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LES MODELLING OF PROPAGATING TURBULENT PREMIXED FLAMES USING A DYNAMIC FLAME SURFACE DENSITY MODEL

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Abstract. *A Dynamic flame surface density (DFSD) model, developed recently from experimental images for transient turbulent premixed flames, is implemented and tested using the large eddy simulation (LES) modelling technique. Numerical predictions from DFSD model are compared with those predicted using the flame surface density (FSD) sub-grid scale (SGS) model for reaction rate. In the SGS-DFSD model, dynamic formulation of the reaction rate is coupled with the fractal analysis of the flame front structure. The fractal dimension is evaluated dynamically from an empirical formula based on the sub-grid velocity fluctuations. A laboratory scale combustion chamber with inbuilt solid obstacles is used for model validation and comparisons. The flame is initiated from igniting a stoichiometric propane/air mixture from stagnation. The results obtained with the DFSD model are in good comparisons with experimental data and the essential features of turbulent premixed combustion are well captured. It has also been observed that the SGS-DFSD model for reaction rate found to capture the unresolved flame surface density contributions. Further investigations are planned to examine and validate of the SGS-DFSD for different flow geometries.*

1 INTRODUCTION

Combustion is the most important process of energy production in engineering. Understanding the process of combustion is very essential and important in order to produce most efficient combustion devices such as gas turbine combustors, industrial burners, I.C engines etc. Simulating the real time turbulent combustion using numerical techniques is ever growing in the course of revealing the physics of combustion. Among the numerical techniques available to simulate combustion, large eddy simulation (LES) is gaining more popular and delivering confidence because of its unique feature of filtering the flow field. In

LES, large eddies are computed explicitly and the smallest eddies are modelled by sub-grid scale (SGS) models. In applying LES to premixed turbulent flames, there is a requirement of SGS model for reaction rate. Flame surface density (FSD) models developed in the context of RANS^{1, 2} and LES^{3, 4} has achieved good confidence in accounting the reaction rate, for the application of fast chemistry problems. However, previous investigations^{5, 6} has reported certain drawbacks in predicting the peak over pressure and the time of its occurrence, by using FSD model for LES. A dynamic sub-grid scale model for reaction rate, formulated from mathematical and experimental analysis of Knikker⁷, following the similarity ideas is implemented and tested during this investigation. This model has dynamism in calculating the flame surface density and expected to predict the SGS contributions of reaction rate accurately.

In the present work, the large eddy simulation (LES) technique is used to model transient premixed propagating turbulent flame. The flame is initiated from igniting a stoichiometric propane/air mixture from stagnation. The objective of the present study is to conduct a preliminary test on dynamic flame surface density (DFSD) model⁷ in the context of LES. Performance of the SGS-DFSD model for the reaction rate is evaluated and compared with the experimental measurements. The simulations are carried out for a laboratory scale premixed combustion chamber⁸ having repeated built-in solid obstacles as shown in figure 1. The purpose of the built-in solid obstacles is to enhance the level of turbulence and hence increase the flame propagating speed. This chamber has been selected with particular interest of investigating the interactions between the flame movement and the solid obstacles. From previous investigations⁵, these interactions between flame movement and solid obstacles are 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. The SGS-DFSD model employed in this investigation accounts for the influence of such local events on flame propagation and generated overpressure.

2 COMBUSTION MODELLING

In LES, Favre filtered (density weighted) equations for conservation of mass, momentum, energy and a reaction progress variable coupled with the state equation are solved for turbulent premixed flames. The chemical reaction is modelled by assuming the single step irreversible chemistry between the reactants and products with a unity Lewis number. Favre filtered governing equations are closed by the sub-grid scale models for turbulence and reaction rate. The SGS contributions of turbulence are modelled by the standard Smagorinsky⁹ model. Smagorinsky model coefficient is calculated from the instantaneous flow conditions using the dynamic determination procedure developed by Moin¹⁰ for compressible flows following the similarity ideas of Germano¹¹.

