Flame propagation and heat transfer characteristics of a hydrogen–air premixed flame in a constant volume vessel

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Abstract

Direct numerical simulation of a stoichiometric hydrogen–air turbulent premixed flame in a rectangular constant volume vessel has been conducted to gain fundamental insights into turbulence–flame interactions and heat loss characteristics under a pressure rising condition. The turbulent vortices are significantly weakened in the burnt side due to expansion and viscosity increase. The conditionally averaged turbulent kinetic energy is suppressed near the wall and it takes mostly constant in the rest of the domain which suggests that there is no significant turbulence production near the wall, and the wall just damps the turbulence in the present simulation's set up. It is found that the turbulent kinetic energy still takes a significant value in the burnt side due to the velocity induced by the expansion, not much inherent to the turbulent eddies. Temporal evolution of the wall heat loss characteristics is studied. Although the heat loss induced by the burnt gas

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dominates the total heat loss at the end of combustion, the heat loss induced by flame impingements contributes to substantial portion of total heat loss. Finally, turbulence–flame interactions modeling is studied using a conventional flamelet model for reaction rate closure. The result shows that turbulence–flame interaction mechanism does not change significantly under pressure rising conditions, suggesting that this model could be also used in a pressure-evolving combustion system without further modifications.

Keywords: Direct numerical simulation (DNS), Turbulent premixed combustion, Flame–wall interactions, Flamelet model

1. Introduction

Designing high thermal efficiency and low emission combustion devices such as spark ignition (SI) engines is a challenging task as emission standards becomes more stringent. One of the challenges to meet the standards is to reduce pollutants of hydrocarbon fuels such as CO, CO₂ and NO_x. Employing lean premixed combustion in SI engines is one way to achieve this. With a lower fuel air ratio, pollutant reduction is improved due to a lower peak flame temperature. Utilizing lean premixed flames with diluents has been found to improve the knock resistance as well as improving thermal efficiency as the end gas temperature is further decreased [1, 2]. However, the characteristics of lean premixed flames are different from stoichiometric flames, similar to which is seen in Moderate or diluted Intense oxygen Dilution (MILD) combustion [3]. Further investigations into turbulence–flame interactions are needed for developing a better insight in lean diluted combustion.

Hydrogen as the next generation fuel has gained particular interest as it has unique characteristics and various advantageous over hydrocarbon fuels such as a faster burning rate, lower lean operational limits and more importantly no CO and CO₂ emissions. These features show that hydrogen can play a prominent role in clean combustion technology in the future. Many studies have been conducted to investigate the characteristics of hydrogen–air premixed flames with a detailed chemistry by employing direct numerical simulation (DNS) under different flow configurations such as planar flames [4, 5, 6, 7], V-flame [8, 9], swirl flames [10, 11, 12] and jet flames [13, 14]. Flame–turbulence interaction characteristics, which are difficult to model due to its nonlinearity, have been studied in these studies. The scalar dissipation rate, an important quantity that characterizes molecular mixing at micro scale, is directly related to reaction rate, and a relationship of these two quantities was proposed by Bray [15] to close the reaction rate for high Damköhler number premixed flames. However, whether this reaction rate closure model can be applied for flames in a constant volume configuration with temporal pressure change, has not been studied yet by means of DNS, hence this should be investigated.

To achieve cleaner and high efficiency in combustion devices, it is also crucial to understand heat loss characteristics and flame–wall interactions as heat transfer through the wall during combustion significantly affects thermal efficiency. For hydrogen flames, flame–wall interaction has been studied by DNS with detailed chemistry [9, 16, 17]. It has been shown that reaction rate peaks near the cold wall region and wall heat flux (ϕ_q) shows a quick rise when the flame impingement occurs. The above mentioned DNS studies

have been conducted under constant atmospheric pressure conditions due to enormous computational resources required by this simulation technique. In SI engines, however, the pressure in the vessel rises and it significantly affects chemical reactions, fluid dynamics, flame propagations and wall heat transfer characteristics. In our previous study [18], three-dimensional DNS of hydrogen–air premixed flames has been conducted under a pressure rising condition for the first time. The results have shown that the maximum ϕ_q , which is induced by flame impingement, increases with mean pressure increase, and the maximum ϕ_q can be described as a function of mean pressure for hydrogen–air premixed flames. It is known that the wall heat flux induced by burnt gas temperature contributes the total heat loss the most, although ϕ_q induced by flame impingement is the largest in magnitude. This is because the time scale of ϕ_q induced by burnt gas is much larger than that of induced by flame impingement during combustion. Measurement of wall heat flux is a difficult task, especially in a pressure evolving system. By using the DNS data, however, the time evolution of wall heat flux induced by burnt gas and flame impingement, and their contributions to total heat loss can be quantified and examined, and this is also of our interest in the present study.

