Direct Numerical Simulation of Flame/spontaneous Ignition Interaction Fueled with Hydrogen under SACI Engine Conditions

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Abstract

In spark assisted homogeneous charge compression ignition (SACI) engines a premixed flame is first established; the propagating flame results in compression heating of the end gas and finally auto-ignition of the gas. Two dimensional direct numerical simulation (2D DNS) and one dimensional (1D) detailed simulations of flame/spontaneous ignition interaction in a lean hydrogen/air mixture under a constant volume enclosure relevant to SACI engine conditions are performed using detailed chemistry and detailed transport properties. In a 2D outward propagating spherical flame, thermal-diffusive instability is observed and once auto-ignition starts a low temperature region in the preheat zone of the flame is formed. Subsequently, the ignition in the preheat zone is suppressed. Then 1D flame/ignition interactions in H₂/air, syngas/air and methane/air mixtures are studied using detailed numerical simulations. The results reveal that due to preferential diffusion of hydrogen, heat and mass transfer in the preheat zone inhibits the ignition process, yielding a slower reaction rate hence an even lower temperature in the region. It is shown further that the low temperature region is not affected by the domain size and one step chemistry but it will disappear at very low initial temperature conditions. This is due to the absence of auto-ignition under low temperature conditions.

Keywords: direct numerical simulation, flame/ignition interaction, hydrogen, thermal-diffusive instability, SACI engines

1. Introduction

HCCI has the advantage of low nitric oxides (NO_x) emission and simultaneously high efficiency [1,2], however due to the absence of an external ignition control, the combustion phasing is hard to control instead the auto-ignition is governed by chemical kinetics of the charge. Also, the misfire in low load and too high pressure-rise-rate (PRR) at high load hinder the development of commercializing HCCI (homogeneous charge compression ignition) engines. Spark assistance has been used to

control combustion phasing and to extend the engine operation from part load to high load. This technology is referred to as SACI (spark assisted HCCI). By employing a spark to initiate the combustion in SACI engines the combustion process can be considered as a hybrid process of regular flame propagation, as in a spark ignition (SI) engine, and auto ignition as in a HCCI engine [5-6]. In addition, hydrogen is a cleanest promising fuel for IC engines [7] and had been intensively studied for its high burning velocity, wide flammable range and transport property [8].

Bentsson and Denbratt [9] demonstrated that the spark assistance provides a potential way to control HCCI combustion. The flame front propagation initiated by a spark is followed by HCCI combustion; therefore it can extend the operating range of HCCI combustion but confront the problem that the initial flame propagation front are strongly influenced by the thermodynamic state of the end gas. Also, the large cycle-to-cycle variation is observed but the knowledge about the transition between flame propagation and auto-ignition is limited [10-12]. Wang et al. [13] showed that higher intake temperature would increase early flame propagation significantly and also the ensuing auto-ignition. The expansion velocity of self-ignition in the unburnt mixture can be around 25 m/s [14]. Normally, EGR (exhaust gas recirculation) is implemented to meet the thermal state and used for combustion control [6,15] for SACI combustion. Daw et al. [15] used nonlinear EGR feedback to achieve stable transition between SI and HCCI modes and avoid large cycle-to-cycle variation. It seems that the mode switch from SI to HCCI is more difficult than from HCCI to SI because HCCI mode is more sensitive to the charge temperature and composition [10]. It is well accepted that turbulence plays a role on flame propagation so that it may have effects on SACI engines. Persson et al. [16] showed an enhanced turbulence by swirl will increase the expansion speed of SI flame and slow down the HCCI burning rate. Recently, in a constant volume combustor relevant to SACI engines, four distinctive regimes during the combustion process, including the laminar flame stage, the cellular flame stage, the squish flame stage and the auto-ignition stage were present [17]. Besides the above studies, a part of researchers focused on knocking in SACI engines [18,19], indicating dramatic pressure oscillation and the induced detonation development which is different from SACI combustion mode and beyond the scope of the current paper.

