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LARGE EDDY SIMULATION OF HYDROGEN-AIR PROPAGATING FLAMES

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Abstract

The future use of hydrogen as a clean fuel and an energy carrier brings in safety issues that have to be addressed before community acceptance can be achieved. In this regard, availability of accurate modeling techniques is very useful. This paper presents large eddy simulations (LES) of propagating turbulent premixed flames of hydrogen-air mixtures in a laboratory scale combustion chamber. A Dynamic flame surface density (DFSD) model where the reaction rate is coupled with the fractal analysis of the flame front structure, is implemented and tested. The fractal dimension is evaluated dynamically based on the instantaneous flow field. The main focus of the current work is to establish the LES technique as a good numerical tool to calculate turbulent premixed hydrogen flames having an equivalence ratio of 0.7. Developing this capability has practical importance in analyzing explosion hazards, internal combustion engines and gas turbine combustors. The results obtained with the DFSD model are compare well with published experimental data. Further investigations are planned to examine and validate the LES-DFSD model for different flow geometries with hydrogen combustion.

Introduction

The environmental concerns of fossil fuel combustion have generated interest in hydrogen as a suitable replacement fuel and an energy carrier. This is because of its availability from many resources and zero carbon emissions. However, to enable its widespread usage in practical applications, tough challenges must be overcome regarding hydrogen and further studies are needed to develop an improved understanding of the issues affecting the generation, storage, distribution as well as combustion of hydrogen. The objective of the present work is to contribute to hydrogen safety by developing numerical capabilities to compute the overpressures resulting from hydrogen combustion. The study uses the large eddy simulation technique to calculate the structure of lean hydrogen flames propagating inside a vented chamber while interacting with solid obstructions. The results are validated against experimental measurements reported by Masri et al [8].

Large Eddy Simulation (LES) technique is now accepted as a high fidelity computational tool to study turbulent flames both premixed and non-premixed [1-6] despite its added computational cost. A key advantage of LES lies in its ability to compute the complex dynamics of turbulent flows and resolve transient processes such as flame propagation, instability, extinction, as well as ignition. The cost and accuracy of LES solutions lie between DNS and RANS techniques. A crucial challenge to the advancement of LES lies in the development of adequate sub-grid-scale (SGS) models, which are capable of representing combustion over a wide range of flow and combustion conditions. This paper makes a contribution towards this objective.

As the reaction zone thickness of the premixed flame to be resolved is thin, with a characteristic length scale much smaller than a typical LES filter width, an appropriate SGS model is vital to account for chemical reaction. Earlier studies [7, 8] using DFSD model based on laminar flamelets were promising in predicting key characteristics of propagating turbulent premixed flames with built-in solid obstructions. The work presented in this paper is a continuation of previous research [7, 8] where progress has been made in the development of a dynamic flame surface density (DFSD) model to account for the SGS chemical reaction rate. Here, the same strategy is applied where the DFSD model is used to simulate transient turbulent premixed flames of a hydrogen-air mixture with equivalence ratio of 0.7, propagating in a small vented chamber having 3 baffles and a square solid obstacle. The experimental test facility [9] offers the capability to configure various geometries with a range of turbulent flow conditions. The LES, simulations use a grid independent resolution and the results are validated against the available experimental data.

Test Case

The experimental chamber used in this study was developed by the University of Sydney, Australia [9]. The combustion chamber has dimensions of 50 x 50 x 250 mm and consists of 3 baffle plates located at equidistance and a solid square obstacle of size 12 x 12 mm at about 96 mm from the ignition end (Figure 1a). In the experiments the hydrogen-air mixture enters the atmospheric pressure chamber, where the mixture is allowed to settle before being ignited by focusing the infrared output from a Nd:YAG laser 2 mm above the base. A hinged flap on top of the chamber contains the mixture during fill time prior to ignition. This flap is raised just before ignition and is maintained through the combustion process to allow venting.