This paper is organized as follows: The details of the DNS database is explained in Sec. 2, and the results are discussed in Sec. 3, beginning with flame propagation and flow characteristics, and followed by the detailed discussion on heat loss characteristics. Finally, the relationship between the mean reaction rate and the scalar dissipation rate is discussed. The conclusions are summarized in the final section.

2. Direct Numerical Simulation

2.1. Governing Equations

The fully-compressible governing equations are for the conservation equations of mass, momentum, energy and chemical species mass fractions and can be written respectively as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (1)$$

$$\frac{\partial \rho \vec{u}}{\partial t} + (\nabla \rho \vec{u} \vec{u}) = -\nabla \cdot \mathbf{P}, \quad (2)$$

$$\begin{aligned} \frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho \vec{u} T) &= \frac{1}{\bar{c}_v} \nabla \cdot (\lambda_k \nabla T) - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} \left(\rho Y_i \vec{V}_i c_{p,i} \nabla T \right) \\ &\quad - \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} \left[R_i \nabla \cdot (\rho Y_i \vec{V}_i) \right] - \frac{1}{\bar{c}_v} \mathbf{P} : (\nabla \vec{u}) \\ &\quad - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (h_i w_i) + \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} (R_i w_i), \end{aligned} \quad (3)$$

$$\frac{\partial Y_i}{\partial t} + \vec{u} \cdot \nabla Y_i = -\frac{1}{\rho} \nabla \cdot (\rho Y_i \vec{V}_i) + \frac{w_i}{\rho}. \quad (4)$$

where, ρ , $\vec{u}$, T , λ_k and N_s denote density, fluid velocity vector, temperature, thermal conductivity and the number of chemical species, respectively. Y_i , $\vec{V}_i$, R_i , h_i , w_i , $c_{v,i}$ and $c_{p,i}$ denote, respectively, mass fraction, diffusion velocity, characteristic gas constant, enthalpy, reaction rate, specific heat capacities at constant volume and pressure for chemical species i . The stress tensor, $\mathbf{P}$ is given by

$$\mathbf{P} = \left[p + \frac{2}{3} \mu (\nabla \cdot \vec{u}) \right] \mathbf{I} - \mu \left[(\nabla \vec{u}) + (\nabla \vec{u})^T \right], \quad (5)$$

where p , μ and $\mathbf{I}$ denote pressure, dynamic viscosity and the unit tensor, respectively. The mixture averaged specific heat capacity at constant volume, $\bar{c}_v$, is given by

$$\bar{c}_v = \sum_{i=1}^{N_s} c_{v,i} Y_i \quad (6)$$

The Soret effect, the Dufour effect, pressure gradient diffusion, bulk viscosity and radiative heat transfer are neglected.

2.2. Numerical methods

Figure 1 shows the schematic of numerical configuration with a high temperature ignition kernel. The initial temperature distribution, T_{ini} , is given as Gaussian distribution and can be written as:

$$T_{ini} = T_{pre} + (T_{max} - T_{pre}) \exp\left(-\frac{r^2}{2\sigma_T^2}\right) \quad (7)$$

$$\sigma_T = r_c/3 \quad (8)$$

Here, T_{max} , T_{pre} , r_c , r and σ_T denote the maximum temperature of the ignition kernel, preheat temperature, radius of the ignition kernel, distance from center and the distance from center to position at which the temperature gradient is maximum, respectively. T_{max} is 2000 K, T_{pre} is 700 K and r_c is 0.5 mm in the present DNS.

The present DNS is conducted in a constant volume vessel configuration. Fully-developed homogeneous isotropic turbulence (HIT) is used for initial velocity field and the initial flow field is obtained through preliminary DNS of decaying HIT by using the spectral method with periodic boundary conditions. The Reynolds number of HIT is: $Re_l = u'_{rms} l / \nu = 516$ and $Re_\lambda = u'_{rms} \lambda / \nu = 97.1$, where u'_{rms} , l , λ and ν denote the root-mean-square of