Furthermore, in a hydrogen combustion process it is well known that the reaction zone is affected by preferential diffusion since the diffusivity of hydrogen is much larger than other species in a typical combustion system [20]. Some key parameters are investigated to show that equivalence ratio affects unequal diffusion instability via varying Lewis number; higher temperature will retard the onset of instability and pressure has minor effect on thermal-diffusive instability [21]. According to Law et al. [22,23], lean hydrogen flames exhibit cellular instabilities immediately after the initiation of flame because of the simultaneous excitation of the thermal-diffusive instability.

Despite the numerous studies devoted to researching SACI engines, some key mechanisms, such as flame/auto-ignition interactions which determine SI-HCCI-SI mode transition and the effect of flame propagation on the auto-ignition process are still unavailable. This lack of understanding is mainly because such a small scale interaction is difficult to measure even with advanced laser diagnostics. Modeling but only direct numerical simulation (DNS) method can provide the most useful and detailed information. Yoo et al. [24] studied a lean iso-octane mixture under HCCI and SACI conditions using two-dimensional (2D) DNS. It was found that, for SACI combustion, turbulence with higher intensity advances the overall combustion by increasing the turbulent flame area and only deflagration wave is observed before the onset of maximum heat release rate. In a 1D configuration, Martz et al. [25] studied the laminar flame front propagating during end gas auto-ignition. The interaction between flame and spontaneous ignition front was examined by burning velocity and temperature gradient. However, it is too quick to find the apparent auto-ignition front during the end gas consumption and more realistic engine conditions should be investigated in the future.

In this paper, 2D DNS of SACI combustion in a lean H_2 /air mixture is conducted in a constant volume enclosure. The interaction between flame front and auto-ignition process is captured by intermediate species and budget terms. In addition, 1D simulations are performed to elucidate the effects of fuel type, Lewis number, flame residence time and initial temperature on the interaction between the propagating flame front and auto-ignition front.

2. Mathematical formulation and numerical methods

The turbulent reacting flow in a SACI engine is governed by a system of partial differential equations representing (species) mass conservation, momentum conservation and energy conservation (in temperature form). The main physical processes involved in a typical SACI process include the flame deflagration and auto ignition of lean mixture. The flow velocity is relatively low; the low Mach number assumption can therefore be used to remove the stiffness caused by the high speed acoustic wave. With this assumption the physical pressure can be decomposed into a thermodynamic pressure and a hydrodynamic pressure; the former is used to update density via the equation of state, and the latter is used to compute pressure gradient term in the momentum equations. Furthermore, the body force, the Soret/Dufout effects and radiation are neglected, the species diffusion obeys Fickian law.

The above system of equations is numerically solved using an in-house reacting-flow DNS solver [26] taking into account detailed chemistry and transport. With low Mach number assumption, a large overall time step can be used to advance the discretized system. The integration of the above convection-diffusion-reaction (CDR) problem is performed with a 2nd order Strang splitting [27] algorithm. During one step of temporal advancement of the CDR system, a full step of detailed chemistry computation is placed in between two half steps calculation of the effect of the convective and

diffusive transport. The chemistry calculation taking account of detailed elementary reactions is performed with a high order, general purpose, stiff ordinary differential equations (ODE) solver – DVODE [28]. The computation of diffusion terms is further split into multiple sub-steps of explicit integration with a sub-step size determined by diffusion stability limit. The sub-step integration starts with a 2nd order Runge-Kutta step then continues with the 2nd order Adams-Bashforth steps. The overall temporal accuracy is limited by the Strang splitting algorithm, higher order symmetrical splitting method is possible but with a price of much higher computational costs.