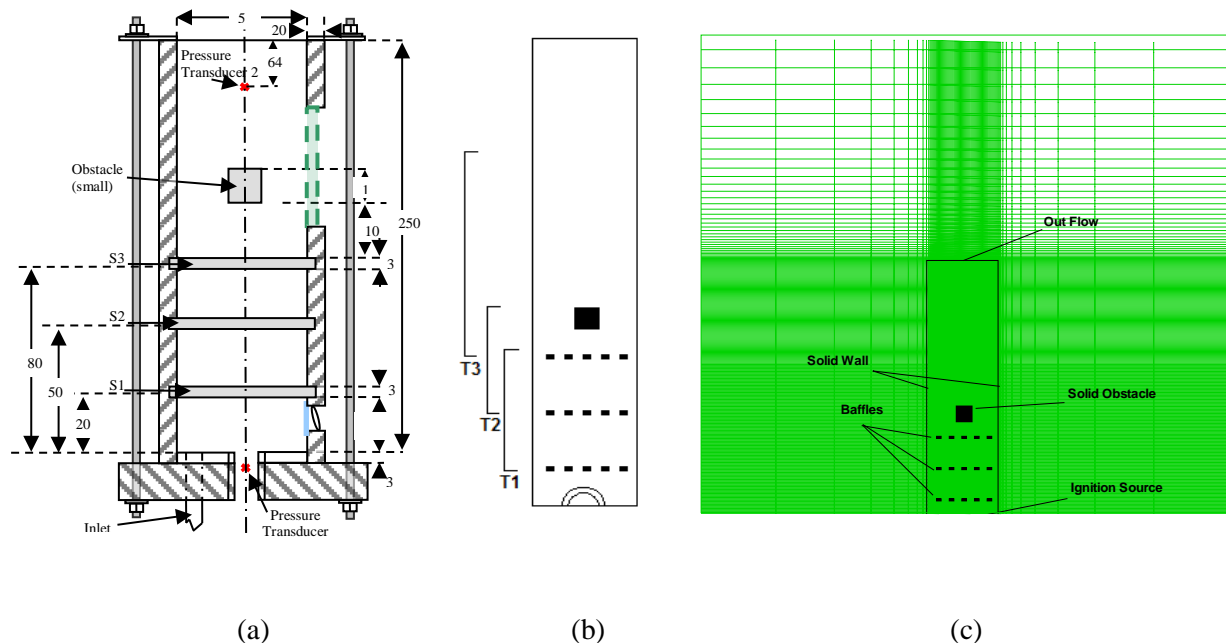


Figure 1. (a) Schematic diagram for the Sydney combustion chamber. (b) The three imaging tiers used to capture the maximum viewable height [9]. (c) Illustration of the computational domain with the combustion chamber and the obstacles are superimposed over grid resolution.

The LES Model

In LES, modelling the mean chemical reaction rate in turbulent premixed flames is very challenging due to its non-linear relation with chemical and thermodynamic states. It is often characterized by propagating thin reaction layers thinner than the smallest turbulent scales. In the present simulations, the SGS chemical reaction rate is accounted for by using a recently developed DFSD model [2, 7, 8] modified for hydrogen flames. Brief details of the model are given here. More details can be found elsewhere [7].

The mean SGS chemical reaction rate ($\bar{\omega}_c$) is the source term, which is modelled by following the laminar flamelet approach as:

$$\bar{\omega}_c = \rho_u u_L \bar{\Sigma} \quad (1)$$

Where (ρ_u) is the density of unburned mixture, (u_L) is the laminar burning velocity, and (Σ) is the flame surface density (FSD). The filtered flame surface density in Eq. (1) can be split into two terms as resolved and unresolved:

$$\bar{\Sigma} = |\bar{\nabla}c| = \underbrace{\Pi(\bar{c}, \bar{\Delta})}_{Resolved} + \underbrace{f(\bar{c}, \bar{\Delta}, \Pi(\bar{c}, \bar{\Delta}))}_{Unresolved} \quad (2)$$