turbulent velocity, the integral length scale, the Taylor micro scale and the kinematic viscosity, respectively. The size of the vessel is $L_x \times L_y \times L_z = 20.0 \text{ mm} \times 5.0 \text{ mm} \times 20.0 \text{ mm}$. $N_x \times N_y \times N_z = 1025 \times 257 \times 1025$ grid points are used. The closed vessel is assumed to have a rectangular configuration, which is a simple idealized model for a combustion chamber such as an automobile engine. This domain length (L_y) of the vessel represents the state when the piston head is at the top dead center (TDC) at the end of the compression stroke. Although this length scale is smaller than that in practical applications, the present configuration of the vessel is chosen to make the simulation more computational affordable. With this configuration, the effects of pressure increase on flame propagation and time-varying chemical properties can be addressed. Each wall is named as follows: left wall ($x = 0$), right wall ($x = L_x$), lower wall ($y = 0$), upper wall ($y = L_y$), front wall ($z = 0$) and back wall ($z = L_z$), respectively. Spatial resolution is determined based on the laminar flame thickness and characteristics of turbulence in addition to the care of near wall phenomena. As the pressure increases, the Kolmogorov length scale (η) averaged in the unburnt side decreases to about $14 \text{ } \mu\text{m}$ at 3 atm. The grid size in the present study is Δx : $19.5 \text{ } \mu\text{m}$; this corresponds to $k_{max}\eta = 2.2$, where k_{max} is the maximum wave number in DNS. This resolution is well enough to resolve the smallest scale of turbulent eddies which corresponds to the well-known resolution limit $k_{max}\eta > 1.2$ for DNS of turbulence. More than 24 grid points are within the laminar thermal flame thickness δ_{th} and decreasing flame thickness due to pressure increase is also taken into account. In the final part of the simulation, when the flames reach all four corners of the vessel and the combustion is almost finished,

more than 10 grid points are still within δ_{th} . Therefore the spatial resolution in the present study is justified. The detailed kinetic mechanism [19] including 12 reactive species (H_2 , O_2 , H_2O , O , H , OH , HO_2 , H_2O_2 , N_2 , N , NO_2 and NO) and 27 elementary reactions is used for the hydrogen-air reaction. Temperature dependence of the viscosity, the thermal conductivity and the diffusion coefficients are taken into account by using the CHEMKIN-II packages [20, 21]. The governing equations are discretized using fourth-order central finite difference scheme in all directions. The fourth order compact finite difference filter [22] is applied to eliminate unphysical oscillations with higher spatial frequencies than the spatial resolution. The time integration is implemented by the third order Runge-Kutta scheme. Only the chemical source terms in species conservation equations are advanced by using the implicit method [23]. For the boundary condition, isothermal, no-slip and fully-reflecting wall boundary conditions given by the Navier-Stokes characteristic boundary condition (NSCBC) [24, 25] are used on the walls and the wall surfaces are chemically inactive. The wall temperature, the equivalence ratio and the initial pressure are set to 450 K, 1.0 and 0.1 MPa, respectively. With this configuration, the phenomena of flame propagation under isochoric process after the mixture ignition while the piston is at the TDC can be simulated. The initial distribution of species is assumed to be uniform. Other numerical parameters at initial condition are $u'_{rms}/S_L = 1.80$ and $l/\delta_F = 281$, where S_L and δ_F denote the laminar burning velocity and the Zel'dovich thickness. The present case is classified as corrugated flamelets in the turbulent combustion diagram [26].

3. Results and discussions

3.1. Flame and turbulence characteristics

The temporal development of the mean pressure (P_m) in the constant volume vessel is shown in Fig. 2. Note that P_m shows a slight decrease until $t = 100 \mu\text{s}$ since the total heat loss from the wall is slightly higher than the total heat generated by the chemical reactions during this period. P_m starts to increase approximately $100 \mu\text{s}$ after the ignition, and it increases up to threefold as the stoichiometric mixture is preheated to 700 K at the initial condition. Figure 3 shows flame and vortical structures indicated by iso-surfaces of temperature and second invariant (Q) of the velocity gradient tensor. The second invariant is defined by $Q = (W_{ij}W_{ij} - S_{ij}S_{ij})/2$, where $S_{ij} = 0.5(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ and $W_{ij} = 0.5(\partial u_i/\partial x_j - \partial u_j/\partial x_i)$ represent the symmetric and the antisymmetric parts of the velocity gradient tensor, $A_{ij} = \partial u_i/\partial x_j$. The temperature iso-surface indicates $T = 1282 \text{ K}$ at which the heat release rate peaks in the corresponding laminar flame of the initial condition. The mixture ignites from the high temperature kernel at the center of the computational domain, and then flame front propagates with distortion by the turbulent motion. In the burnt side, for a better visualization, the value of iso-surface of Q is set to one tenth of that in the unburnt side because the vortices are weakened due to expansion and viscosity increase, which is shown by density of vortical structures. The color bar shows the minimum and maximum values of the wall heat flux, ϕ_q , through the lower wall. ϕ_q is defined as the product of thermal conductivity of the gas mixture and temperature gradient on the wall, and can be given as:

$$\phi_q = -\lambda_k \nabla T|_{wall} \quad (9)$$

As shown in Fig. 3, ϕ_q shows high values in the region of the wall exposed to the burnt gas and flame front. The instantaneous maximum heat flux on a wall can be observed in the region with flame attachment, and increases with pressure increase [18]. On the other hand the heat flux on the region exposed to the burnt and unburnt gas does not change significantly with the increase of the pressure. The wall heat flux of each region and their contributions to the total heat loss with pressure change will be discussed in detail in Sec. 3.2.

To investigate the flow and flame characteristics in a constant volume vessel, temporal developments of averaged quantities of the flow within probes are obtained. Each probe contains 4 grid points δ (volume: $\delta^3 = 58.6^3 \mu\text{m}^3$) in each direction with total of 64 points. The position of the first probe is in the center of the vessel, and the next 31 probes are equally distributed in the x direction, hence the distance between each probe is $16\Delta x$ where $\Delta x = L_x/N_x$. The probe P_1 is located in the center of the vessel and P_{32} is the closest probe to the right wall. A certain averaged quantity of the flow in a P_i can be computed from

$$\bar{F} = \frac{1}{\delta^3} \sum_{\delta x, \delta y, \delta z=0}^{\delta} F(x_i + \delta x, y_i + \delta y, z_i + \delta z) \quad (10)$$

where (x_i, y_i, z_i) is the starting location of Probe P_i . The Favre average of the quantity $\tilde{F}$ can be given as $\tilde{F} = \overline{\rho F} / \bar{\rho}$.

Figure 4 shows the turbulent combustion diagram [26]. Each data point in this figure is computed from a probe, and the color changes from blue to red represents the probe location from the center of the vessel to the wall. The integral length scale is obtained using $l = u_{\text{rms}}'^3 / \tilde{\epsilon}_{\text{turb}}$, where $\tilde{\epsilon}_{\text{turb}}$ is the

mean turbulence energy dissipation rate. In Fig. 4, it is clear that the local flames located in high Damköhler number regimes where local Re_l is also relatively high.

Figure 5 shows the temporal developments of several quantities of the flow in a P_i . For clarity, one in every 5 probes is plotted. As shown in Fig. 5a, $\tilde{T}$ in P_1 , which is located in the center, is about 2000 K at the beginning of the simulation, since the high temperature ignition kernel is located in this part of the domain. The Favre averaged $\tilde{T}$ in other probes which are away from the center and closer to the right wall, shows about 700 K, and start to increase rapidly where flame passes each probe. In Fig. 5b, the Favre averaged mass fraction of H_2 , $\tilde{Y}_{H_2}$, is the same for the probes away from the flame, and shows a sharp decrease as the flame passes through. The smoothness in Figs. 5 is related to the time interval of the sampling data. Only 12 μs of data interval is used due to the large amount of dataset of the present DNS. It should be noted that the conclusions do not change by the choice of the time interval.

As the flame propagates in the vessel, turbulence in the burnt side is weakened. This turbulence weakening is seen more clearly in Figs. 5 (c) and (d) which show temporal evolution of ν and the Kolmogorov length scale η . Comparing with temperature plot in Fig. 5a, ν at each probe starts increasing when flame passes. This is then reflected in the increase of η . In Fig. 5a, $\tilde{T}$ shows slight increase where flame is still away from the probe, which is indicated by the dashed arrow. This is due to the compression in the unburnt side as the flame propagates, results in increase in density, hence decline in ν before flame passes the probe, as shown by the dashed arrow in Fig. 5c.

It should be noted that the variables are also obtained using a larger probe size (8 grid points in each direction with total of 512 grid points) and similar results were obtained.

