Numerical Study on the Effects of Turbulence Scale on Spherically Propagating Hydrogen Flames within Multiple Flame Radii

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ABSTRACT: Three-dimensional direct numerical simulations of spherically propagating premixed turbulent hydrogen flames were carried out to clarify the influence of turbulence scale on propagating hydrogen/air flame. In a previous study (1), results suggested that an optimum integral length scale exists to promote flame propagation, with which the maximum burning velocity was obtained. This study investigates the influence of variation of turbulence scale on turbulent flame propagation and burning velocity within multiple turbulent flame radii. Results of the work suggest that an integral length scale was found where the maximum turbulent burning velocity exist. Also, it got larger as flame propagated.

KEY WORDS: Heat Engine, Spark Ignition Engine, Combustion Analysis Hydrogen Flame, Turbulence scale (A1)

1. Introduction

Turbulence has significant influence on flame in both structure and propagation. Turbulence intensity and scale have the major contribution on premixed turbulent combustion. Peters categorized premixed turbulent flame characteristics, by considering those two parameters, into several regimes (2).

Turbulent eddies may wrinkle and/or distort the flame front and increase its area. An increase in flame front area will result in increasing the turbulent burning velocity. In itself, the turbulent burning velocity has become a basic feature of premixed turbulent combustion. Hence, it received considerable attention through decades of research.

Most of those investigations were dedicated to examining the influences of turbulence intensity on flame development and burning velocity. The influence of moderate turbulence intensity on turbulent burning velocity is well established through numerous experimental researches (3), (4). As turbulence intensity increases, turbulent burning velocity increases. The increment is reasoned to the gain in local flame front area by turbulent eddies (5).

On the other hand, direct experimental researches related to turbulence scale and its implications on premixed flame combustion are scarce. In an early study, Ballal and Lefebvre (6) have investigated premixed combustion in a grid generated turbulence in a channel. They investigated a variety of turbulence scales within three turbulence intensity regions; weak, intermediate and strong turbulence. While maintaining turbulence intensity constant in each of those regions, integral length scale was varied and burning velocity was obtained. In the weak turbulence region, burning velocity increased linearly with the increase in turbulence scale. In the intermediate turbulence intensity region, turbulence scale had no influence on flame structure and burning velocity. In the strong turbulence region, burning velocity declined with the increase in turbulence scale. Ting et al. (7) did their investigation in a more applicable setting. They considered flame propagation ignited with a spark in a spatially uniform, decaying turbulence in a similarity to what can be found in engine combustion chambers. They varied turbulence scale using different moving grids to generate turbulence. While maintaining all other variables constant, burning velocity decreased with increasing turbulence scale. In a recent numerical study, Fogla et al. (8) investigated multiple combinations of initial turbulence intensities and scales in a two-dimensional flow field. For weak turbulence intensities, a favorable turbulence scales were found, with which a maximum burning velocity can be obtained.

Since available data on the topic of turbulence scale and its influence on the development of premixed flames and burning velocities are limited and are in real need to be updated. This research is committed to focus on such topic. As recent computational capabilities got remarkably developed, leading to the possibility of simulating premixed combustion with detailed chemistry in three-dimensional flow fields (9). In this research, spherically propagating premixed hydrogen/air flames were investigated using three-dimensional direct numerical simulation. The aim is to investigate the influence of turbulence scale,
characterized by integral length scale, on spherically propagating flame with intermediate turbulence intensity.

Hydrogen and hydrogen-enriched fuels has received substantial interest in recent years. Those fuels are considered as clean alternative to conventional petroleum and natural gas fuels. Hence, the focus on hydrogen/air flames in this study.

2. Methodology

By utilizing direct numerical simulations, spherically propagating hydrogen/air premixed turbulent flames were investigated. The considered flow is a compressible reactive flow, and can be described using the following governing equation, Eqs. (1-5).

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \mathbf{P} + \nabla \cdot \mathbf{\sigma}
\]

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \mathbf{u}) = \nabla \cdot (\rho D_k \nabla T) + \dot{\omega}
\]

\[
\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \mathbf{u}) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}
\]

Hydrogen/air flames were implemented using an improved H2-O2 reaction mechanism by Hong et al. An in-house code, FK3, was used in this study. The premixed turbulent flames propagated in a three-dimensional cubical geometry. Each edge was set to 60 mm in length, and resolved within 600 grids, resulting in a grid resolution of 0.10 mm per grid.