Where (\bar{c}) is the mean reaction progress variable, ($\bar{\Delta}$) is the filter width. The over-bar describes application of the spatial filter. The unresolved term in the above equation is evaluated using the following expression:

$$\lambda = \bar{\Sigma} - \Pi(\bar{c}, \bar{\Delta}) = |\bar{\nabla}c| - \Pi(\bar{c}, \bar{\Delta}) \quad (3)$$

Defining (γ) as a ratio of test filter to grid filter, taken here equals 2 and applying the test filter ($\hat{\cdot}$) to flame surface density Eq. (2) leads to:

$$\hat{\bar{\Sigma}} = |\hat{\nabla}c| = \underbrace{\Pi(\hat{c}, \hat{\Delta})}_{Resolved\ at\ test\ filter} + \underbrace{[|\hat{\nabla}c| - \Pi(\hat{c}, \hat{\Delta})]}_{Unresolved\ at\ test\ filter} \quad (4)$$

From the above equation, the unresolved flame surface density contribution at the test filter level can be written as:

$$\Lambda = [|\hat{\nabla}c| - \Pi(\hat{c}, \hat{\Delta})] \quad (5)$$

Assuming the sub-grid scale contribution of unresolved flame surface density at test filter is the same as that at grid filter and relating (λ) and (Λ) by using Germano identity [10]:

$$\begin{aligned} \Lambda - \hat{\lambda} &= [|\hat{\nabla}c| - \Pi(\hat{c}, \hat{\Delta})] - [|\bar{\nabla}c| - \Pi(\bar{c}, \bar{\Delta})] \\ \Lambda - \hat{\lambda} &= [\Pi(\bar{c}, \bar{\Delta}) - \Pi(\hat{c}, \hat{\Delta})] \end{aligned} \quad (6)$$

The sub-grid scale flame surface density contribution from the above equation can be added to the resolved flame surface density in Eq. (4) with a model coefficient (C_s) in order to obtain total flame surface density. Hence the flame surface density can be expressed as:

$$\bar{\Sigma} = \Pi(\bar{c}, \bar{\Delta}) + C_s [\Pi(\bar{c}, \bar{\Delta}) - \Pi(\hat{c}, \hat{\Delta})] \quad (7)$$

The model coefficient (C_s) in above equation is dynamically obtained by identifying sub-grid scale flame surface as a fractal surface [4] as follows:

$$C_s = \frac{1}{1-\gamma^{2-D}} \left[\left(\frac{\bar{\Delta}}{\delta_c} \right)^{D-2} - 1 \right] \quad (8)$$

Where (δ_c) is the lower cut-off scale, (γ) is the ratio of test filter to grid filter and (D) is the fractal dimension, calculated dynamically from [2].

$$D = 2.0 + \frac{\log(\langle \Pi(\bar{c}, \bar{\Delta}) \rangle / \langle \Pi(\hat{c}, \hat{\Delta}) \rangle)}{\log(\hat{\Delta} / \bar{\Delta})} \quad (9)$$

The angular brackets ' $\langle \rangle$ ' in the previous equation indicates conditional averaging within the flame bounded by $\bar{c} = 0$ to $\bar{c} = 1$.

The other parameters used in the LES are summarized in the following table:

Table 1. Model parameters used in the present work

Equivalence ratio	$\Phi = 0.7$
Lower Heating Value (kJ/kmol)	286,000
Un-strained laminar burning velocity (m/s)	1.3
Ignition radius (mm)	3.0

The numerical model described above, has been implemented using a modified in-house LES code [10]. The numerical results presented in this work are carried out using a grid independent resolution of 90 x 90 x 336 (2.7 million) cells in 3 dimensional space (Figure 1c). The simulations are performed using an initially stagnant hydrogen-air mixture of equivalence ratio $\Phi = 0.7$. Other mathematical details of the code are not described here but available in our earlier publications [7, 8].

