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LES Modelling of Explosion Propagating Flame inside Vented Chambers with Built-in Solid Obstructions

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1 Introduction

This paper presents large eddy simulations (LES) of the transient interaction between propagating turbulent premixed flames and solid obstructions mounted inside a laboratory scale combustion chamber. Interactions between the flame movement and the obstacles found to create both turbulence by vortex shedding and local wake/recirculation whereby the flame is wrapped in on itself, increasing the surface area available for combustion and the rate of local reaction rate. Accounting the influence of such local events in order to predict overall flame spreading speed, flame behaviour and the generated overpressure as a measure of reaction rate are extremely useful in combustion analysis in order to develop new models. The rise in the reaction rate due to the local nature of the flow and the increase in overall pressure due to the enhanced turbulence flame interactions as the flame travels through the unburned fuel air mixture are presented and discussed. The main focus of the current work is to establish the LES technique as a good numerical tool to calculate turbulent premixed propagating flames of propane/air mixture having equivalence ratio of 1.0, which is of practical importance in analysing explosion hazards and gas turbine combustors.

2 LES models

In applying LES to turbulent premixed flames, there are two basic requirements for sub-grid-scale modelling of scalar fluxes and chemical reaction. The standard Smagorinsky [1] model developed in 1963 has been widely used to model the sub-grid fluctuations in the velocity field. Germano *et al* [2] extended this model by devising an automated procedure for determining the Smagorinsky model coefficient. In the present simulations model coefficient is calculated from the instantaneous flow conditions using the dynamic determination procedure developed by Moin *et al* [3] for compressible flows. Chemical reaction can be modelled by either a simple Eddy-Break-Up (EBU) [4] assumption which gives a reaction rate proportional to the time scale of turbulent mixing or by using more advanced models based on the flame surface density, Σ . In these approaches, the mean reaction rate per unit volume ($\bar{\omega}$) is given by: $\bar{\omega} = R\Sigma$. Here R is a mean reaction per unit surface area and Σ is either modelled [5] or obtained by solving a full transport equation for the flame surface density [6]. Mean reaction rate per unit surface area R can be written as $\rho_u u_L$, where ρ_u is unburned mixture density and u_L is laminar flame velocity. Following the DNS analysis of thin premixed flames Boger *et al* [7] deduced an algebraic expression for Σ as:

$$\Sigma = 4\beta \frac{\tilde{c}(1-\tilde{c})}{\bar{\Delta}} \quad (1)$$

where \tilde{c} is Favre filtered reaction progress variable, $\bar{\Delta}$ is the filter width and β is the model constant. This approach is implemented in the preset simulation and the model constant, β is taken as 1.2 [7, 8]. The above expression is similar to the Bray-Moss-Libby (BML) expression for flame surface density in RANS [9]. The ratio $\bar{\Delta}/\beta$ represents the degree of sub-grid scale flame wrinkling. Potentially, this combustion model can predict localised extinctions should the local stretch exceeds certain limit [5, 9].

3 LES calculations

Transient calculations of turbulent premixed flames propagating over solid obstructions mounted inside a laboratory scale combustion chamber has been carried with the compressible version of the LES code PUFFIN [8]. PUFFIN solves strongly coupled Favre-filtered mass, momentum, energy and reaction progress variable equations along with the state equation, which are written in boundary fitted coordinates and discretized by using a finite volume method. The discretization is based on control volume formulation on a staggered non-uniform Cartesian grid. A second order central difference approximation is used for the diffusion advection and pressure gradient terms in the momentum equations and for gradient in the pressure correction equation. Conservation equations for scalars use second order central difference scheme. The third order upwind scheme of Leonard, QUICK [10] and SHARP [11] are used for advection terms of the scalar equations to avoid problems associated with oscillations in the solution. The equations are advanced in time using the fractional step method. Crank-Nicolson scheme is used for the time integration of momentum and scalar equations. Solid boundary conditions are applied at the bottom, vertical walls, for baffles and obstacle, with the power-law wall function of Werner and Wengle [12] used to calculate the wall shear layer and a constant temperature along all solid walls. A non-reflecting boundary condition is used to prevent reflection of pressure waves at these boundaries. Outflow boundary conditions are used at the open end of the combustion chamber. The initial conditions are quiescent with zero velocity and reaction progress variable. Simulations were carried in three dimensional non-uniform Cartesian co-ordinate system for compressible flow and having low Mach number. Since this type of flow involves large changes in density, high velocities and significant dilatation, all terms in the transport equations must be retained.