A high temperature region was placed at the center of the computational domain, as a substitute for spark energy. The high temperature region had a spherical geometry with an outer diameter of 3.0 mm, and contained unburned mixture with a maximum temperature of 1500 K. This maximum temperature was set throughout the spherical geometry, from the center of the region to an outer diameter of 1.5 mm.

Homogeneous and isotropic turbulent flows introduced to the domain were generated through spectral method based on the energy spectrum function in Eq. (6) (12).

\[
E(k) = \frac{32}{3} \left( \frac{2 n^2}{k_e} \right)^{3/2} \exp \left[ -2 \left( \frac{k}{k_e} \right)^2 \right]
\]

Where \( k_e \) was calculated with corresponding to the desired integral length scale as in Eq. (7) (13).

\[
k_e = \frac{8}{3T} \sqrt{\frac{2}{\pi}}
\]

Periodic conditions were imposed on all boundaries of the computational domain. The governing equations were discretized using second-order central finite difference scheme in all directions. QUICK scheme was implemented for species transport.

As for time integration, it was carried out using third order Runge-Kutta scheme.

Premixed turbulent hydrogen/air flames were investigated in stoichiometric conditions, \( \phi = 1.0 \), with an initial temperature, \( T_i \) and pressure, \( P_i \) of 298 K and 0.10 MPa respectively. Four turbulent conditions were investigated, as listed in Table 1, with a moderate turbulence intensity of \( u' = 4.0 \text{ m/s} \), and four integral length scales, \( l = 0.4, 0.6, 0.8, 1.0 \text{ mm} \). A preliminary computation was conducted to ensure that total kinetic energy is maintained by the end of combustion event. Hence, a non-reactive freely decaying turbulent flow was simulated with the initial turbulent field of case A04 as it holds the fastest energy decay rate within computing conditions. Result of that computation showed that total kinetic energy was maintained at a reasonable value.

Figure 1 shows all initial conditions on Peters diagram. All computed cases fall within the corrugated flame regime. Flame thickness, \( \delta \) here follows Peters definition as shown in Eq. (8).

\[
\delta = \frac{\gamma}{u_l}
\]

| Condition | \( u' \) | \( l \) | \( \eta \) |
|-----------|-------|-----|---|
| A04       | 4.0 m/s | 0.4 mm | 0.042 mm |
| A06       | 4.0 m/s | 0.6 mm | 0.051 mm |
| A08       | 4.0 m/s | 0.8 mm | 0.059 mm |
| A10       | 4.0 m/s | 1.0 mm | 0.066 mm |

Fig. 1: Peters Diagram showing all investigated premixed turbulent flames

Laminar burning velocities of hydrogen/air flame was obtained by means of propagating premixed laminar flame. The computation was done for stoichiometric condition with the same initial pressure and temperatures as turbulent conditions.
Symmetric conditions were applied to all boundaries of the domain. Laminar burning velocity, for spherically propagating flames, was obtained from the evolution of laminar flame radius, $r_f$, following Eq. (9).

$$u_a = \frac{\rho_b}{\rho_u} \frac{d r_f}{d t} \quad (9)$$

Obtained laminar burning velocity in Eq. (9) was subjected to flame stretch. Flame front curvature and hydrodynamic strain are sources of flame stretch $^{(14),(15)}$. Flame stretch rate, which is the time rate of change of flame front area per unit area was calculated as in Eq. (10).

$$\alpha = \frac{1}{A_f} \frac{dA_f}{dt} = \frac{2}{r_f} \frac{d r_f}{d t} \quad (10)$$

Following experimental approach, the unstretched laminar burning velocity, $u_t$, was then obtained for a stretch rate of zero $^{(16)}$.