Flame Structure

Figure 2 shows a sequence of images for the development of the propagating flame at different times after ignition from the numerically obtained reaction rate contours compared with the measured LIF-OH images [9]. It is clear (not shown in experimental images), that the leading edge of the flame starts to expand hemi-spherically in the axial direction and the flame edge elongates in the radial direction. Once the flame hits the baffle plate, the laminar hemi-spherical structure is distorted and flame starts protruding through narrow vents. As a result, the surface area of the flame brush increases, hence, consumes more fuel/air mixture per unit time and propagates at relatively higher velocity through the un-burnt fuel/air mixture.

It is obvious that the LES technique is capable of reproducing turbulent flame structure and the propagation rate with high level of accuracy. For instance at 4.2 ms, both LES and

measurements demonstrate the entrainment of un-burnt mixture on the upstream edge of the obstacle as it is surrounded by the flame. This trapped mixture is seen to burn between 4.2 and 4.4 ms. However, there is some un-burnt mixture trapped in the formed recirculation zone downstream the solid obstacle and this burns after the leading edge of the flame has exited the chamber. It should be noticed here that experimental images are captured using the defined image tiers as shown in (Figure 1b) [9].

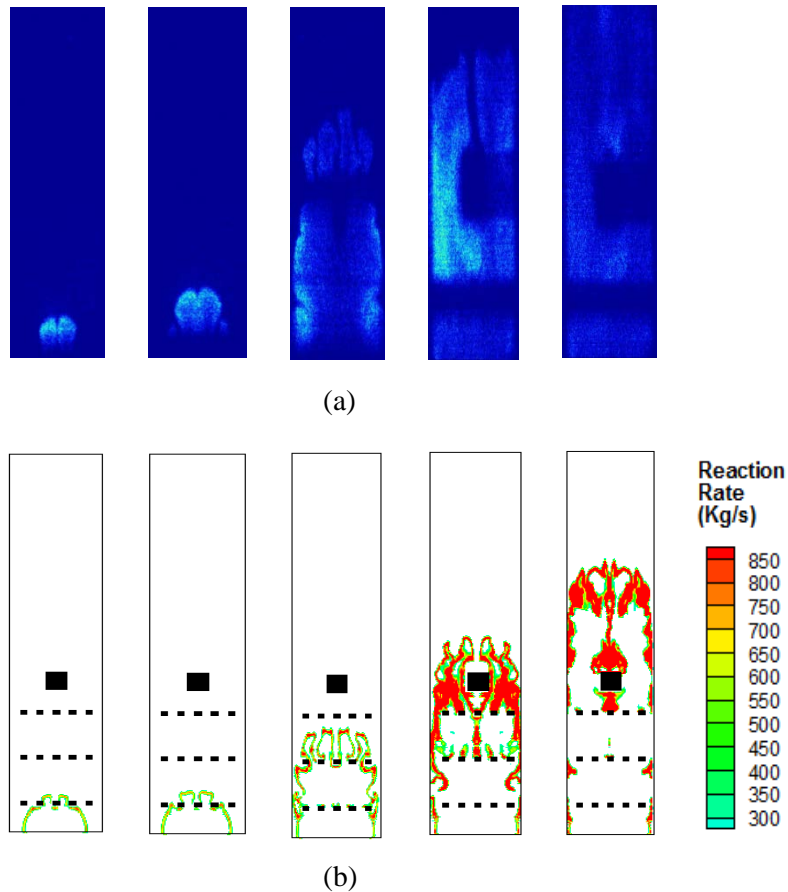


Figure 2. Comparison between sequence of images showing flame structure after ignition. (a) LIF-OH images from experiments [9]. (b) Numerical snapshots for reaction rate contours generated at 2.2, 2.4, 3.6, 4.2 and 4.4 ms.

