Numerical Simulations of CNG, LPG & H_2 Lean Premixed Deflagrating Flames

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1 Introduction

This paper presents large eddy simulations (LES) for transient propagating premixed flames inside a laboratory scale combustion chamber. During combustion, a number of instabilities can occur that will alter the shape of the flame and can lead to localized flame acceleration/deceleration. If this fact is not included in the combustion model, the predicted pressure will be under- or over-predicted and may cause major safety threats. In studying explosion hazards, thermo-diffusive instability should be considered. The main focus for the current work is to examine the effects of thermos-diffusive instability, expressed by Lewis number (*Le*) and the assumption of neglecting that effect (i.e. unity and non-unity values), on the generated pressure, flame location and speed for 3 different fuels namely, CNG, LPG and Hydrogen at lean conditions with equivalence ratio of 0.8. The numerical results obtained are validated against published experimental data of [1, 2] for the selected chamber configuration.

2 The Model

For the present work the Large Eddy Simulation (LES) technique is used here. In LES, modelling the reaction rate in turbulent premixed flames is a difficult task due to its non-linear relation with chemical and thermodynamic states. It is often characterized by propagating thin reaction sheets or layers thinner than the smallest turbulence scales. In the present simulations, the SGS reaction rate is accounted for by using the developed DFSD model [3-6]. Due to space limitations, brief details of the model are given here. More details can be found elsewhere [3-6]. However, in the present simulations, the SGS reaction rate, $\overline{\dot{\omega}}_c$ is the source term in the Favre filtered reaction progress variable equation (see Eq. (1)) and this is modelled using the laminar flamelet concept. The filtered conservation equation for the reaction progress variable and enthalpy may be written as:

$$\frac{\partial \overline{\rho}\tilde{c}}{\partial t}+\frac{\partial\left(\overline{\rho}\tilde{u}_j\tilde{c}\right)}{\partial x_j}+\frac{\partial\left(\overline{\rho u_j c}\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\overline{\mu}}{Sc}\frac{\partial \tilde{c}}{\partial x_j}\right)+\overline{\dot{\omega}}_c \tag{1}$$

$$\frac{\partial\left(\overline{\rho}\tilde{h}\right)}{\partial t}+\frac{\partial\left(\overline{\rho}\tilde{u}_j\tilde{h}\right)}{\partial x_j}+\frac{\partial\left(\overline{\rho u_j h}\right)}{\partial x_j}=\frac{\partial \overline{P}}{\partial t}+2\overline{\mu}\left[S_{ij}-\frac{1}{3}\delta_{ij}\tilde{S}_{kk}\right]:\frac{\partial \tilde{u}_j}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\frac{\tilde{\mu}}{Pr}\frac{\partial \tilde{h}}{\partial x_j}\right]+\overline{\dot{q}_c} \tag{2}$$

$$\overline{\dot{q}_c}=h_f^{\circ}\,\overline{\dot{\omega}}_c Y_{fu}^{\circ} \tag{3}$$

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$$Le = \frac{Sc}{Pr} \tag{4}$$

where (c) is the reaction progress variable,(h) is the enthalpy, (P) is the pressure, Sc and Pr are the Schmidt and Prandtl numbers respectively, (Y_{fu}) is the local mass fraction, (h_f) is the lower heating value and ($\overline{\dot{q}_c}$) is the chemical source term and it is represented by eq. (3). The basic idea here is to use the actual values for Schmidt and Prandtl numbers to represent the effects of non-unity Lewis number. The values used in the present work are obtained from [7-9] and are listed in table 1 below.

The SGS reaction rate ($\overline{\dot{\omega}_c}$) in eq. (1) is modelled as:

$$\overline{\dot{\omega}_c} = \rho_u u_L \overline{\Sigma} \tag{5}$$

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. (4) is expressed as

$$\overline{\Sigma} = \prod\left(\overline{c}, \overline{\Delta}\right) + Cs\left[\widehat{\prod\left(\overline{c}, \overline{\Delta}\right)} - \prod\left(\hat{\overline{c}}, \hat{\overline{\Delta}}\right)\right] \tag{6}$$

The model coefficient (Cs) in above equation is dynamically obtained by identifying subgrid-scale flame surface as a fractal surface [3] as follows:

$$Cs = \frac{1}{1-\gamma^{2-D}}\left[\left(\frac{\overline{\Delta}}{\delta_c}\right)^{D-2} - 1\right] \tag{7}$$

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 [3].

$$D = 2.0 + \frac{\log\left(\widehat{\prod\left(\overline{c}, \overline{\Delta}\right)} / \prod\left(\hat{\overline{c}}, \hat{\overline{\Delta}}\right)\right)}{\log\left(\hat{\overline{\Delta}} / \overline{\Delta}\right)} \tag{8}$$

Table 1: Summary of the parameters used in the present work for the 3 fuels; CNG, LPG and H_2.