4 Results

LES results presented in this paper are for unsteady turbulent premixed flame. The flame is initiated by igniting an initially stagnant stoichiometric mixture of propane in air. Following ignition, the flame propagates past built-in solid obstructions inside an open end rectangular premixed combustion chamber. Present work aims to investigate the modelling issues associated with applying LES to calculate turbulent premixed flames. The computational domain has the dimensions of 50x50x250 mm and this domain is extended to 325 mm in x, y and 250 mm in z direction with the far-field boundary conditions. Parametric studies are performed with different grid sizes for configuration 1 in order to examine sensitivity of the results to the grid resolution. However, results from all grid resolutions are not presented here due to space limitations. For the present analysis, LES results of five different configurations shown in Figure 1 are considered from the finest grid simulations, having 2.7 million grid points with 90x90x336 in x, y and z directions respectively, with 67x67x300 grid points within the chamber. However, due to the space constrain, only results for configuration 1 and 5 are presented and explained. These results reveal the significance of the interaction between the flow and the propagating flame and their effects on both: the level of turbulence and generated over pressure.

Details of the flame positions and flame speeds corresponding to the peak over pressure for various configurations employed in this study are presented in Table 1. Figure 2 (a & b) shows the snapshots of the reaction rate from LES simulations compared with the high speed video images of the experiments for

configuration 1 & 5 respectively at various times during the flame propagation. Both the configurations use a square obstruction running through the explosion chamber with the only difference in the number of baffle plates used. Configuration 1 uses three baffle plates (S1, S2 & S3) and configuration 5 uses only one baffle plate (S3) near the solid square obstruction. The time traces of over pressure, flame speed and position for both the configurations with experimental measurements are shown in Figure 3 (a, b & c). For the same configurations flame speed and position are plotted against experimental measurements and shown in Figure 3 (d). This plot gives quantitative difference of flame speed in both the cases for any chosen flame front position.

The propagating speed of the flame in case of configuration 1 is around 4 m/s and is approximately constant until flame reaches the first baffle plate. Once the flame hits the baffle plate, a rapid increase in flame speed followed by a sharp decrease is observed because of the local obstructions. After hitting the first baffle plate the laminar hemispherical structure of the flame is distorted and flame starts protruding through the narrow vents. As a result, surface area of the flame brush increases as it propagates through the un-burnt fuel/air mixture, hence increase in the flame speed observed. This also results in wrapping and wrinkling of the flame around the local obstruction and on itself, which traps the un-burnt mixture by the burnt gases. The trapped un-burnt gases will have significant contribution in increasing the over pressure at later stages (after third baffle plate). The flame front reaches the second plate at a progressive flame speed. Eventually flame experiences wrinkling, stretching and increase in surface area at a higher degree as it propagates further. At this stage, it can be noticed that the flame propagation speed increases rapidly and the flame front appears to be turbulent and more corrugated as it accelerates towards the third baffle. Increase in propagation speed due to the local turbulence causes further stretching and wrinkling of the flame. At this stage flame jets out of third baffle plate and encounters the solid square obstruction, flame is further distorted and wrinkled, followed by an increase in surface area thereby boosting the reaction rate. Highly wrinkled flame starts wrapping around the solid square obstacle, which subsequently results in trapping of a high volume of un-burnt fuel/air mixture by flame at the up stream and the down stream of the square obstacle with in the recirculation zone. The highly wrinkled flame propagates past the obstacle and gets reconnected quickly with in the recirculation zone. The trapped gases will start burning as the flame combines together and this has significant contribution in increasing the over pressure. The flame structure and the entrapment of the un-burnt gases is very well predicted at various stages by LES simulations in comparison with the high speed video images as shown in 2 (a).