The instantaneous turbulent burning velocity, $u_t$, of spherically propagating premixed turbulent flame was obtained from evolution of mean turbulent flame radius of $r_{tf}$ as in Eq. (11).

$$u_t = \frac{\rho_b}{\rho_u} \frac{d r_{tf}}{d t} \quad (11)$$

In experimental approach $^{(17)}$, mean turbulent flame radius, $r_{tf}$ was derived from a spherical surface with an equivalent volume to the reconstructed flame volume. The flame volume was reconstructed by using simultaneous Mie-scattering tomography and 2-Views Schlieren technique. In a similar manner, we derived mean turbulent flame radius from the sphere of volume equivalent to the burned gas volume. Burned gas volume was defined to be all volume within the flame front. Flame front was defined as an isotherm of 1000 K.

### 3. Results and discussion

#### 3.1. Laminar burning velocity

Laminar burning velocity for hydrogen/air flame is shown in Fig. 2. At early stage of flame development, burning velocity was affected by energy release of high temperature region. Hence, those values were not recorded. As laminar flame propagated, that effect decayed and burning velocity monotonically increased.

Laminar burning velocity was plotted against its corresponding flame stretch rate in Fig. 3. Unstretched laminar burning velocity, $u_t$, was obtained by extrapolating to flame stretch rate of zero. Obtained value was the same as in experimental results $^{(16),(18)}$.

#### 3.2. Turbulent burning velocity

Figure 4 shows the time history of turbulent burning velocities. Burning velocities varied based on integral length scale for each case. Fully developed burning velocities were not obtained except for the case of $l =$0.4 mm, A04. It can be seen in the figure that at early stage of flame development, turbulent flame of the case of $l =$0.4 mm, A04 had the largest burning velocity value. Later on, and as flame propagated, turbulent flame of the case of $l =$0.6 mm, A06 had the largest burning velocity value. Simultaneously, burning velocity of case of $l =$0.4 mm, A04 stopped increasing.
a) Developed turbulent flame at radius of 10 mm
b) Developed turbulent flame at radius of 12.5 mm
c) Developed turbulent flame at radius of 15 mm

Fig. 5: Flame front contours, represented by 1000 K isotherm, at the upper panels, and two-dimensional slices of temperature profile at the lower panels
That change is contributed to turbulent eddies and their interaction with flame front as flame propagated, as will be explained later on.

In order to investigate the impact of integral length scale on flame front-turbulent eddies interactions and burning velocity, turbulent flames with an equivalent flame radius of 10, 12.5 and 15 mm were investigated.

Morphology and temperature profiles of all computed conditions are shown in Fig. 5. In all cases, the initially spherical flame got quickly perturbed through interactions between turbulent eddies and flame front, and wrinkling structure started to appear. Wrinkling formation got more complex as flame propagated. That can be seen through the increase in wrinkles’ count with time. However, a distinctive difference between all cases was clearly observed. Although quantitative analysis of wrinkles had not been done, it is seen through visual observation that wrinkles formed on flame fronts were different in their relative lengths and count. For the case of \( l = 0.4 \) mm, A04, formed wrinkles were relatively the smallest in length and largest in count, while those formed in the case of \( l = 1.0 \) mm, A10 were the largest in length and least in count. That is a reasonable observation since interacting turbulent eddies had the smallest integral length scale in the case of \( l = 0.4 \) mm, A04, and the largest in the case of \( l = 1.0 \) mm, A10.

Figure 6 shows the variation of turbulent burning velocity with integral length scale for multiple mean turbulent flame radii. By looking at the line of mean turbulent flame radius of 10 mm, as integral length scale increased, turbulent burning velocity decreased. Since the case of \( l = 0.4 \) mm, A04 had the smallest turbulent eddies within computed conditions, those eddies made more wrinkles on flame front. Thus, flame front area was larger than other cases. Therefore, and within computed conditions, the maximum turbulent burning velocity for flames with mean turbulent flame radius of 10 mm was obtained for the case of \( l = 0.4 \) mm, A04.

As flames grew larger, and for mean turbulent flame radius of 12.5 mm, all burning velocities increased. However, the maximum burning velocity belonged to the case of \( l = 0.6 \) mm, A06. That means, making more wrinkles on the flame front for the case of \( l = 0.4 \) mm, A04 was not enough to obtain the maximum turbulent burning velocity. Clearly, there is a relative connection between turbulent eddies size and flame front area. If flame front area is small, then small turbulent eddies are effective to obtain the maximum burning velocity. As flame grew larger, larger turbulent eddies would be the effective ones to obtain the maximum turbulent burning velocity.