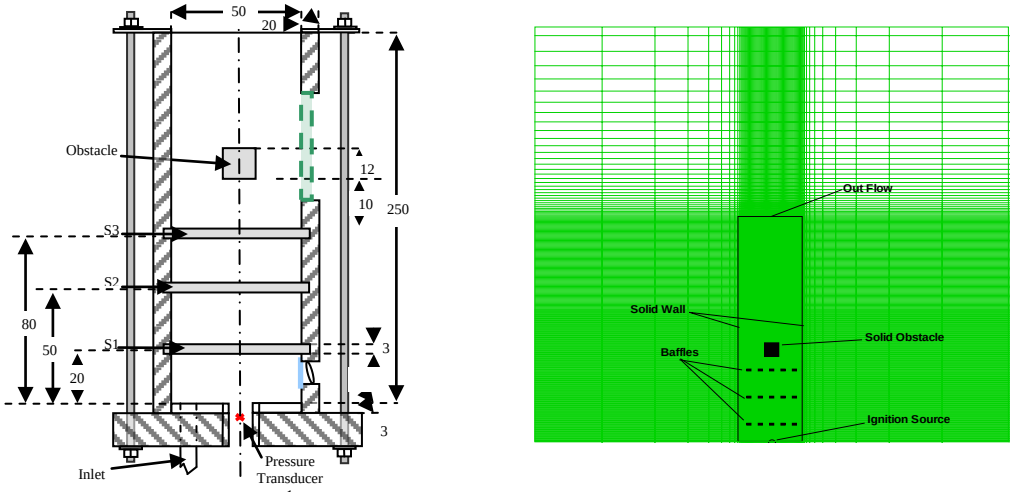
Fuel	**CNG**	**LPG**	**H_2**
Equivalence Ratio (φ)	0.8	0.8	0.8
Sc	0.742	1.260	0.353
Pr	0.798	0.810	0.531
Lewis No.	0.93	1.55	0.67

It should be mentioned that, for the cases of unity Lewis number, the Schmidt and Prandtl numbers were assumed as 0.75 for both CNG and LPG, and 0.70 for hydrogen case.

3 The Combustion Chamber

The experimental chamber used in this study was developed by the University of Sydney, Australia [1, 2]. The combustion chamber has dimensions of 50 x 50 x 250 mm and has 3 baffle plates and 1 solid obstacle. The baffles are located at various distances from the base plate where ignition occurs and the solid square obstacle is placed further downstream of the baffle plates as shown in Fig. 1a. The

numerical model described above, has been employed using an in-house LES code [10, 11] with an independent grid [12] of size 90 x 90 x 336 (2.7 million) cells in 3 dimensional space (Fig. 1b).



(a) (b)

Figure 1. (a) Schematic diagram for the Sydney combustion chamber (dimensions in mm). (b) Illustration of the computational domain with the combustion chamber, baffles and obstacle are superimposed over grid resolution.

4 Results and Discussions

In the model, the flame is initiated by igniting an initially stagnant mixture of fuel in air. This is done numerically by setting the reaction progress variable to 0.5 within a definite radius at the bottom centre of the chamber. Following ignition, the flame propagates past the built-in solid obstructions inside an open ended rectangular premixed combustion chamber. However, from table 1 it is obvious that Lewis numbers vary in value for both LPG and Hydrogen and are away from unity. For CNG its value is very close to unity [13]. From Fig. 2, it is clear that there is almost no change in the overpressure for CNG when using unity or non-unity *Le* number and for both cases a reasonable agreement is obtained. While for LPG, using unity *Le* number assumption tends to over-predict the overpressure when compared with experiments. However, for the non-unity *Le* case, good agreement was achieved. For Hydrogen, the unity *Le* number assumption under-predicts the pressure, while for the non-unity *Le* number better agreement was obtained with the experimental results. This is very crucial in accidental explosions as the over/under prediction of the overpressure may lead to critical problems in designing the industrial, commercial or domestic facilities.

Results shown in Fig. 3 support the above conclusion. The reason for over/under predictions is mainly due to diffusivity. In the hydrogen case, higher diffusivity do exist in the non-unity *Le* number case rather than the unity one. This is led to have a faster flame. An inverse effect happened for the LPG where non-unity *Le* number led to a slower flame. For CNG, a negligible effect is observed.

5 Conclusions

A method to account for the effect of Lewis number and its effect of overpressure, flame position and speed by using the calculated values of Schmidt and Prandtl numbers is proposed. 3 different fuel-air

mixtures at equivalence ratio 0.8 (lean conditions) are investigated, mainly; CNG, LPG and Hydrogen. The effect of Lewis number is observed on both LPG and Hydrogen. While for CNG, slight effect is noted. Also, LES results using the proposed method give better agreement when validated with the experimental data.