In case of configuration 5 with only one baffle plate near square obstruction, propagating flame maintains laminar profile until it reaches baffle plate near the square obstacle. As the flame propagates through the narrow vents, surface area of the flame increase due to the flame distortion and the generated vortices. Unlike in configuration 1, variation in the flame speed is very little as the flame has enough time to interact with the baffle plate. Also it can be noticed from the snapshots of LES predictions and experimental images shown in 2(b) that hemispherical structure of the flame started changing before hitting the baffle plate. Distorted flame propagates further and encounters square obstacle which further distorts flame. Distorted flame wrinkles the flame surface and generates vortices, which subsequently traps the un-burnt gases upstream and down stream of the square obstacle. It is noteworthy at this point that the volume of the trapped un-burnt fuel/air mixture is less than that of the configuration 1. This is because of the strength of the local turbulence encountered due to the flow conditions.

The peak over pressure for configuration 1 as shown in Figure 3 (a) from LES predictions is 109.53 mbar at 11.06 ms against the experimental measurements of 138.28 mbar at 10.3 ms. Peak over pressure in case of LES and experiment is corresponds to the reconnection of the flame after the square obstacle and burning of the trapped un-burnt gases down and upstream of the obstruction. The time shift of the peak over pressure in case of the experiment could be because of establishing the time zero setting of ignition. However there is no such problem with the LES predictions as ignition is initialized by setting reaction progress variable to 0.5 with in the radius of 4 mm. In case of configuration 5, peak over pressure from LES simulation is 63.82 mbar which is much less than in configuration 1 (approx. 41% lesser) and experiences at 13.97 ms which confirms that flame is travelling at lesser speed. Experimental measurements of peak over pressure for configuration 5 is 82.03 mbar

occurring at 13.25 ms. Experimental peak pressure for configuration 5 is 41% less than of configuration 1 and occurs at later time. In this case peak pressure is occurring as flame propagates furthest of the square obstacle and half way through to exit the chamber. This is just because flame has travelled inside the chamber with laminar profile until it encounters vented plate. Similar time shift in the incidence of the peak over pressure can be observed in this case and it is evident from the details of other configurations presented in table 1, that the time shift is dependent on the condition of the individual experimental configuration. From these simulations it is evident that the magnitude of the over pressure generated in combustion chamber is dependent on the number and the position of solid obstructions with respect to the ignition point in combustion chamber.

Simulations of turbulent premixed flames by LES are qualitatively well predicted on par with the experimental measurements. These simulations substantiate the good representation of the flame position, speed, structure, interactions between flow and turbulence and reaction rate for various configurations. However, peak over pressure and its time of occurrence are predicted slightly less than that of experimental measurements. One of the reasons might be the sub-grid scale model employed to account the reaction rate. In case of thin premixed flames, chemical reaction takes place in thin propagating layers, referred as flamelets and this phenomenon is mostly in sub-grid scales. It is evident that the flame is thinner than the grid resolution. Employing a complex model may account most of the sub-grid reaction rate. The second reason may be the laminar flame speed u_L used in this model. Although instantaneous flame remains laminar with in these flamelets, the local flame speed can be affected by the flame stretch and curvature. Implementing the stretched laminar flame speed into the flame surface density model may produce good results. Further investigation in this direction has to be carried out to assess the predictability of this model. Overall, LES simulations of premixed turbulent flames by flame surface density are very promising.

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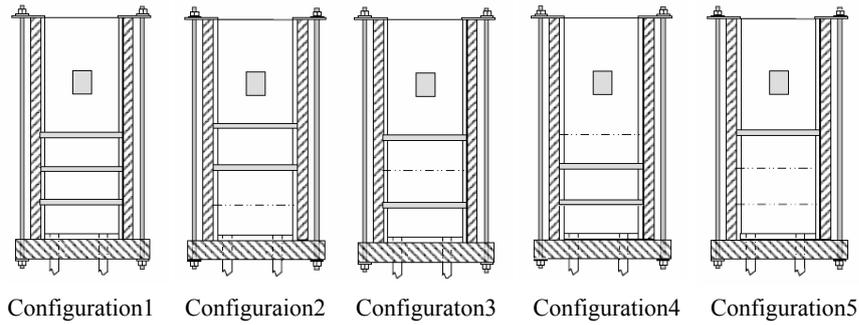


Figure 1 Schematic diagram of the explosion chamber with 5 different built-in solid obstructions.