Figure 6 demonstrates the velocity distributions near the wall ($y = 90 \mu\text{m}$ away from the lower wall). As indicated, the velocity vectors in the unburnt side are pointing in various directions while they are pointing mostly in the same direction in the burnt side due to the burnt gas expansion. In the burnt side, the velocity is induced by expansion of the burnt gas and the velocity magnitude is still comparable to that in the unburnt side. In Fig. 7, cuts of the temperature distribution in $x - y$ plane at the center z plane ($z = 10 \text{ mm}$) are shown and the velocity profiles in y at different x locations indicated by solid black lines, are shown for a better visualizations of the burnt side of the vessel. It is clear that the turbulence is significantly weakened where the combustion is almost finished. In Fig. 7a, at $t = 120 \mu\text{s}$, the fluid velocity near the flame front at $x = -6.0 \text{ mm}$, tends to show the outward component while it can possess the inward component in the burnt side at the same location just after $84 \mu\text{s}$ in Fig. 7c. Near the lower and upper walls, the velocity profile at one x position also takes back and forth in different instants. Figure 8 shows the profiles of the turbulent kinetic energy k conditionally averaged on the unburnt and burnt sides of the domain separated by temperature iso-surface at $T = 1282 \text{ K}$. The profiles of k from $t = 120 \mu\text{s}$ to $240 \mu\text{s}$ are averaged. k is given as $k = 3u_{\text{rms}}'^2/2$. In the both sides, k is suppressed near the wall $y < 0.4 \text{ mm}$, and it takes mostly constant in the rest of the domain. This suggests that there is no significant turbulence production near the wall, and the wall just damps the turbulence in the present configuration. It is

noted that the turbulent kinetic energy still takes a significant value in the burnt side. However, this is mostly attributed to the velocity induced by the expansion, not much inherent to the turbulence, which is demonstrated in Fig. 3 and Fig. 6.

3.2. Heat loss characteristics

It is important to clarify the heat loss characteristics as heat loss through engine walls during combustion greatly affects the work output. It was shown that the majority of the heat loss occurs during combustion and expansion stroke, where about 14% of fuel energy is lost through the engine walls during combustion and 10% during expansion in a diesel engine [27].

As shown in Fig. 3, the temporal development of wall heat flux, ϕ_q demonstrates three distinctive regions in terms of its magnitude. This characteristics can be seen more clearly in Fig. 9 (a)-(c). These figures show the instantaneous distribution of ϕ_q on the lower wall. Here, in Fig. 9 (a)-(c), these regions can be classified as, burnt (cyan-yellow), unburnt (blue) and reaction (orange-red) regions. ϕ_q through these three distinctive regions will be investigated quantitatively to study the characteristics of each region's heat loss and their contribution to total heat loss at the end of combustion. From now on, these regions will be defined as follows: (i) reaction regions correspond to location where flame impingement occurs; (ii) unburnt region is the wall heat flux induced by the difference between the unburnt gas temperature and the wall temperature; and (iii) burnt regions correspond to wall heat flux induced by the burnt gas temperature. These regions can be defined based on the mass fractions of H_2O normalized by its instantaneous maximum value. The instantaneous distributions of $Y_{\text{H}_2\text{O}}$ on the lower wall

are shown in Fig. 9 (d)-(f). The region with $0.15 < Y_{\text{H}_2\text{O}}^* < 0.90$ is defined as (i) the reaction region, $Y_{\text{H}_2\text{O}}^* \leq 0.15$ for (ii) the unburnt region and $Y_{\text{H}_2\text{O}}^* \geq 0.90$ for (iii) the burnt region. The asterisk denotes normalization by its instantaneous maximum value. Within these ranges, the three regions can be well separated, as shown in Fig. 9 (g)-(i). Note that regions separation based on the temperature distribution (one grid point away from the lower wall) have also been done, and the results are similar to those discussed below. It should be also noted that this is not a method to separate each regions for heat flux measurements in experiments, but an effective way to evaluate ϕ_q quantitatively by conditional average in the unburnt, reaction and burnt regions using the present DNS data.

Figure 10a shows the development of the mean value of ϕ_q through each region. It can be seen that the mean value of heat flux in the reaction region increases with time; this is because the flame becomes thinner in the increasing pressure condition which will lead to a shorter quenching distance and higher temperature gradient [18]. In the burnt and unburnt regions, the dependency of ϕ_q on the mean pressure is much less pronounced. The mean value of the wall heat flux in the reaction region is the highest amongst the three regions, and at higher pressure condition it is around twice of the value of that induced by the burnt region. ϕ_q in the unburnt region increases only slightly, due to the increased unburnt temperature of the fuel during compression. In Fig. 10b, the contribution of each region to instantaneous total heat loss Φ_q is shown. The heat loss contribution from the burnt region increases which is largely due to the increase in the area of this region, which is shown in Fig. 10c. Figure 10d shows the temporal developments of total

heat loss $\int_0^t \Phi_q dt$ of each region through the lower wall. It can be seen that heat loss through the burnt region increases over time and is responsible about 72% of the total heat loss at the end of combustion. Heat loss in the reaction region is dominant in the early period, and saturates as the flame quenches. This is because in this period most of the flames have already reached the four corner of the vessel. And the area of the reaction region also decreases quickly after 250 μs as shown in Fig. 10c. At the end, ϕ_q through the reaction region is responsible for 22% of the total heat loss through the lower wall.