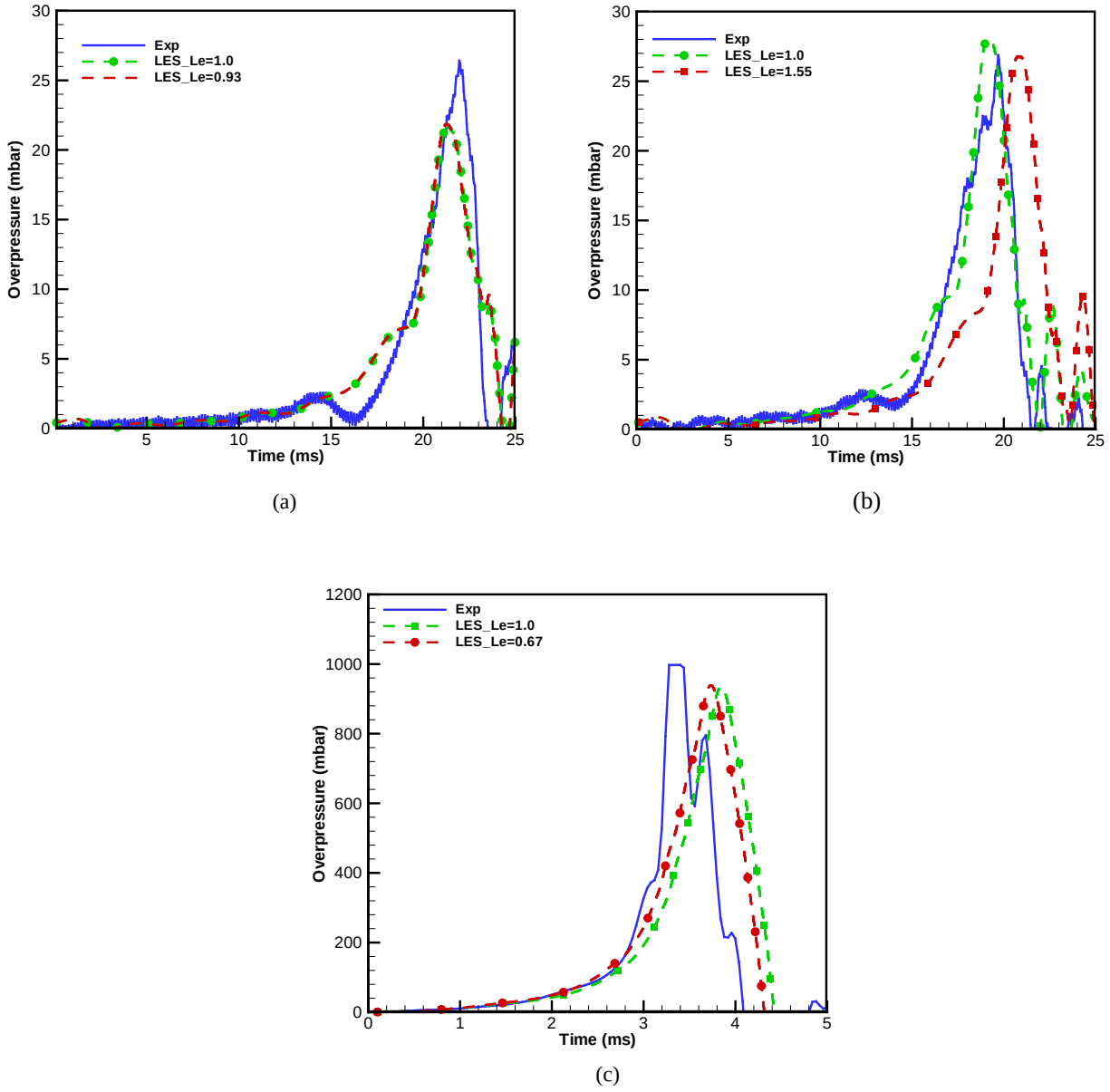
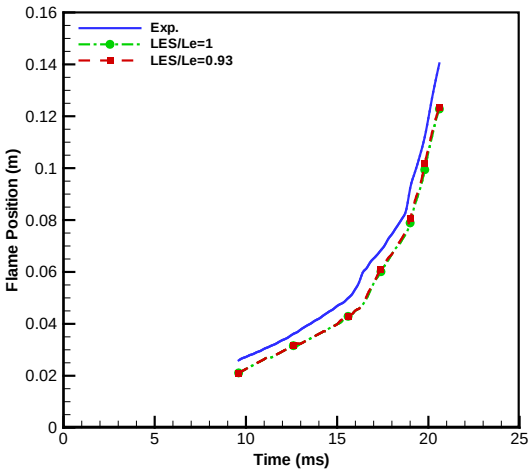
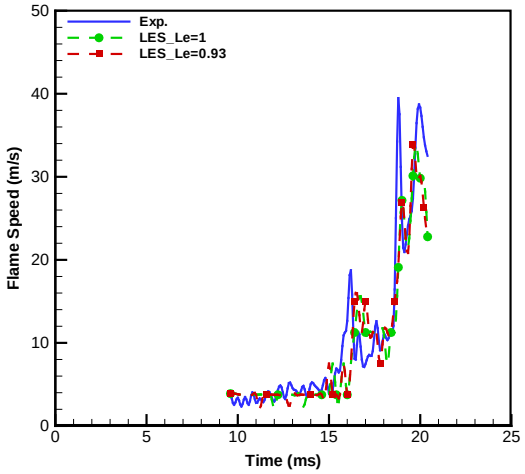