The reaction progress variable c defines the complete chemical state of the air/fuel mixture from completely burned ($c = 1$) to unburned ($c = 0$) based on the value of fuel mass fraction.

Mathematically it can be represented as, $c = 1 - \frac{Y_{fu}}{Y_{fu}^0}$. Here Y_{fu} is the local fuel mass fraction and Y_{fu}^0 is the fuel mass fraction in unburned mixture. Favre-filtered transport equation for reaction progress variable can be written as:

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_j \tilde{c})}{\partial x_j} + \frac{\partial (\overline{\rho u_j'' c''})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}}{Sc} \frac{\partial \tilde{c}}{\partial x_j} \right) + \bar{\tilde{\omega}}_c \quad (1)$$

In the above equation ρ is the density, u_j is the velocity component in x_j direction, μ is the viscosity, c is the reaction progress variable and $\tilde{\omega}_c$ is the reaction rate. An over-bar describes the application of the spatial filter while the tilde denotes Favre filtered quantities. The last term on right-hand side in the above equation is the filtered reaction rate. Sub-grid scale models are required to account this reaction rate. The SGS reaction rate is modelled by following the flamelet approach. The reaction rate zone can be viewed as collection of the thin propagating reaction layers having the structure of laminar flames. Therefore the mean reaction rate per unit volume, $\tilde{\omega}_c$ can be modelled as $\tilde{\omega}_c = R\Sigma$. Here R is a mean reaction per unit surface area and Σ is the flame surface density (or the flame surface area per unit volume), which is either modelled¹ or obtained by solving a full transport equation for the flame surface density^{12, 13}. The work presented in this report is carried by employing two different models for Σ , the first one is flame surface density model based on flamelet concept⁴ and the second is dynamic flame surface density model⁷ following the similarity ideas¹¹.

In the context of LES, mean reaction rate per unit surface area R can be modelled using the formulation of flame front propagation into the fresh gases developed as in G-equation approach¹⁴⁻¹⁶. Hence R can be expressed as $\langle \rho u \rangle_s$, which is surface averaged, density weighted displacement speed of the propagating flame into the fresh gases. Assuming that individual flamelet is propagating at laminar flame speed, u_L into the fresh gases of density, ρ_u , and the mean reaction rate can be modelled as $\rho_u u_L$. Laminar flame speed u_L experiences the contributions of flame curvature and strain with in the flame surface due to the local nature of flame. Therefore, flame curvature and strain must be accounted to calculate the laminar flame speed u_L from the unstrained laminar flame speed u_L^0 . Following, the algebraic expression of Metghalchi & Keck^{17, 18} laminar flame speed u_L is calculated in the present work.

$$u_L = u_L^0 \left(\frac{T_R}{T_o} \right)^\alpha \left(\frac{P}{P_o} \right)^\beta \quad (2)$$

where u_L^0 is the reference or un-strained laminar burning velocity taken as 0.45 m/s for stoichiometric propane/air mixture, T_o and P_o are reference temperature and pressure 298.15

K and 1.01 bar respectively and T_R is the reactant temperature. α and β are constants can be calculated from the expressions stated below^{17,18}.

$$\alpha = 2.18 - 0.8(\phi - 1.0) \text{ and } \beta = -0.16 + 0.22(\phi - 1.0) \quad (3)$$

where ϕ is the equivalence ratio.

2.1 Flame surface density model

The flame surface density (FSD) model developed by Boger⁴ is based on the assumption of an evolving thin flame front into fresh gases. Boger⁴ proposed a simple algebraic model for flame surface density, $\bar{\Sigma}$ from the analysis of 3-D DNS database of flame in a decaying isotropic and homogeneous turbulence. $\bar{\Sigma}$ is defined as a function of filtered reaction progress variable \tilde{c} , filter width $\bar{\Delta}$ and β which is a model coefficient.