The spatial discretization in the DNS solver is based on a staggered Cartesian grid on which the velocity is defined on cell surfaces and the scalars on the cell center. The approximation of spatial derivatives and variable interpolations is largely based on 6th order center scheme; nevertheless, the convective terms in the species mass and temperature equations are discretized with a 5th order WENO scheme [29] to handle flame induced large gradient and inhibit numerical wiggles. A six order polynomial interpolation is used for approximating the variable from the cell center to the surface in most of the first derivatives. The discretization of the second derivative follows the first derivative with the half-cell shift so that the total numerical stencil becomes compact. The velocity-pressure decoupling results in a variable-coefficient equation for the hydrodynamic pressure that is solved by an efficient multi-grid method [30]. The temporal and spatial accuracy of the DNS solver are verified by performing grid/time-step dependence tests by comparing the results from successive step refining, the solver has been applied in [31,32]. Further numerical details are reported in [33].

3. Problem definition and initial condition

A model SACI combustion process is considered in this study. A square box domain is considered with the size of 0.614 mm $\times$ 0.614 mm. The domain is within a large constant volume enclosure filled with a perfectly premixed lean H₂/air/EGR mixture. The mixture has an equivalence ratio of $\phi=0.6$ with 50% EGR and the initial mixture is set to an elevated pressure (60 bar) and different initial temperature (1050-1300 K) similar to an engine operation condition in 2D DNS cases. The EGR is assumed to be composed of combustion product of the unburned mixture surrounding the flame. The boundary of the box domain satisfies the periodic condition; therefore there will be no net mass flux through the boundaries of the domain. An initial laminar cylindrical flame is placed at the domain center. A grid made up of 1024 $\times$ 1024 cells is used to discretize the domain, leading to a uniform grid resolution of 0.6 μ m. Such fine resolution is needed to capture the thin reaction zones associated with the flame.

The initial cylindrical flame is implemented by simply imposing the temperature and species profiles of a modified 1D premixed flame solution along the radial coordinate with the origin set at the domain center, with the higher temperature side at the origin. The radius of the cylindrical flame is set as 0.06 mm. The fresh mixture of the above 1D problem is set the same as the ambient mixture

condition. Different from the flame propagation in a chemically inert unburned mixture, the fresh mixture at elevated temperature and pressure is undergoing ignition reactions. At a given location if the time required for the flame to propagate to the location is longer than the ignition delay time the mixture would auto-ignite before the flame front propagates to the location. In the 1D simulation for the initial flame profile, in order to avoid auto-ignition in the unburned mixture, we stabilize the flame front at a location 2 mm downstream of the inflow boundary. The thermal thickness of the initial flame is 15 μm which is resolved with 23 grid points. The initial turbulent flow field is generated using a synthesis turbulence method. The integral scale is 0.154 mm and the rms (root mean square) velocity is 0.5 m/s, which yields a turbulence eddy turnover time about 0.308 ms.

4. Propagation of the flame front

Figure 1 shows the evolution of the mass fraction of OH, H_2O_2 and heat release rate (HR) at five consecutive instances of time with un-burnt temperature 1200 K in the 2D DNS case. Starting from a small and smoother surface the flame front propagates outward with cellular structures developed. The disturbance of the turbulent eddies to the flame front in the present case may be negligible since the eddy turnover time is significantly (10 times) longer than the evolution time shown in the figure. The observed cellular structures are owing to the inherent flame instability. Considering the small size of the flame ball limited in the currently investigated domain, the major contributing flame instability mechanism would be the thermal-diffusive instability [34], rather than the hydrodynamic instability. In the first three instances of time heat release is seen in the thin cellular shaped flame, where the mass fraction of OH and H_2O_2 are highly non-uniform. It is clearer to see at 0.025 ms at the center of a flame cell they are significantly higher and at the cusp region they are significantly lower. Later at 0.067 ms, the homogenous mixture in the surrounding area is undergoing chemical reactions, as seen the formation of H_2O_2 , which is produced at the early stage of combustion. The significant accumulation of H_2O_2 can be found at 0.09 ms. Due to the high reactivity of end gas, fuel consumption is finished quickly so that at the last instance of time shown in the figure (0.094 ms), a large amount of OH radicals and low level of heat release rate can be found in the domain outside of the flame, indicating that the mixture in front of the flame is auto-ignited. However, one still can see the transition from a flame propagation to auto-ignition.