Figure 2. Overpressure-time traces of LES simulations using unity and non-unity Lewis no. for the 3 fuel-air mixtures. (a) CNG, (b) LPG and (c) H_2 compared with experimental data of [1, 2].



(a)



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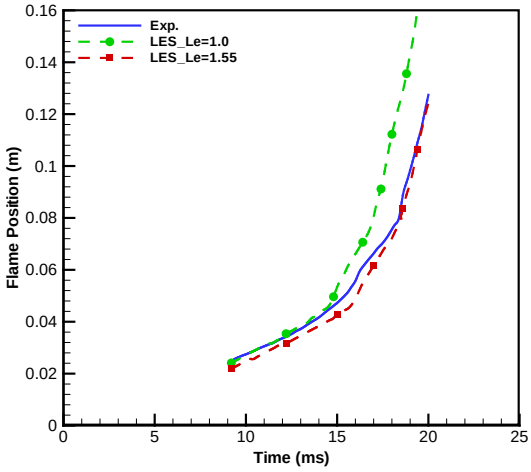

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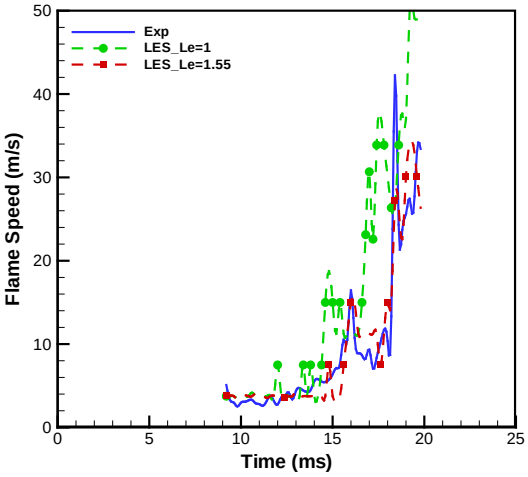

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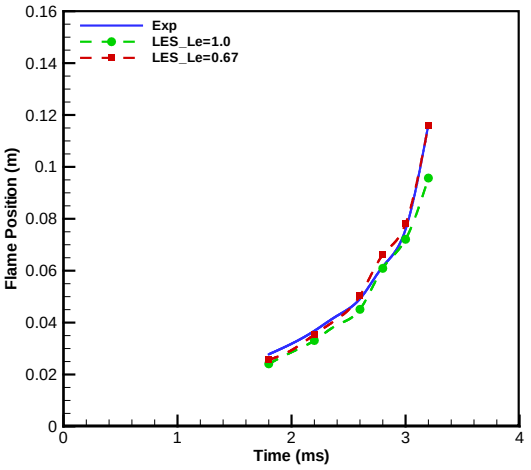
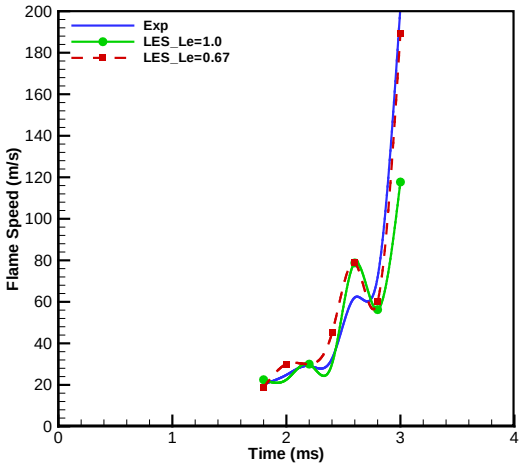


(c)



(c)

Figure 3. Flame Position (left) and Flame Speed (right) time traces of LES simulations using unity and non-unity Lewis no. for the 3 fuel-air mixtures. (a) CNG, (b) LPG and (c) H_2 compared with experimental data of [1, 2].

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