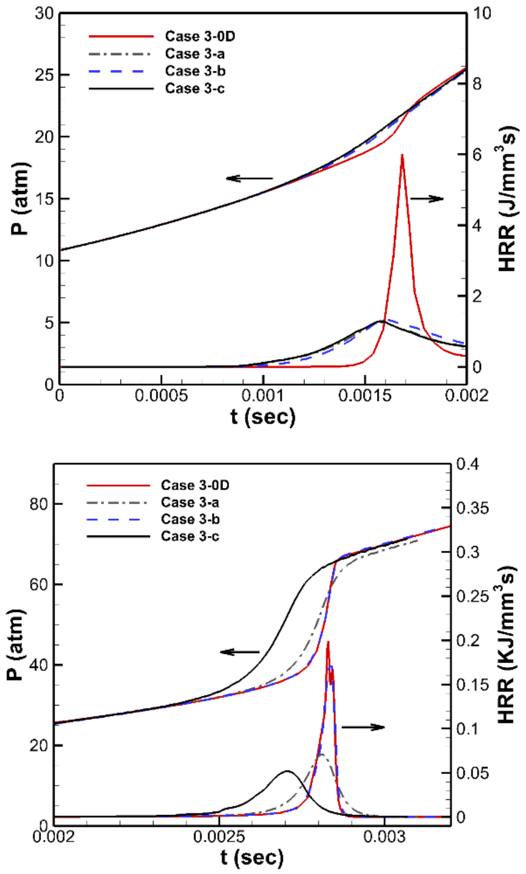


Figure 4: Time evolutions of mean Heat release rate for mixtures with different temperature and composition stratifications

4 Conclusions

This paper reports direct numerical simulations of autoignition of dimethyl ether (DME) and hydrogen blends in high pressure stratified turbulent conditions relevant to HCCI engines. Inert mass source terms were added to the governing equations to mimic isentropic pressure rise that occurs in a practical internal combustion engine. A reduced chemical mechanism consisting of 30 species was used. Simulations of 0-D homogeneous autoigniton of the DME/H_2/Air blends are first conducted. It is found that ignition of DME and all the blends studied exhibits a typical multistage heat release. Hydrogen addition has a negative effect in the DME low temperature ignition, leading to a declined maximum of the heat release rate and a retarded ignition timing. The ignition at higher temperature is significantly delayed by hydrogen addition, however, the maximum of heat release rate increases a lot for higher hydrogen blending ratio.

The ignition characteristics of thermally stratified mixtures is then investigated. It can be found that the mean HRR in the turbulent cases is more spread out over time while its peak is significantly reduced compared to the corresponding values of 0-D autoignition. The ignition occurs sooner for the first stage in the turbulent cases, however, it is still retarded with addition of hydrogen. The mean heat release rates during the second and third stage ignition overlap in time, and therefore only a single peak is observed for the thermally stratified cases. And the overall pressure rise rate is smoothed.

The ignition characteristics of thermally- and compositionally-stratified mixtures are briefly discussed. The negatively-correlated and uncorrelated cases present a similar advanced first stage ignition and reduced maximum of HRR during the low temperature reaction as the thermally-stratified only case. For the uncorrelated case, the high temperature reaction is significantly advanced, while the volume averaged pressure and heat release rate appear to be consistent with the 0-D ignition for the negatively correlated case.

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