In Fig. 2(a) the budget terms of the transport equation for the mass fraction of H_2 along line A extracted normal to the flame front at 0.067 ms in Fig. 1 show that both terms are in the same order. Contrary to this, the counterparts extracted from line B in Fig. 1 at 0.094 ms appear that the diffusion term both at flame front and the region far away is negligible but the consumption rate of H_2 is significantly higher, see Fig. 2(b), because of the spontaneous auto-ignition at the end gas region. It has shown that owing to the initial high temperature and the compression effect of the flame propagation

in the constant volume enclosure, the mixture farther away from the flame is undergoing auto-ignition from 0.067 ms.

Intuitively, it is expected that in the preheat zone of the flame heat and products generated in the flame are transferred from the flame, which would enhance the ignition of the mixture. However, an unusual non-monotonic distribution is observed both in the temperature and H_2 mass fraction profiles in Fig.3. A lower temperature region is formed in between the center burned products and the adjacent unburned gas, where transport of heat and mass from the flame is seen rather significant. This region is often referred to as the preheat zone of the premixed flame. Figure 3 also shows the fuel in this preheat zone is at a higher mass fraction than those in the burned gas (zero mass fraction, $x < 0.54$ mm) and in the end gas farther away from the flame ($x > 0.57$ mm).

Furthermore, it is well recognized that the enhancement in initial temperature can decrease end-gas auto-ignition time and increase flame propagation speed [35,36]. Here, 2D DNS results in Fig. 4 display consistent results showing a trend of increased displacement speed with higher temperature. The corresponding end-gas auto-ignition time decreases as well as the distance indicating the flame can propagate at most before ignition at higher temperature conditions.

5. One dimensional detailed numerical simulation of flame/ignition interaction

To understand the underlining physics involved in the retarded ignition behavior in the preheat zone of the flame we have performed detailed numerical simulations under various conditions in a simple 1D configuration that is relevant to the 2D constant volume condition present in the previous section. The 1D constant volume domain has a periodic condition applied on the boundaries. In the initial field a 1D twin-flame is placed in the domain center, in a similar way as in the 2D case. Figure 5 shows the profiles of temperature and mass fraction of H_2 in the initial field.

Eight cases (A-H) are investigated in which the fuel type, equivalence ratio, initial temperature and diffusivity are varied. For comparison, cases I and J use one-step global chemistry mechanism and the pressure is reduced to 1 bar for hydrogen and 10 bar for methane, respectively. Table 1 summarizes ten cases setup. The domain size is 5 mm – 50 mm, much larger than that in the 2D case discussed earlier, which ensures a longer flame propagation time before the transition to auto-ignition. With longer flame propagation time one can also study conditions under which the ignition delay time is longer, thus, in cases A-C, F and G the initial temperature is lower than the 2D case (which is 1200 K). To investigate the effect of preferential diffusion in hydrogen/air mixture we have deliberately set in case B the diffusivity of H_2 to be equal to the diffusivity of N_2 . Note that 1 bar, 10 bar and 30 bar for lean hydrogen/air cases are also performed but not shown for brevity because they present consistent results with case A under 60 bar pressure, while holding all other initial conditions the same. For all cases the initial flame size is set to 0.4 mm, which is a small fraction of the total domain length. In total three different fuel/air mixtures are investigated: hydrogen/air, syngas (a mix-

ture of CO and H₂ with 50% each on volume basis), and methane/air. In all cases 50% of EGR is mixed with the fuel and air. For the various cases the EGR is made up of the major combustion products (O₂, CO₂, H₂O, and N₂) of the corresponding unburned mixture assuming a complete combustion.

