Proceedings of the 7th World Congress on Momentum, Heat and Mass Transfer (MHMT'22)
~~Lisbon, Portugal~~ Virtual Conference – April 07 – 09, 2022
Paper No. ICMFHT 129
DOI: 10.11159/icmfht22.129

Numerical Studies of Hydrogen and LPG Turbulent Premixed Flames

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Abstract **-** This paper presents numerical studies of turbulent premixed flames for lean hydrogen and stoichiometric LPG mixtures. The transient flames under investigation propagate past repeated solid baffle plate(s) and a square obstruction with varied area blockage ratios in a lab-scale combustion chamber. The chamber allows for up to three removable baffle plates to be equipped in addition to a square obstacle to increase turbulence intensity within the chamber. The hydrogen mixture is studied at an equivalence ratio of 0.7 and the LPG mixture is investigated at an equivalence ratio of 1.0. An in-house computational fluid dynamics (CFD) model is applied to numerically evaluate transient flame propagation. The large eddy simulation (LES) technique is applied for turbulence modelling. Reaction rate calculations are carried out using a dynamic flamelet model for turbulent premixed flames. Four flow configurations with different area blockage ratios (ABRs) are used to investigate combustion overpressure. Numerical results are compared against published experimental data to ascertain the ability of the numerical model in reproducing key combustion events for hydrogen and LPG. A conclusion is drawn that the increase in blockage ratio raises peak combustion overpressure and the maximum rate of pressure rise. Hydrogen combustion, albeit at a lower equivalence ratio, results in higher maximum overpressures and peak rate of pressure rise when compared with LPG.

Keywords**:** Combustion, hydrogen, dynamic flame surface density, large eddy simulation, area blockage ratio, LPG.

1. Introduction

While hydrocarbons remain the main source of energy in most economies, emission legislation is resulting in funding and research being invested towards alternative and renewable energy sources. Hydrogen is a renewal fuel, which unlike hydrocarbons, does not produce emissions as a result of the combustion process. As a fuel, hydrogen produces significantly higher combustion overpressures, and has a wide flammability range and a low requirement for ignition energy when compared with fuels such as LPG. In this study and in several application, the overpressure generated from combustion occurs as a result of obstacles in the path of the flame which generate a turbulent flow. The danger is increased when there are multiple or repeated obstruction in the path of the transient flame.

Numerical results presented in this paper are validated against published experimental data produced using a lab-scale combustion chamber configured at The University of Sydney in Australia [1]. Experimental data indicates that hydrogen produces significantly higher overpressures and flame speeds when compared with CNG and LPG. Additionally, experiments concluded that decreased obstacle separation distances and using a higher obstacle Area Blockage Ratio (ABR) leads to higher peak combustion overpressure, increased maximum rate of pressure rise and higher flame speeds.

Computational fluid dynamics (CFD) through various approaches of numerical modelling has become a plausible alternative to expensive, dangerous and time-consuming experiments [2]. The large eddy simulation (LES) approach has been used with the dynamic flame surface density (DFSD) model and a suitable sub-grid scale (SGS) to study turbulent premixed flames for configurations using a solid obstacle with an ABR of 0.24. The Reynolds-Averaged Navier-Stokes approach is capable of producing results in a relatively small timeframe, however the averaging nature of this approach means that it is usually only applicable to large-scale applications. On the other hand, direct numerical simulations (DNS) can produce very accurate results, however it typically requires a significant amount of computational resources. Published numerical results confirm the capability of the LES technique and DFSD model to produce results for hydrogen and LPG turbulent premixed flames [3], [4].This paper further investigates turbulent premixed flames for a lean hydrogen mixture and a stoichiometric LPG mixture, comparing both mixtures and impact of an increased ABR through the combustion overpressure and flame speeds.

2. Experimental Setup

Experimental data obtained from the lab-scale combustion chamber at The University of Sydney in Australia is used to validate numerical results [1], [5], [6]. The combustion chamber measures 50 x 50 x 250 mm and has a volume of 0.625 litres. The chamber can be equipped with three interchangeable baffle plates and a small or large square obstacle. Baffles can be placed 19 mm, 49 mm and 79 mm for the chamber base. Each baffle is 3mm thick and is made of 5 strips which are 4 mm in width with 5 mm gaps resulting in an ABR of 0.4. The square obstacle is positioned 96 mm from the base of the chamber. The small square obstacle has a side length of 12 mm for an ABR of 0.24, and the large obstacle has a side length of 25 mm resulting in an ABR of 0.5.