Looking at flames with mean turbulent flame radius of 15 mm, although all burning velocities increased, for the case of \( l = 0.4 \) mm, A04 that increment was insignificant. Turbulent eddies of this size had no further contribution on flame front, as flame front grew too large compared to turbulent eddies’ size. Hence, burning velocity value stopped increasing in Fig. 4. The maximum burning velocity belonged to the case of \( l = 0.6 \) mm, A06. At the same time, burning velocity of the case \( l = 0.8 \) mm, A08 was almost as large.

Thus, it can be easily perceived that, soon after ignition, turbulent eddies with small integral length scale hugely contributed in wrinkling the flame front. Therefore, increasing its’ area and turbulent burning velocity. While turbulent eddies with large integral length scale would hardly wrinkle the flame front. Therefore, their contribution to increase the flame front area and turbulent burning velocity was limited.

Soon after that, and as flame propagated, it reached an adequate size to be able to experience the contribution of turbulent eddies with large integral length scale. Thus, wrinkling of the flame front increased. And with it, the area of the flame front and turbulent burning velocity got increased. At the same time, turbulent eddies with small integral length scale had no further influence on the flame front; to increase its’ area nor turbulent burning velocity.

4. Conclusion

In this study, influence of integral length scale on spherically propagating premixed hydrogen/air flames was investigated using three-dimensional direct numerical simulation. Computed conditions were within the corrugated flamlets, with a single moderate turbulence intensity, and four different integral length scales.

Varying integral length scale influenced wrinkle formation on turbulent flame front. As integral length scale increased, number of wrinkles formed on flame front decreased, and length of wrinkles increased.
Within computed conditions, an integral length scale was found, where the maximum turbulent burning velocity is associated. For mean turbulent flame radius of 10 mm, that integral length scale was $l=0.4$ mm. As flame propagated, it grew larger to $l=0.6$ mm. There is a clear relation between flame front area and turbulent eddies’ size. Turbulent eddies with small integral length scale hugely contributed in wrinkling the flame front of initially ignited flame. Therefore, increasing its area and turbulent burning velocity. Thereafter, and as the flame reached an adequate size, it could experience the contribution of turbulent eddies with large integral length scale. Thus, wrinkling of the flame front increased. And with it, the flame front area and turbulent burning velocity increased.

### Nomenclature

- $A_F$: Flame front area
- $C_P$: Specific heat at constant pressure
- $D_k$: Diffusivity coefficient of species $k$
- $E(k)$: Turbulent kinetic energy spectrum
- $h$: Enthalpy
- $J_h$: Enthalpy transport coefficient of diffusive fluxes
- $k$: Wavenumber corresponding to $l$
- $k_z$: Wavenumber corresponding to desired $l$
- $K_a$: Karlovitz number
- $l$: Integral length scale
- $P$: Pressure
- $P_i$: Unburned mixture initial pressure
- $R$: Universal gas constant
- $r_f$: Laminar flame radius
- $r_{f,z}$: Mean turbulent flame radius
- $Re$: Reynolds number
- $T$: Temperature
- $T_i$: Unburned mixture initial temperature
- $t$: Time
- $u$: Fluid velocity vector
- $u'$: Turbulence intensity
- $u_n$: Stretched laminar burning velocity
- $u_l$: Unstretched laminar burning velocity
- $u_t$: Turbulent burning velocity
- $Y_k$: Mass fraction of species $k$

### Greek symbols

- $\alpha$: Flame stretch rate
- $\delta$: Flame thickness
- $\eta$: Kolmogorov length scale
- $\omega$: Source term due to reactions
- $\lambda$: Thermal conductivity
- $\nu$: Kinematic viscosity
- $\rho$: Density
- $\rho_b$: Burned gas density
- $\rho_u$: Unburned mixture density
- $\sigma$: Viscous stress tensor
- $\phi$: Equivalence ratio

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