3.3. Turbulence–flame interaction modeling

The relationship between mean reaction rate and scalar dissipation rate has been studied in previous studies [12, 15, 28, 29, 30, 31]. However not many studies are performed for pressure-evolution conditions. At high turbulent Reynolds number Re and Damköhler number Da flames, it was proposed that the mean reaction rate can be written as [15]:

$$\bar{\omega}_c = \frac{2\bar{\rho}}{2C_m - 1} \tilde{\epsilon}_c, \quad (11)$$

where C_m is a model parameter defined as:

$$C_m \equiv \frac{\int_0^1 c \omega_c P(c) dc}{\int_0^1 \omega_c P(c) dc}, \quad (12)$$

where $\bar{\omega}_c$ and $\tilde{\epsilon}_c$ are the mean reaction and scalar dissipation rates and $P(c)$ is the probability density function of a progress variable c . Here, a model parameter C_m is usually computed using Eq. (12) based on a corresponding laminar flame. Although, Bray [15] reports that $C_m \sim 0.7$ when the probability density function is bimodal using an asymptotic flame, it is uncertain

whether C_m remains to be constant during the pressure increase that influences thermochemical condition of unburnt mixtures in the present DNS. One way to evaluate this is to compute the model parameter using Eq. (11) instead of Eq. (12), and examine it at different times. The parameter computed using Eq. (11) is denoted by C'_m and this represents the balance of $\bar{\omega}_c$ and $\tilde{\epsilon}_c$, which need to be nearly constant if the flamelet model in Eq. (11) is used straightforwardly. In the present study, two progress variables are considered:

$$c_T = \frac{T - T_u}{T_b - T_u}, \text{ and } c_Y = \frac{Y_{H_2} - Y_{H_2,u}}{Y_{H_2,b} - Y_{H_2,u}}. \quad (13)$$

Here, the subscript u and b denote the unburnt and burnt side of the domain. The scalar dissipation rate ϵ_c computed from c_T is given as $\epsilon_{c_T} = \alpha_c |\nabla c_T''|^2$, where α_c is the thermal diffusivity. Whereas ϵ_c computed from c_Y can be written as $\epsilon_{c_Y} = \alpha_Y |\nabla c_Y''|^2$, where α_Y is the mass diffusivity of H_2 .

As shown in Fig. 4, the present combustion condition at large Da with large Re, and Eq. (11) is exact for large Da and large Re limit [15]. Therefore, it is interesting to investigate the relationship between the mean reaction rate and the scalar dissipation rate where flame propagates in a constant volume configuration using Eq. (11). Figure 11 shows variations of the model parameter C'_m ($=\bar{\rho} \tilde{\epsilon}_c/\bar{\omega}_c + 0.5$) computed using Eq. (11) based on $\bar{\omega}_c$ and $\tilde{\epsilon}_c$ directly obtained from DNS. Here, $\bar{\omega}_c$ and $\tilde{\epsilon}_c$ are collected at the location of each probe P_i , (x_i, y_i, z_i) , when the probe observes reaction zones of the flame passing through. Thus, this plot includes effect of pressure evolution on turbulence–flame interaction at different times and locations. Clearly, C'_m shows values ~ 0.6 , and this value seems to be almost constant throughout the sampling period, suggesting that the turbulence–flame interaction

mechanism does not significantly change. Also, this suggests that the model parameter C_m does not need to be computed for different pressure instants. This constant variation of C'_m is shown for both c_T and c_Y . This indicates that once exact C_m is computed using Eq. (12) based on the initial mixture condition, the same parameter value can be used for the entire simulation period regardless of the change of mixture and turbulence conditions caused by the pressure rise as discussed in Fig. 5. Thus, this flamelet formulation for the averaged reaction rate could be also used in a pressure-evolving combustion system without further modifications. Note that similar results of C'_m were also obtained using a larger probe size, which is discussed in Sec. 3.1.

4. Conclusions

DNS of a stoichiometric hydrogen–air turbulent premixed flame in a rectangular constant volume vessel has been conducted to gain fundamental insights into turbulence–flame interactions and heat loss characteristics under a pressure rising condition.