The chemical kinetic mechanisms employed in the 1D studies are the H₂/air mechanism of Li et al. [37] (9 species, 21 reactions), the CO/H₂/air mechanism of Davis et al. [38] (14 species, 38 reactions), and the CH₄/air mechanism of Smooke et al. [39] (16 species, 35 reactions). In case I a one-step H₂/air chemistry mechanism by Marinov et al. [40] is employed. In case J a one-step CH₄/air chemistry mechanism provided in OpenFOAM [41] is used.

In the H₂/air mechanism of Li et al. [37] elementary reactions involved in the formation of OH radicals include the R1, R2, R4, R7, R11, R12 and R16 reactions, listed below,

The elementary reactions of R3, R8, R13 and R20 are responsible for the consumption of OH,

Reaction R14 is found to be important in the ignition process,

These reactions will be used below to interpret the flame/ignition interaction.

5.1 Flame/ignition interaction in lean H₂/air mixtures

In order to highlight the interaction of flame/spontaneous ignition front, temporal evolution of the spatial profiles of temperature, mass fractions of OH and HO₂, gas velocity and the rate of the elementary reaction R14 are shown in Figure 6 for case A and R14 profile for case B. The data are extracted from the right-hand-side half of the domain; the left-hand-side half profile is totally symmetric.

Until time 1 ($t < 0.794$ ms) the flame front is seen to propagate towards the unburned mixture where auto-ignition is at its early stage as indicated by the low HO₂ formed in the region. The spike of OH in the reaction zone of the flame separates the burned gas (left) where OH is at its equilibrium

level and unburned gas (right) where OH is absent. Reaction R14 is significant only in the reaction zone of the flame. The flame front continues propagating to the right-hand-side mixture until time 3 (1.227 ms), thereafter the flame front is seen to move leftwards owing to the gas expansion due to heat release in the flame, which results in negative velocity (flowing leftwards).

At time 5 a slightly lower temperature is observed in the preheat zone of the flame, which corresponds well to the 2D flame reported in the previous section. At time 5 the OH radicals are rather low in the mixture on the right-hand-side of the flame where HO₂ formed in the ignition process is at a level higher than that at the flame front. As a result, reaction R14 is also at a high rate, which initiates a dramatic increase of H₂O₂ in the region and eventually an explosive formation of OH through reaction R16 at time 6. It is seen that the preheat zone of the flame at time 6 has a much lower temperature than the mixture far away from the flame. It appears that heat and mass transfer from the reaction zone of the flame to the preheat zone of the flame has inhibited the reaction progress in the preheat zone. This phenomenon is consistent with that observed in the 2D case, and the question is, what is the physical reason that causes the inhibition?

5.2 Flame/ignition interaction in lean H₂/air mixtures with $D_{H_2}=D_{N_2}$

One may speculate that the high diffusivity of hydrogen in the lean hydrogen/air/EGR mixtures is the reason that causes the inhibition of ignition in the preheat zone of the flame. To investigate this, in case B, the diffusivity of hydrogen is set to the diffusivity of nitrogen ($D_{H_2}=D_{N_2}$). The corresponding results are shown in Fig. 7. As seen, as the flame is propagating to the fuel/air/EGR mixture while auto-ignition takes place in the mixture. Temperature and H₂ mass fraction vary monotonically across the flame through out the ignition region of the mixture; the preheat zone has a faster reaction progress than the mixture farther away from the flame. The heat and mass transfer from the flame improved the ignition of the mixture in the preheat zone. It is clear that the inhibition of ignition of the mixture in the preheat zone in lean hydrogen/air/EGR mixtures is owing to the high diffusivity of hydrogen in the mixture.