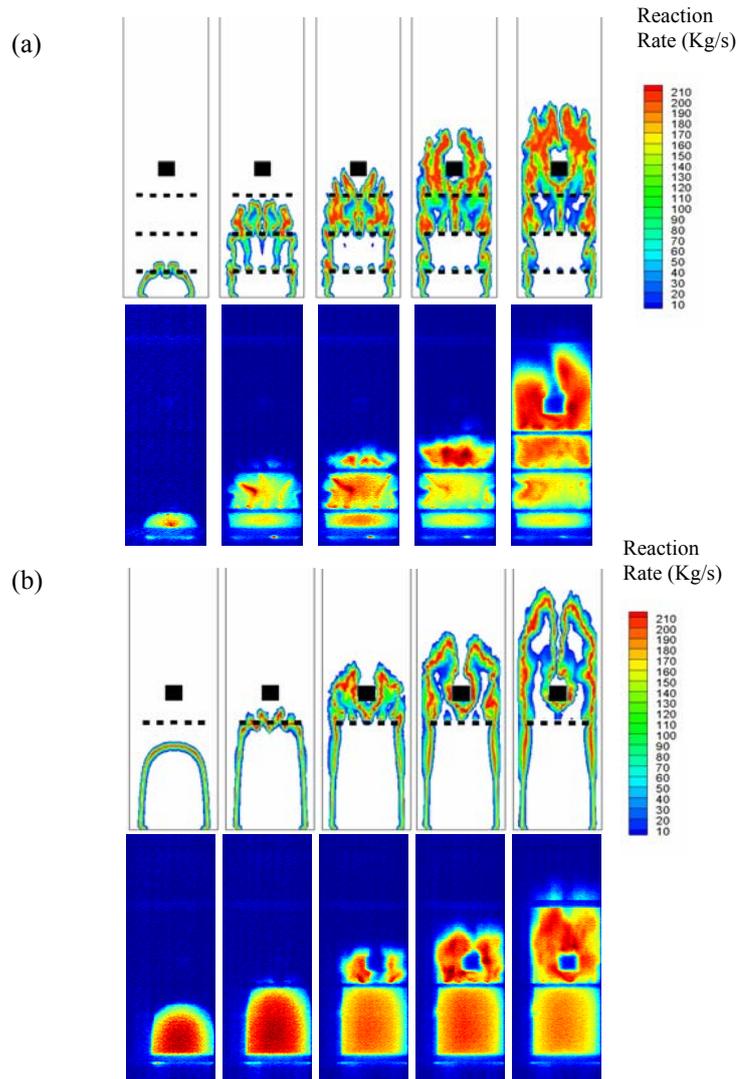


Figure 2 Sequence of images to show flame structure at different times after ignition. Reaction rate contours generated from LES predictions are presented against high speed recorded video images of experiments. (a) Numerical snap shots for configuration 1 at 6, 9.5, 10.0, 10.5, and 10.8 ms are compared with experimental images at 6, 9.5, 10, 10.5 and 11.5 ms. (b) Numerical snap shots for configuration 5 at 10.5, 12.0, 13.0, 13.5, and 14.0 ms are compared with experimental images at 10.5, 12.0, 13.0, 13.5, and 14.0 ms.

Table 1 Results form the LES simulations and experimental measurements are presented for various configurations.

Configu- ration	Turbulence generating grid				Experimental data sets				LES Predictions				Time shift LES – Exp
	S1	S2	S3	Sq. Ob.	Peak over pressu- re (mbar)	Time (ms)	Corres- pondi- ng Flame positio- n (m)	Corres- pondi- ng Flame speed (m/s)	Peak over pressu- re (mbar)	Time (ms)	Corres- pondi- ng Flame positio- n (m)	Corres- pondi- ng Flame speed (m/s)	
1	Y	Y	Y	Y	138.28	10.3	0.1	53.94	109.53	11.06	0.1785	81.83	0.74
2	-	Y	Y	Y	118.46	11.96	0.1	50.72	95.70	12.53	0.1815	76.582	0.57
3	Y	-	Y	Y	80.47	11.42	0.13	49.52	82.21	11.99	0.1805	80.728	0.57
4	Y	Y	-	Y	77.15	9.79	0.08	30.0	80.11	10.95	0.1555	64.92	1.16
5	-	-	Y	Y	82.03	13.25	0.176	75.2	63.82	13.97	0.1675	63.33	0.72