The mean pressure increases up to 3.2 atm in the combustion process. The turbulence structures represented by the second invariant of the velocity gradient tensor are significantly weakened in the burnt region due to expansion while the velocity induced by expansion is observed in this region. The conditionally averaged k is suppressed near the wall and it takes mostly constant in the rest of the domain which suggests that there is no significant turbulence production near the wall, and the wall just damps the turbulence in the present configuration. The large k in the burnt side is mostly at-

tributed to the velocity induced by the expansion, not much inherent to the turbulence. In SI engines, there are both swirl and tumble flows during combustion. Since there is no mean flow in the present simulation's set up, the effects of mean flow on near wall turbulence production will be investigated in future research.

The contributions of the unburnt, reaction and burnt regions to the total heat loss to the wall are evaluated quantitatively. The heat loss through the reaction region (flame impingement) plays a major role in the early stage. The contribution of the burnt region (burnt gas) to the total heat loss becomes more pronounced in the later stage due to the increased area in this region. At the end, the heat loss through the reaction region is about 22% of the total heat loss. The burnt region is responsible about 72% of the total heat loss. Although these results show that the heat loss induced by the burnt gas is dominant in the combustion process, heat loss induced by the flame front (flame impingement) contributes to substantial portion of the total heat loss.

Finally, turbulence–flame interactions modeling is studied using Eq. (11). The model parameter shows almost constant values for entire domain and time. This suggests that turbulence–flame interaction mechanism does not unduly change under pressure rising conditions. Therefore, this model could be also used in a pressure-evolving combustion system without further modifications.

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References

- [1] S. Ratnak, J. Kusaka, Y. Daisho, K. Yoshimura, K. Nakama, *Int. J. Automotive Eng.* 6 (2015) 97 – 104.
- [2] B. Hoepke, S. Jannsen, E. Kasseris, W. Cheng, *SAE Int. J. Engines* 5 (2012) 547 – 559.
- [3] A. Cavaliere, M. de Joannon, *Prog. Energy Combust. Sci.* 30 (2004) 329–366.
- [4] M. Tanahashi, M. Fujimura, T. Miyauchi, *Proc. Combust. Inst.* 28 (2000) 529 – 535.
- [5] Y.-S. Shim, N. Fukushima, M. Shimura, Y. Nada, M. Tanahashi, T. Miyauchi, *Proc. Combust. Inst.* 34 (2013) 1383 – 1391.
- [6] A. Poludnenko, E. Oran, *Combust. Flame* 157 (2010) 995 – 1011.
- [7] Y.-S. Shim, S. Tanaka, M. Tanahashi, T. Miyauchi, *Proc. Combust. Inst.* 33 (2011) 1455 – 1462.
- [8] Y. Minamoto, N. Fukushima, M. Tanahashi, T. Miyauchi, T. D. Dunstan, N. Swaminathan, *Phys. Fluids* 23 (2011) 125107.

- [9] A. Gruber, R. Sankaran, E. R. Hawkes, J. H. Chen, *J. Fluid Mech.* 658 (2010) 5–32.
- [10] S. Tanaka, M. Shimura, N. Fukushima, M. Tanahashi, T. Miyauchi, *Proc. Combust. Inst.* 33 (2011) 3293 – 3300.
- [11] H. Wang, K. Luo, K. Qiu, S. Lu, J. Fan, *Int. J. Hydrogen Energy* 37 (2012) 5246 – 5256.
- [12] Y. Minamoto, K. Aoki, M. Tanahashi, N. Swaminathan, *Int. J. Hydrogen Energy* 40 (2015) 13604 – 13620.
- [13] M. Shimura, K. Yamawaki, N. Fukushima, Y. S. Shim, Y. Nada, M. Tanahashi, T. Miyauchi, *J. Turbulence* (2012) N42.
- [14] T. Jin, K. Luo, S. Lu, J. Fan, *Int. J. Hydrogen Energy* 38 (2013) 9886 – 9896.
- [15] K. Bray, *Symposium (International) on Combustion* 17 (1979) 223 – 233.
- [16] F. Dabireau, B. Cuenot, O. Vermorel, T. Poinso, *Combust. Flame* 135 (2003) 123 – 133.
- [17] R. Owston, V. Magi, J. Abraham, *Int. J. Hydrogen Energy* 32 (2007) 2094 – 2104.
- [18] B. Yenerdag, N. Fukushima, M. Shimura, M. Tanahashi, T. Miyauchi, *Proc. Combust. Inst.* 35 (2015) 1277–1285.