From Figs. 6 and 7 one can estimate the time needed for the transition from the flame to ignition. For case A, the transition took about 1.256 ms whereas for case B, the transition took about 0.923 ms. The inhibition of ignition in the preheat zone is shown to significantly slow the flame propagation and the transition from the flame to ignition.

5.3 Reaction path analysis

To look into the details of the transition from flame to ignition in lean hydrogen/air/EGR mixtures, we plot the rates of formation and consumption of OH radicals in various elementary reactions for case A (Fig. 8) and case B (Fig. 9) at the time of flame transition to ignition. As shown in Fig. 8 (case A), in the reaction zone of the flame the dominant reactions for the formation of OH radicals are R1, R4 and R16, whereas the consumption is through R3 and R13 (in which H₂ and HO₂ are oxi-

dized by OH to form H₂O). In the mixture farther away from the flame R3 and R16 are the two dominant reactions consuming and producing OH radicals, respectively. It appears that at time 5 (1.253 ms) the lowest temperature in case A, the flame is located in the preheat zone around $x \sim 0.995$ mm, see Fig. 8, where the two dominating reactions R16 and R3 are at their local minima. The heat and mass transfer from the flame has inhibited particularly these two reactions. For case B with $D_{H_2}=D_{N_2}$, it is seen in Fig. 9 that all reaction rates varies monotonically from the reaction zone of the flame to the preheat zone and to the mixture farther away from the flame. What's more, the distribution of ϕ is the same over x position and temperature decreases monotonically from burnt to unburned zone in case B compared with those in case A, c.f. Fig. 8.

Therefore, we propose here a mechanism of flame/ignition interaction in the lean hydrogen/air mixtures. The interaction can be summarized as the following:

(a) Heat and mass transfer between the reaction zone and the unburned mixture; in the proximity of the flame on the unburned side, the mixture is heated and combustion intermediates are transferred from the reaction zone, meanwhile reactants in the preheat zone are diffused to the reaction zone. Owing to the high diffusivity of hydrogen molecules the diffusion of hydrogen is faster than oxygen and other species, as a result, hydrogen in the preheat zone is relatively in deficit, as noted in the equivalence ratio profile, Fig. 8.

(b) Chemical reactions in the preheat zone and unburned mixtures farther away from the flame; in the preheat zone ϕ is lower in a initially fuel lean mixture, which results in a lower heat release compared with the mixture further away from the flame. As the ignition processes throughout the unburned mixtures, the temperature in the preheat zone is gradually becoming lower than that in far field. Reactions R3 and R16 are both slowing down, leading to a slower oxidation of the fuel.

One can envisage that in a rich hydrogen/air mixture, the effect of high diffusivity of hydrogen will lead to a decrease of hydrogen in the preheat zone, which will enhance the heat release in the zone. This will speed up the ignition in the preheat zone leading to a speed up of the flame speed. The result of case C ($\phi=2$) confirms this speculation. For brevity the results of case C are not shown here. A brief summary of the results of case C is the following. First, there is no local low temperature minima in the preheat zone throughout the flame-to-ignition transition process; second, the flame speed is significantly higher than that of lean flame case A.

For brevity, the results of cases D-J are omitted here. The results confirm the observation of case A. In particular, in cases D, F and H we have observed the inhibition of ignition by the heat and mass transfer to the preheat zone. In case G the initial temperature in the unburned mixture is too low to have a substantial transition from flame to ignition, hence, the inhibition of ignition in the preheat zone is not identifiable. For one-step chemistry in cases I and J, it shows little effect on the diffusive-thermal instability, which leads to the same result as that in case A and case E, respectively.

