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Large Eddy simulation of hydrogen–air premixed flames in a small scale combustion chamber

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ABSTRACT

While hydrogen is attractive as a clean fuel, it poses a significant risk due to its high-reactivity. This paper presents Large Eddy Simulations (LES) of turbulent premixed flames of hydrogen–air mixtures propagating in a small scale combustion chamber. The sub-grid-scale model for reaction rate uses a dynamic procedure for calculating the flame/flow interactions. Sensitivity of the results to the ignition source and to different flow configurations is examined. Using the relevant parameter from the calculations, the flames are located on the regimes of combustion and are found to span the thin and corrugated flamelet regimes, hence confirming the validity of flamelet modelling. The calculations are compared to published experimental data for a similar configuration. It is found that both the peak overpressure and flame position are affected by the number of baffles positioned in the path of the flame and this is consistent with earlier findings for hydrocarbon fuels. Also, the LES technique is able to reproduce the same flame shape as the experimental images. A coarse study of sensitivity to the ignition source shows that the size of the ignition kernel does not affect the flame structure but influences only the time where the peak overpressure appears while moving the ignition source away from the base plate leads to a decrease in the peak overpressure.

Introduction

The usage of hydrogen as a clean fuel and energy carrier brings into consideration the safety problems related to its use. The current interest in hydrogen is due to its availability from many resources and to the fact that it leads to no 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 overpressure and flame evolution resulting from its deflagration. The present work uses the LES technique to calculate the structure of lean hydrogen flames propagating inside a vented combustion chamber while interacting with solid obstructions. The results are validated against experimental measurements of Masri et al. [1] and Al-Harbi et al. [2].

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The importance to study deflagrating flames came from the fact of their wide applications in industry and accidental explosions. However, there are already a significant amount of studies reporting data in vented explosions in laboratory chambers [3–12]. Different parameters are reported in these studies, mainly pressure and/or velocity, but the information remains limited because of the difficulty of making detailed measurements [13]. Laboratory-size vented chambers with obstacles represented in various configurations, e.g. Fairweather et al. [14,15] studied chambers with repeated circular rings and concluded that unreacted mixture which trapped behind the obstruction rings and this reacted violently, after the main flame front leaves the vessel leading to high overpressures. Moen et al. [16] used wires placed in the chamber to obstruct the propagating flames. In all of these studies the overpressure increases with increasing overall blockage ratio through one or more obstacles. Also, the spacing between obstacles is a factor because the flame re-laminaries quickly so if the spacing increases, the overpressure decreases.

The LES technique is now accepted as a common computational tool for modelling both premixed and non-premixed turbulent flames [17–22]. The added computational cost of LES remains an issue particularly for detailed combustor calculations. However, this is outweighed by key advantages such as the 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 direct numerical simulation (DNS) and Reynolds Averaged Navier–Stokes (RANS) techniques. A vital challenge to the improvement of LES lies in the development of relevant sub-grid-scale (SGS) models capable of representing combustion over a wide range of flow and combustion conditions. In most turbulent flames, the reaction zone thickness to be resolved is thin and the characteristic length scale is much smaller than a typical LES filter width. Therefore, an appropriate SGS model is needed to account for reaction rate. A range of approaches to model combustion at the SGS are being used with a varying degree of success depending on the combustion problem being addressed. The flamelet approach [23] was used by many researchers in the past in various forms [24–26] and, although limited to thin reaction zones, it remains applicable to a wide range of applications. Recent developments of this approach involve flame generated manifolds (FGM) tabulated in terms of mixture fraction, reaction progress variable as well as other parameters such as a measure of flow strain [27]. These formulations enable the application of flamelet modelling in premixed, non-premixed, as well as partially premixed flames. Two variations of the laminar flamelet approach are the flame surface density (FSD) where a transport equation for the FSD is solved [28] and the thickened flamelet model [29,30]. The approaches based on FSD are more reasonable in terms of computational cost yet well recognized in accounting for chemical reactions in the context of LES [31,32] with reaction rate being modelled as a function of the reaction progress variable and filter width. Recently, Di Sarli et al. [33,34] showed the importance of FSD based SGS models [17] to predict deflagrations in a vented chamber using LES. Other SGS models that are seen as alternatives to flamelets include the filtered density functions (FDF) [35], and probability density function approaches (pdf-like methods) which include transported pdf [36,37], multiple mapping conditioning (MMC) [38,39], the conditional moment closure [40,41], the linear Eddy model (LEM) [42–44], the renormalization group (RNG) [7,45]. While pdf-like methods are likely to be relevant across the entire mixture fraction space, they remain computationally intensive particularly if detailed chemistry is to be accounted for.

Flame surface density model is considered in the present investigation with a dynamic formulation [18] in order to account for the unresolved part of the SGS reaction rate. Earlier

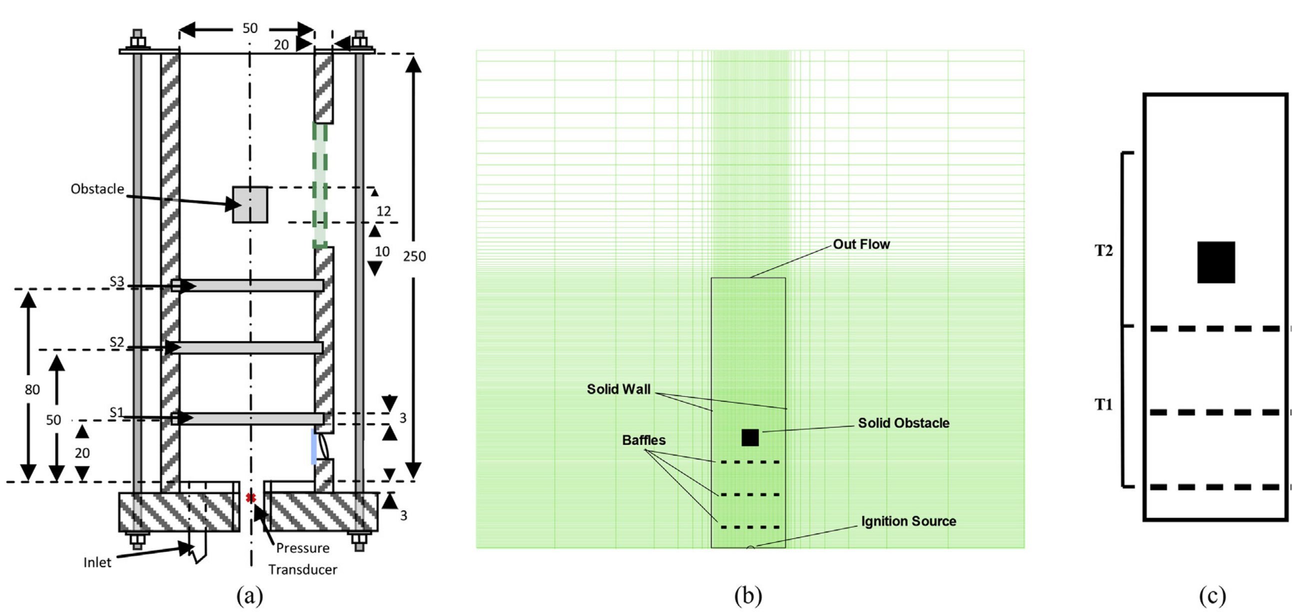

Fig. 1 – (a) Schematic diagram for the Sydney combustion chamber. All dimensions are in mm. (b) Illustration of the computational domain with the combustion chamber, baffles and obstacle are superimposed over grid resolution. (c) The two imaging tiers used to capture the maximum viewable height.