- [19] E. Gutheil, G. Balakrishnan, F. Williams, in: N. Peters, B. Rogg (Eds.), *Reduced Kinetic Mechanisms for Applications in Combustion Systems*, volume 15 of *Lecture Notes in Physics Monographs*, Springer Berlin Heidelberg, 1993, pp. 177–195.
- [20] R. J. Kee, G. Dixon-Lewis, J. Warnatz, M. E. Coltrin, J. A. Miller, Sandia National Laboratories (1986) Report No. SAND86-8246.
- [21] R. J. Kee, F. M. Rupley, J. A. Miller, Sandia National Laboratories (1989) Report No. SAND89-8009B.
- [22] S. K. Lele, *J. Comput. Phys.* 103 (1992) 16 – 42.
- [23] P. Brown, G. Byrne, A. Hindmarsh, *SIAM J. Sci. Stat. Comput.* 10 (1989) 1038–1051.
- [24] T. Poinso, S. Lele, *J. Comput. Phys.* 101 (1992) 104 – 129.
- [25] M. Baum, T. Poinso, D. Thevenin, *J. Comput. Phys.* 116 (1995) 247 – 261.
- [26] N. Peters, *Turbulent Combustion*, Cambridge Monographs on Mechanics, Cambridge University Press, 2000.
- [27] G. Borman, K. Nishiwaki, *Prog. Energy. Combust. Sci.* 13 (1987) 1 – 46.
- [28] N. Swaminathan, K. Bray, *Combust. Flame* 143 (2005) 549 – 565.
- [29] H. Kolla, J. W. Rogerson, N. Chakraborty, N. Swaminathan, *Combust. Sci. Technol.* 181 (2009) 518–535.

- [30] N. Chakraborty, N. Swaminathan, *Combust. Sci. Technol.* 182 (2010) 1201–1240.
- [31] T. Dunstan, Y. Minamoto, N. Chakraborty, N. Swaminathan, *Proc. Combust. Inst.* 34 (2013) 1193 – 1201.

Figure 1: The schematic of the numerical configuration with a high temperature ignition kernel in the center (red), and probe locations (shown one in every 4 probes).

Figure 2: Temporal development of the mean pressure in the vessel

Figure 3: Temporal developments of turbulence and flame structures. Bottom half of the computational domain is presented. White and gray iso-surfaces indicate the second invariant of velocity gradient tensor at 1.0×10^{10} and 1.0×10^9 ; note that gray surfaces are drawn only in the burnt side for visibility. Orange iso-surface presents the temperature at 1282 K. Color bar represents the heat flux through the lower wall.

Figure 4: Local combustion condition on the turbulent combustion diagram. The data points are computed from a probe P_i for entire sampling period, and the color changes from blue to red indicates the probe locations from the center of the vessel to the right wall.

Figure 5: Temporal developments of $\tilde{T}$ (a), $\tilde{Y}_{H_2}$ (b), ν (c) and η (d). Solid arrow indicates general trend of results when changing P_1 to P_{31} . Dashed arrow indicates the change of unburnt mixture condition due to pressure rise.

Figure 6: Temporal developments of velocity fields near the lower wall; velocity vectors at $y = 90 \mu m$. Bottom half of the computational domain is presented. Color bar represents the velocity magnitude. Orange iso-surface denotes the temperature at 1282 K.

Figure 7: Temporal developments of temperature distributions in the $x - y$ plane at $z = 10$ mm and the velocity profiles indicated by solid black lines, are drawn in x direction at different positions.

Figure 8: Profiles of the conditional averaged turbulent kinetic energy k in the unburnt and burnt sides of the domain which are separated by temperature iso-surface at $T = 1282$ K. The profiles of k from $t = 120 \mu s$ to $240 \mu s$ are averaged.

Figure 9: Distributions of wall heat flux (a, b, c) and mass fraction of H_2O (d, e, f) on the lower wall. The color bars indicate that ϕ_q^* and $Y_{H_2O}^*$ are normalized by their instantaneous maximum values. Separation of unburnt, reaction and burnt regions (g, h, i), three regions are determined based on the corresponding Y_{H_2O} distribution on the lower wall.

Figure 10: Mean values of wall heat flux through the lower wall of unburnt, reaction and burnt regions (a), instantaneous total heat loss through the lower wall of unburnt, reaction and burnt regions (b), temporal development of the surface area on the lower wall of each region (c), temporal development of total heat loss of each region (d).

Figure 11: The model parameter C'_m based on c_T and c_Y as a function of the location of probe P_i when $\bar{\omega}_c$ is the maximum.