5.4 Flame/ignition interaction in lean syngas/air and methane/air mixtures

To identify the fuel effect on the flame/ignition interaction, we have performed simulations for lean syngas/air mixtures (Case D) and lean methane/air mixtures (Case E). Figure 10 shows spatial profiles of temperature, mass fractions of the fuel (H_2 and CO) and HO_2 radicals in Case D at various instances of time. The results are consistent with the previous results in the lean hydrogen/air mixtures. The heat and mass transfer from the flame has inhibited the ignition process in the preheat zone. At time 4 and 5 a locally low temperature is shown in the preheat zone. Corresponding to this local low temperature there is local peak of H_2 and to a less extent a small peak of CO (which indicate a slower reaction progress). At time 5 (0.261ms), even though hydrogen is consumed completely, there is still a CO peak and a local minimum in the temperature in the preheat zone.

Figure 11 shows temporal evolution of temperature, mass fractions of CH_4 , OH , HO_2 , H_2O_2 and CH_2O in the lean methane/air mixture (Case E). From time 3 (1.075 ms) HO_2 , H_2O_2 and CH_2O on the unburned side of the flame start to appear owing to the ignition reactions, leading to a considerable increase of temperature and a considerable decrease of CH_4 . It is seen that the peaks of HO_2 and H_2O_2 that represent the propagating flame front disappear at time 3 and time 4, respectively; and starting from time 4 rapid production of OH radicals is seen in the mixtures farther away from the flame. There is no local minimum of temperature or reaction progress in the preheat zone of the flame. This confirms that the high diffusivity in the lean hydrogen/air and syngas/air mixtures are the reason that causes inhibition of the ignition process in the preheat zone of the flame.

For brevity, the results of cases F, G and H are omitted here. The results confirm the observation of case A. In particular, in cases F and H we have observed the inhibition of ignition by the heat and mass transfer to the preheat zone. In case G the initial temperature in the unburned mixture is too low to have a substantial transition from flame to ignition, hence, the inhibition of ignition in the preheat zone is not identifiable.

5.5 Flame/ignition interaction for one-step chemistry in lean H_2 /air and CH_4 /air mixture

Figure 12 shows the time sequence of spatial distribution of fuel, temperature and equivalence ratio for cases I and J. Due to the fast oxydation process of one-step chemistry mechanism, only 1 bar and 10 bar pressure is used for hydrogen (left column) and methane (right column) in cases I and J, respectively. As such, the ignition delay time is too short and the whole combustion process is dominated by spontaneous auto-ignition. As expected, due to high diffusivity of hydrogen, hydrogen in the preheat zone diffuses faster leading to a slower reaction rate and the temperature tends to be a few kelven lower than the far away homogeneous region. In contrast, the one-step methane mechanism verified that higher Lewis number will not result in the ignition-inhibition in the preheat zone.

6. Conclusions

One and two dimensional direct numerical simulations are performed to study flame and spontaneous ignition interaction in a lean hydrogen/air/EGR mixture under a constant volume enclosure relevant to SACI engine conditions. In 2D DNS cases, it is seen that cellular flame is observed due to thermal-diffusive instability soon after the initial cylindrical flame propagates towards the outer premixed mixture. Then a deeper physical reason underlying the cellular patterns is investigated using a series of 1D simulations for different fuels (H_2 /air, H_2 /CO/air and CH_4 /air mixture) with detailed chemistry and different hydrogen diffusivities. The results show that for lean hydrogen/air flames the heat and mass transfer from the flame to the preheat zone of the flame inhibits the ignition of the mixture in the preheat zone due to the high diffusivity of H_2 , resulting in a slower reaction rates; a local low temperature is observed in the preheat zone where the progress of the fuel oxidation process is slower than that in the region farther away from the flame. Finally, the domain size, initial temperature, one step chemistry and so on are further compared to show that thermal-diffusive instability is affected by initial temperature, fuel properties instead of domain size and multiple reactions.

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Table 1

Table 1 Case setup and initial conditions for 1D cases; DT denotes that detailed transport properties are used.