Results and Discussions

Before going through the results in Figures 4 & 5, an optimization for the ignition source is required. Hence, the analysis shown in Figure 3 is used to provide the most suitable ignition radius. It is found that the peak overpressure is independent of the ignition radius. The only effect found is in the timing of occurrence for the maximum pressure. The ignition radius which found to be most suitable to represent the early phase of flame propagation is 3 mm. Also, for the same ignition area, the shape (i.e. hemi-spherical or spherical) has no effect on either the overpressure or the timing of occurrence, as both shapes have exactly overlapped (as for 3 mm case).

Figures 4 & 5 compare between numerical and published experimental [9] results in terms of time histories for overpressure and flame position. It can be seen that the predicted overpressure shows encouraging comparisons against experimental data. The time traces in

Figure 4 shows that, from LES the peak pressure prediction is about 721 mbar and the experimental measurements is 778 mbar. The peak over pressure in LES and experiments correspond to the reconnection of the flame after the square obstacle and burning of trapped un-burnt gases down and upstream of the obstruction. It should be noted here that, the time shift between the experimental and LES is about 0.43 ms. This discrepancy may be due to the difficulty in establishing the exact time of ignition in the experiments. However, in the LES predictions, ignition is initialized by setting reaction progress variable to 0.5 within a certain radius (3 mm radius is used here) at the start of the computations, i.e. time 0 ms. Figure 5 shows the comparison of predicted and measured time history of the flame position relevant to the ignition closed end. It can be seen that the agreement is remarkably good after some initial discrepancy. This again may be due to the uncertainty and modeling assumptions during the initial phase of flame propagation. These are to be further analysed and improved in further studies.

Conclusion

Overall, good agreements are obtained between the LES predictions and measurements for the case considered here. This proves the ability of the LES based DFSD model to predict characteristics of hydrogen premixed flames. Further extensive work is in progress to validate the model for different flow and combustion configurations.

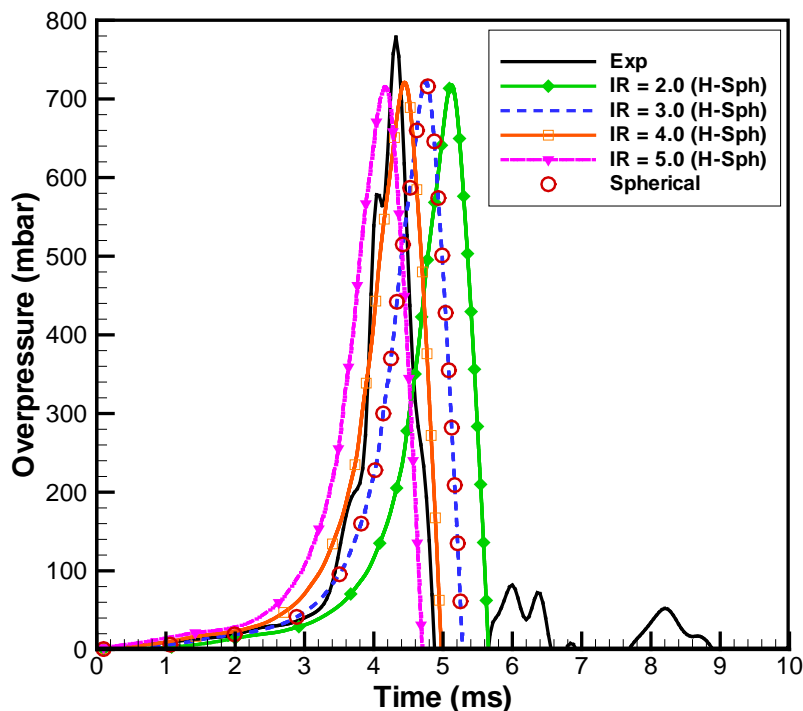


Figure 3. Overpressure time traces of LES simulations using different ignition radii and shapes (IR: Ignition Radius, H-Sph: Hemi-Spherical shape).