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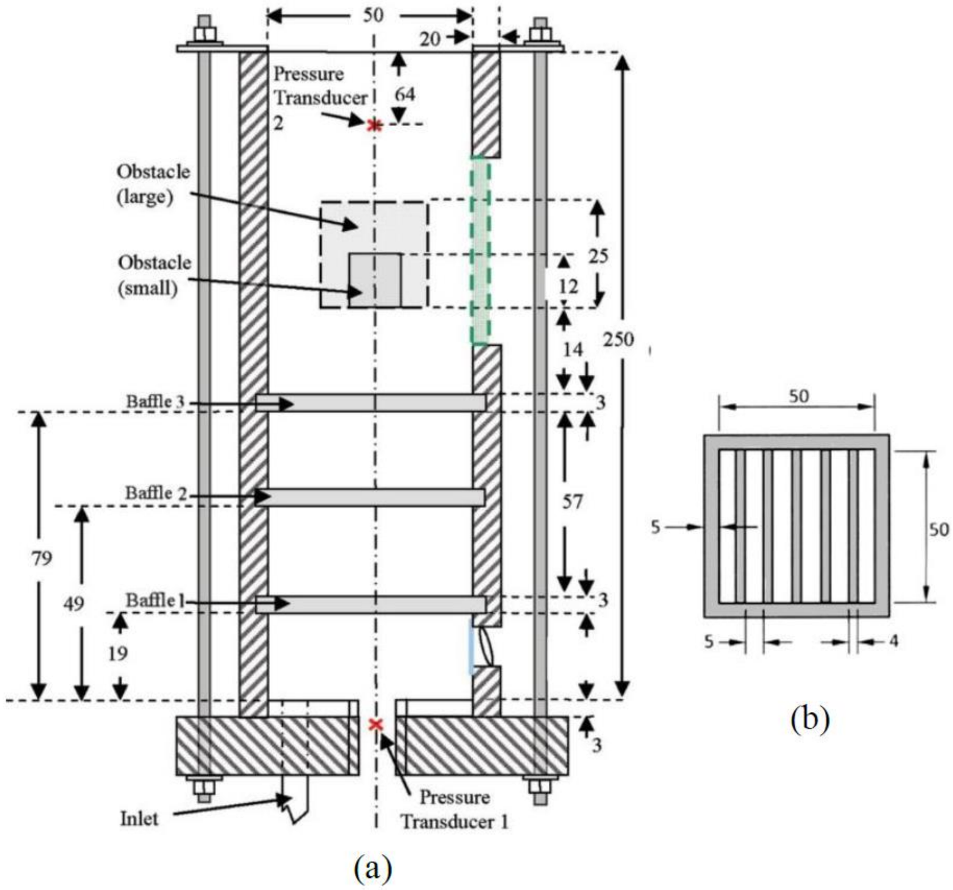

Fig. 1: (a) Combustion chamber and (b) removable baffle plate schematic (not to scale, dimensions in mm).

Each mixture is placed in the chamber through a non-return valve at atmospheric pressure and is allowed to settle before ignition. One second before ignition, the vent at the top of the chamber is opened. An Nd:YAG laser provides ignition via infrared radiation 2mm above the base of the chamber. Pressure readings are provided from two Keller type PR21-SR piezo-electric pressure transducers at a rate of 25 kHz [1]. One transducer is placed in the base of the chamber and the other is placed in the chamber wall 63 mm from the top of the chamber. The 1000 mbar limit of the pressure transducers is retained by using a lean equivalence ratio when using a hydrogen mixture, applying an equivalence ratio which exceeds 0.8 would surpass the pressure transducer limit [5]. Flame images are captured at a rate of 5 kHz using high-speed laser-induced fluorescence (LIF) from OH. Configuration codes are used to identify the baffle positioning and square obstacle size.