Cases	Mixture (50% EGR)	Equivalence ratio	Fuel diffusivi- ty	Initial Tempera- ture [K]	Domain size [mm]
A	H ₂ /air	0.6	DT	1050	5
B	H ₂ /air	0.6	DT, $D_{H_2}=D_{N_2}$	1050	5
C	H ₂ /air	2	DT	1050	5
D	H ₂ /CO/air	0.6	DT	1200	5
E	CH ₄ /air	0.6	DT	1200	5
F	H ₂ /air	0.6	DT	1050	50
G	H ₂ /air	0.6	DT	800	5
H	H ₂ /air	0.6	DT	1200	5
I(one- step)	H ₂ /air	0.6	DT	1200	2.5
J(one- step)	CH ₄ /air	0.6	DT	1200	5

FIGURE 1

FIGURE 2

FIGURE 3

FIGURE 4

FIGURE 5

FIGURE 6

FIGURE 7

FIGURE 8

FIGURE 9

FIGURE 10

FIGURE 11

FIGURE 12

FIGURE CAPTION

Fig. 1 Contour plots of OH, H₂O₂ radical concentration and heat release at five consecutive instances of time. From left to right: 0.0082 ms, 0.025 ms, 0.067 ms, 0.09 ms, and 0.094 ms. The results are obtained from 2D-DNS.

Fig. 2 Budget terms of transport equations of H₂ extracted from selected line A at 0.067 ms (a) and line B (b) at 0.094 ms in Fig. 1.

Fig. 3 Profiles of temperature and mass fraction of H₂ extracted from a selected line B in Fig. 1.

Fig. 4 Displacement speed, end-gas auto-ignition time and flame propagating distance as a function of temperature.

Fig. 5 The initial temperature and fuel mass fraction profiles for the 1D case A.

Fig. 6 Temporal evolution of the profiles of temperature, mass fraction of OH, HO₂, gas velocity for case A and the rate of R14 for cases A and B. The number from 1 to 6 for case A denotes a consecutive time sequence of 0.794 ms, 1.16 ms, 1.227 ms, 1.243 ms, 1.253 ms, and 1.256 ms. The number from 3 to 6 in case B denotes a consecutive time sequence as 0.9, 0.905, 0.907 and 0.923 ms.

Fig. 7 Temporal evolution of the profiles of temperature, mass fraction of H₂, HO₂ and OH for case B. The number from 3 to 6 denotes a consecutive time sequence as 0.9 ms, 0.905 ms, 0.907 ms and 0.923 ms. For brevity time 1 and 2 are not shown in the figure.

Fig. 8 Rates in various elementary reactions for the formation and consumption of OH radicals at time 5 (1.253 ms) in case A (upper row); local equivalence ratio and temperature in cases A and B (lower row).

Fig. 9 Rates in various elementary reactions for the formation and consumption of OH radicals at time 6 (0.923 ms) in case B.

Fig. 10 Temporal evolution of temperature, mass fraction of H_2 , CO and HO_2 in case D. Time sequences: No.1 = 0 ms, No.2 = 0.098 ms, No.3 = 0.196 ms, No.4 = 0.228 ms, No.5 = 0.261 ms, No.6 = 0.391 ms, respectively.

Fig. 11 Temporal evolution of temperature, mass fraction of CH_4 , OH, HO_2 , H_2O_2 and CH_2O at case E. Time sequences: No.1 = 0 ms, No.2 = 0.392 ms, No.3 = 1.075 ms, No.4 = 1.271 ms, No.5 = 1.368 ms respectively..

Fig. 12 left: temporal evolution of temperature, mass fraction of H_2 and ϕ for case I; right: temperature, mass fraction of CH_4 and ϕ for case J. Left: time sequences: No.1 = 0 ms, No.2 = 0.00237 ms, No.3 = 0.00328 ms, No.4 = 0.00408 ms, No.5 = 0.00881 ms, respectively. Right: time sequences: No.1 = 0 ms, No.2 = 0.00278 ms, No.3 = 0.0101 ms, No.4 = 0.0211 ms, No.5 = 0.0348 ms, respectively.