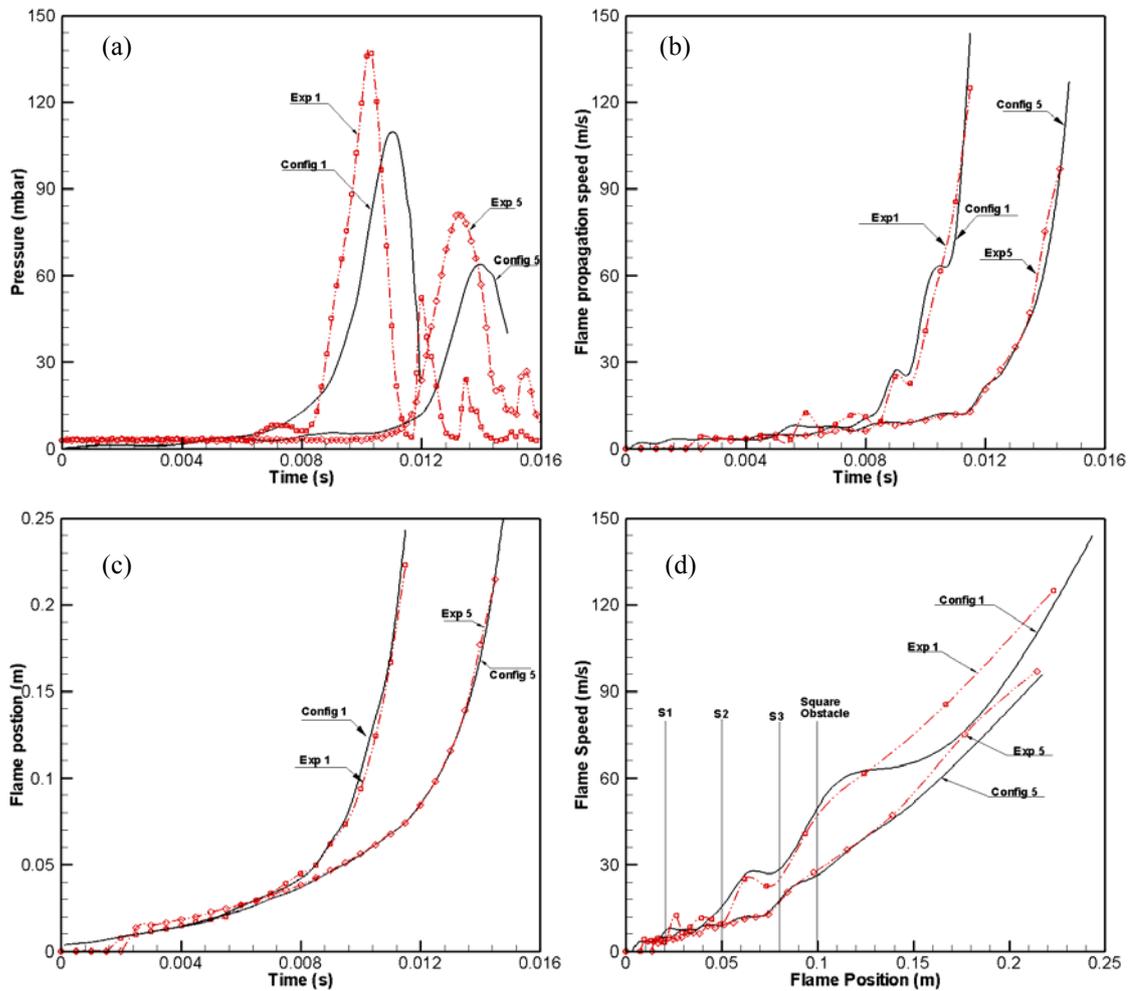


Figure 3 Time traces of LES simulations for two configurations (config1 and config5) with experimental measurements are presented. (a) Peak over pressure (b) Flame speed (c) Flame position (d) Flame speed is plotted against flame position.