3. Numerical Setup

An in-house CFD code is used to perform numerical simulations [7]. An extended numerical domain measures 325 x x 325 x 500 mm with non-reflective boundary conditions used to prevent any pressure reflection effects. The combustion chamber setup in the computational domain measures 50 x 50 x 250 mm. Solid boundaries including the chamber walls, baffles and obstacle have adiabatic and no-slip boundary conditions applied. The computational grid utilises 90 cells in the the x direction, 90 cells in the y direction and 335 cells in the z direction for approximately 2.7 million cells in total. Increased grid refinement is applied in areas of increased flame-obstacle interaction such as where the flame meets the baffles or the square obstacle. The selected grid refinement has been used previously to obtain accurate results in numerical results in published research [3], [8]–[10]. At an equivalence ratio of 0.7, the lean hydrogen-aire mixture has a laminar burning velocity of 1.25 ms/s and a laminar flame thickness of 0.12 mm. At a stoichiometric equivalence ratio, LPG has s a laminar flame thickness of 0.37 mm and a laminar burning velocity of 0.385 m/s [11], [12]. Conservation equations for mass, momentum and energy govern the numerical simulations. The chemical state of the mixtures is identified by the reaction progress variable (c) [13]. Difficulties with modelling the reaction rate for turbulent premixed combustion results in a complex interaction between turbulence levels, chemical and thermodynamic states. Neglecting Zeldovich instability, assuming a unity Lewis number and applying a single-step irreversible chemical reaction between reactants and products reduces system complexity. The mean reaction rate is modelled using the laminar flamelet approach [13]:

$$\bar{\dot{\omega}} = \rho_u u_L \Sigma \tag{1}$$

Where the unburned mixture density is given by ρ_u, the laminar burning velocity is u_L and Σ is the flame surface density (FSD) which is evaluated dynamically. More details on the dynamic flame surface density (DFSD) model can be found elsewhere [8]–[10].

4. Results and Discussion

This section provides a comparison between numerical results and experimental data for a lean hydrogen-air mixture at an equivalence ratio of 0.7 and a stoichiometric LPG-air mixture. Overpressure results including timing, magnitude and the maximum rate of pressure rise will be shown and discussed. Experimental data included is an average of approximately 50 experiments [1]. The configurations studied are BBBL, BBBS, BB0L and BB0S as shown in Fig.2 below. The configuration code helps identify the positioning of the baffles and the size of the square obstacle. For example, configuration BBBL uses Baffle 1, Baffle 2, Baffle 3 and the large square obstacle, whereas configuration BB0S has Baffle 1 and 2 equipped with the small square obstacle.

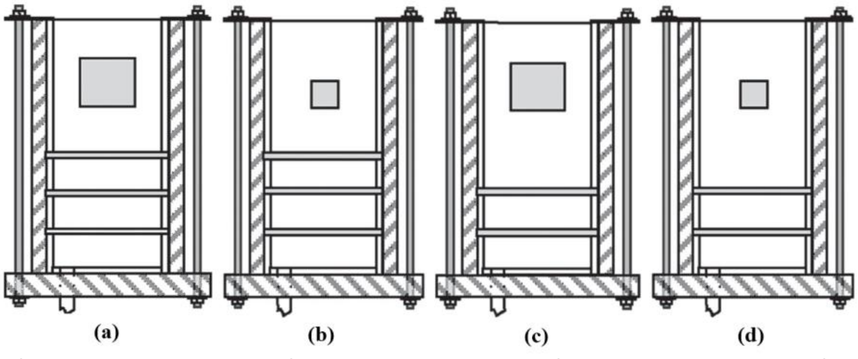

Fig. 2: (a) Configuration BBBL (b) Configuration BBBS (c) Configuration BB0L (d) Configuration BB0S.

Overpressure results convey critical combustion events including the initial pressure rise, peak combustion overpressure magnitude and timing as well as the pressure decay. Comparing the lean (Φ=0.7) hydrogen-air combustion overpressure to a stoichiometric (Φ=1.0) LPG mixture conveys the significantly more reactive nature of hydrogen to a highly turbulent environment within a lab scale combustion chamber.