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

The above expression is similar to the Bray-Moss-Libby (BML) expression for flame surface density in RANS¹⁹. The length $\Delta/4\beta$ is the wrinkling length scale of the sub-grid flame surface. The value of β is dependent on the ratio of filter width to laminar flame thickness and it increases when the flame is infinitely thin compared to grid size. For present analysis the value of β is chosen as 1.2 from the parametric analysis of propagating propane/air flames in the similar type of chambers^{3,6}.

2.2 The dynamic flame surface density model

The Dynamic flame surface density model is an extension to the flame surface density model⁴ discussed in the previous section. Knikker²⁰ has developed a similarity flame surface density (SFSD) model to account the SGS reaction rate following the similarity ideas of Germano¹¹. This model is coupled with fractal theory to determine the model constant K_s . SFSD model is tested on the experimental data extracted from the OH images obtained from planar laser-induced fluorescence technique on propane-air turbulent premixed flames. More details are available in the original paper²⁰. This model precisely predicts the regions where the sub-grid scale contribution to the flame surface density is high. However, this model was not successful in the calculation of the dynamic fractal dimension D . An appropriate value of the fractal dimension has to be used as an input from the experimental analysis in order to obtain good predictions.

Knikker⁷ developed a dynamic flame surface density (DFSD) model, similar to the similarity model²⁰ with the dynamic determination of fractal dimension. This model is also tested on the same experimental data sets stated above. The DFSD-based models are

successful in predicting the global mean flame surface density and also promising in calculating the appropriate fractal dimension. However, these models have never been implemented and tested for LES technique. In the present investigation, a dynamic flame surface density model is implemented in a LES code PUFFIN²¹ and the numerical predictions are validated against experimental data.

For clarity, mathematical details of the the developed DFSD model are presented in this section. The Flame surface density $\bar{\Sigma} = |\overline{\nabla c}|$ is the main term to be modelled in this procedure. It can be split into two terms, resolved and unresolved as follows:

$$\bar{\Sigma} = |\overline{\nabla c}| = \underbrace{\Pi(\bar{c}, \bar{\Delta})}_{\text{Resolved}} + \underbrace{\left(|\overline{\nabla c}| - \Pi(\bar{c}, \bar{\Delta}) \right)}_{\text{Unresolved}} \quad (5)$$

The unresolved component of FSD can be written as $\lambda = |\overline{\nabla c}| - \Pi(\bar{c}, \bar{\Delta})$. Defining a test filter $\hat{\Delta} > \bar{\Delta}$ and the ratio of test filter to grid filter is expressed as γ . Applying the test filter to flame surface density leads to:

$$\hat{\Sigma} = \left| \widehat{\nabla c} \right| = \underbrace{\Pi(\hat{c}, \hat{\Delta})}_{\text{Resolved@testfilter}} + \underbrace{\left[\left| \widehat{\nabla c} \right| - \Pi(\hat{c}, \hat{\Delta}) \right]}_{\text{Unresolved@testfilter}} \quad (6)$$

Unresolved flame surface density contribution at the test filter level can be written as

$$\Lambda = \left[\left| \widehat{\nabla c} \right| - \Pi(\hat{c}, \hat{\Delta}) \right] \quad (7)$$

Following similarity ideas¹¹ and assuming sub-grid scale contribution of unresolved FSD at test filter is same as that at grid filter and relating λ and Λ by using Germano¹¹ identity:

$$\Lambda - \hat{\lambda} = \left[\left| \widehat{\nabla c} \right| - \Pi(\hat{c}, \hat{\Delta}) \right] - \left[\left| \widehat{\nabla c} \right| - \Pi(\bar{c}, \bar{\Delta}) \right] \quad (8)$$

$$\Lambda - \hat{\lambda} = \left[\Pi(\bar{c}, \bar{\Delta}) - \Pi(\hat{c}, \hat{\Delta}) \right]$$