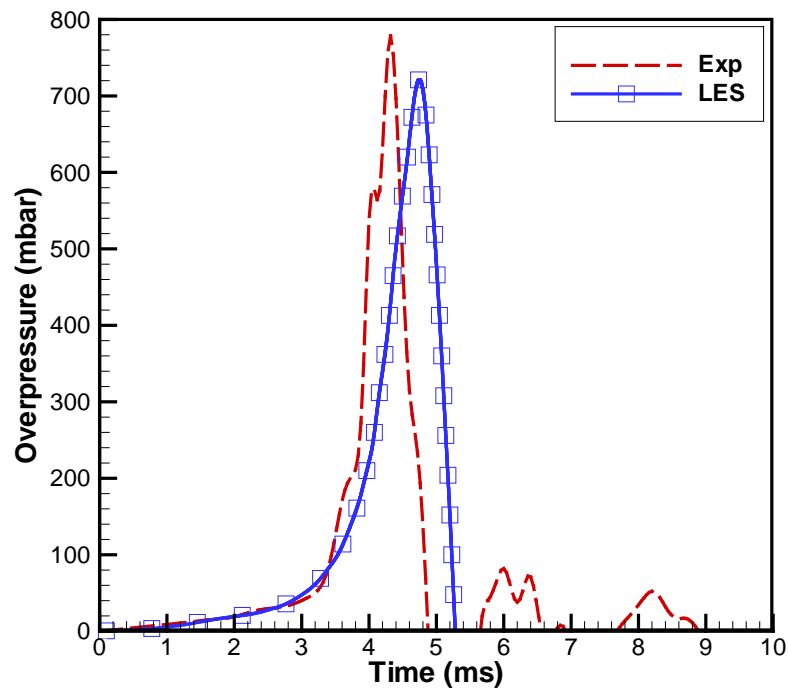


Figure 4. Overpressure time traces of LES simulation compared with experimental data [9].

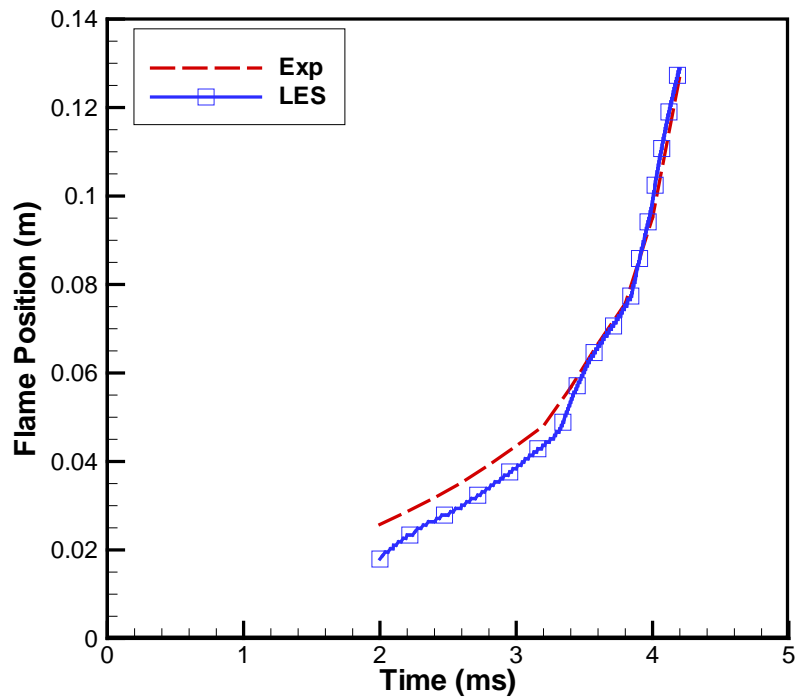


Figure 5. Flame position time traces of LES simulation compared with experimental data [9].

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