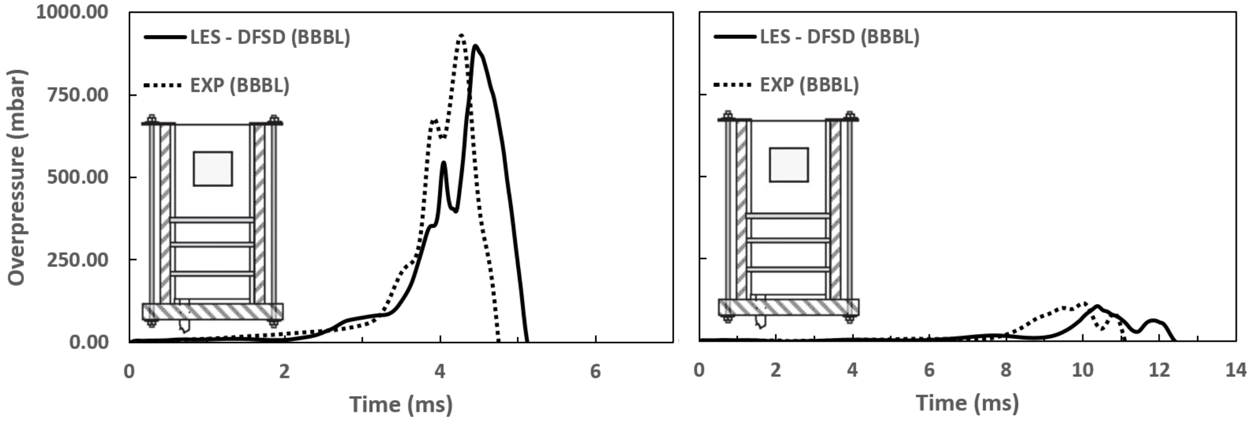

Fig. 3 Overpressure results for hydrogen-air at Φ=0.7 (left) and LPG-air at Φ=1.0 (right) using configuration BBBL.

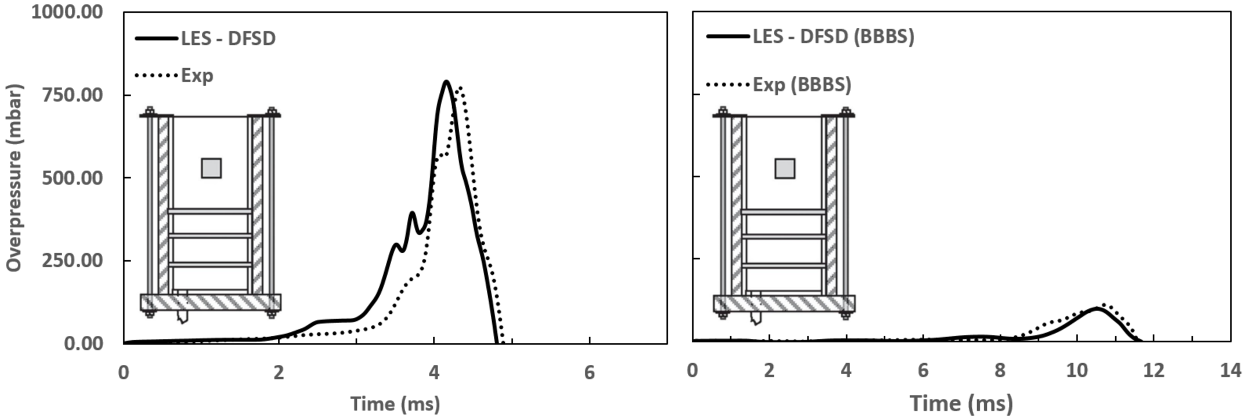

Fig. 4 Overpressure results for hydrogen-air at Φ=0.7 (left) and LPG-air at Φ=1.0 (right) using configuration BBBS.

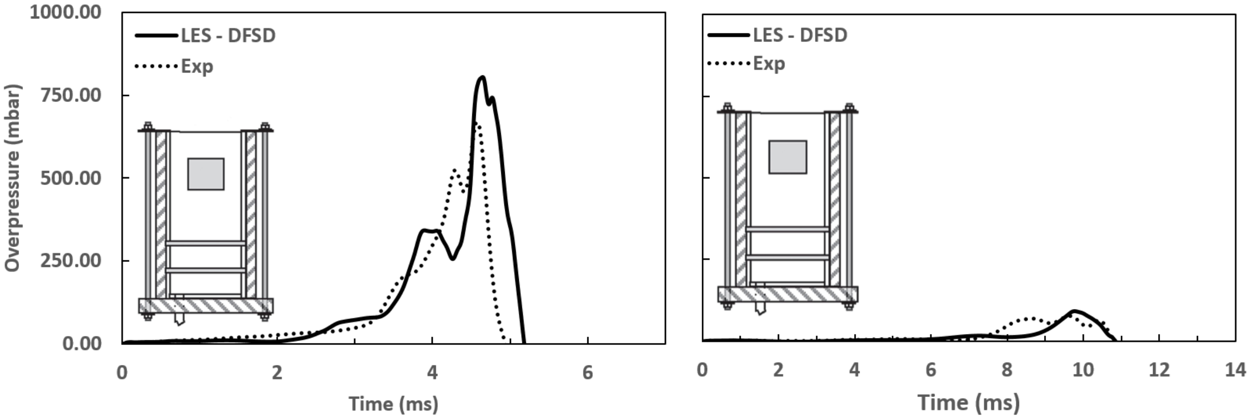

Fig. 5 Overpressure results for hydrogen-air at Φ=0.7 (left) and LPG-air at Φ=1.0 (right) using configuration BB0L.

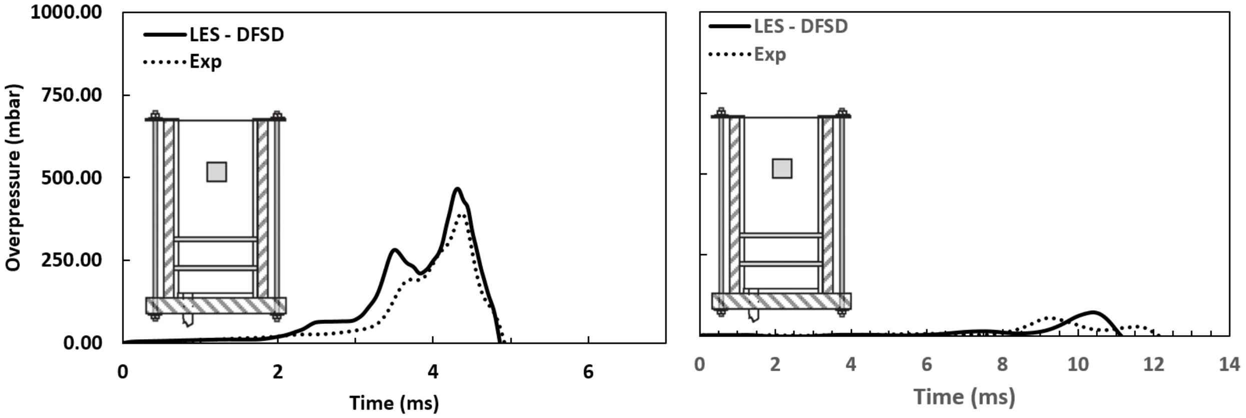

Fig. 6 Overpressure results for hydrogen-air at Φ=0.7 (left) and LPG-air at Φ=1.0 (right) using configuration BB0S.

Comparing Fig. 3 and Fig.4 indicates that using a square obstacle resulted in a higher peak combustion overpressure. For example, when using the lean hydrogen mixture, applying configuration BBBL which applies a square obstacle with an ABR of 0.5 results in a peak overpressure exceeding 890 mbar. On the other hand, configuration BBBS produces a peak of 789 mbar when the square obstacle ABR is reduced to 0.24. Similarly, the peak overpressure for the stoichiometric LPG mixture increases from 99 mbar to 106 mbar when the larger square obstacle is applied. Hydrogen's reactivity means that there is a 12.8% rise in overpressure when the larger obstacle is applied whereas the peak overpressure for the LPG mixture increases by 7%. Additionally, the increased blockage results in a maximum rate of pressure rise which increases from 320.5 MPa/s to 337.2 MPa/s for the hydrogen mixture, and from 8.5 MPa/s to 10.3 MPa/s for the LPG mixture. Figures 5 and 6 remove Baffle 3, which results in an increased obstacle separation distance and reduced turbulence intensity with the combustion chamber. For the hydrogen mixture, the peak overpressure decreases from 890 mbar using configuration BBBL to 806 mbar. The effect of the reduced turbulence intensity is further amplified when the small obstacle is applied, as the peak overpressure falls from 789 mbar using configuration BBBS to 466 mbar when a baffle is removed in configuration BB0S. The maximum rate of pressure rise also drops significantly from 320.5 MPa/s to 110.9 MPa/s. While the stoichiometric LPG mixture is less reactive, the impact of the increased ABR is still notable, as the peak overpressure increases from 72 mbar when using configuration BB0S to 91 mbar when configuration BB0L is applied.

5. Conclusion

This paper presents comparisons between numerical results and experimental data for turbulent premixed hydrogen and LPG flames using a laboratory scale combustion chamber with a built-in square obstacle and two area blockage ratios (ABR) of 0.24 and 0.50. The presented numerical results are validated against published experimental data with the following conclusions drawn:

- Increasing the solid obstacle ABR results in a higher peak combustion overpressure and a raised maximum rate of pressure rise when the lean hydrogen-air mixture or the stoichiometric LPG mixture is applied.
- Removing a baffle, results in an increased obstacle separation distance and reduced turbulence intensity which decreases generated combustion overpressure.
- Hydrogen deflagration, even when a leaner mixture is applied, is found to produce a significantly higher overpressures when compared with LPG.
- Numerical results presented for combustion overpressure show good agreement when compared with experimental data.

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