The sub-grid scale flame surface density contribution from above can be added to resolved flame surface density with a coefficient of K_s to get total FSD. Hence the flame surface density can be expressed as:

$$\bar{\Sigma} = \Pi(\bar{c}, \bar{\Delta}) + K_s \left[\Pi(\bar{c}, \bar{\Delta}) - \Pi(\hat{c}, \hat{\Delta}) \right] \quad (9)$$

where K_s is the model coefficient, which can be determined dynamically by identifying the sub-grid scale flame surface as a fractal surface⁷.

$$K_S = \frac{1}{1 - \gamma^{2-D}} \left[\left(\frac{\bar{\Delta}}{\delta_c} \right)^{D-2} - 1 \right] \quad (10)$$

where D is the fractal dimension, which can be calculated dynamically by following the fractal theory for wrinkled flames. Assuming the flame kernel as a fractal surface, Knikker⁷ developed a dynamic formulation, from the wrinkling factor at grid filter and the conservation of flame surface averaged over a given volume as given in equation 11. In the present simulation, this formulation is not used due to the numerical difficulties in implementation in an LES model. Recent investigations of Fureby²² used an empirical formula to determine the fractal dimension, originally parameterised by North and Santavicca²³ as shown in equation 12. Based on the analysis of wrinkling length scales of propane/air flames, Patel and Ibrahim²⁴ reported the laminar fractal dimension D_L as 2.19.

$$D = 2 + \frac{\log \left(\left\langle \Pi(\bar{c}, \bar{\Delta}) \right\rangle / \left\langle \Pi(\hat{c}, \hat{\Delta}) \right\rangle \right)}{\log \gamma} \quad (11)$$

$$D = \frac{2.05}{\left(\frac{u'}{u_L} + 1 \right)} + \frac{2.35}{\left(\frac{u'_L}{u'} + 1 \right)} \quad (12)$$

Following the work of Patel and Ibrahim²⁴, dynamic determination of the fractal dimension is achieved by replacing the u' with the SGS velocity fluctuations, u'_Δ in case of LES as shown in equation 13. The SGS velocity fluctuations, u'_Δ is calculated from the flow strain rate. In equation 10, δ_c , the lower cut off scale, has to be dynamically modelled. However, following Knikker⁷, we have modelled this to be three times the laminar flame thickness.

$$D = \frac{2.19}{\left(\frac{u'_\Delta}{u_L} + 1 \right)} + \frac{2.35}{\left(\frac{u'_L}{u'_\Delta} + 1 \right)} \quad (13)$$

3 LES CALCULATIONS

The calculations are performed using a compressible version³ of the LES code PUFFIN originally developed by Kirkpatrick²¹. The code solves strongly coupled Favre-filtered flow equations written in a boundary fitted co-ordinate 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 for diffusion terms. The third order upwind scheme of Leonard, QUICK²⁵ and SHARP²⁶ are used for advection terms of the scalar equations to avoid problems associated with oscillations in the solution. The QUICK scheme is also sometimes used for the momentum equations in areas of the domain where the grid is expanded and accurate calculation of the flow is less important. 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. A number of iterations are required at every time step due to strong coupling of equations with one other. Solid boundary conditions are applied at the bottom, vertical walls, for baffles and obstacle, with the power-law wall function of Werner and Wengle²⁷ used to calculate wall shear. A non-reflecting boundary condition is used to prevent reflection of pressure waves at these boundaries. The initial conditions are quiescent with zero velocity and reaction progress variable.

The equations, discretized as described above, are solved using a Bi-Conjugate Gradient solver with an MSI pre-conditioner for the momentum, scalar and pressure correction equations. The time step is limited to ensure the CFL number remains less than 0.5 with the extra condition that the upper limit for δt is 0.3ms. The solution for each time step requires around 8 iterations to converge, with residuals for the momentum equations less than $2.5e-5$ and scalar equations less than $2.0e-3$. The mass conservation error is less than $5.0e-8$.

Simulations are made in three dimensional non-uniform Cartesian co-ordinate system for compressible flow and having low Mach number. Using FSD and DFSD models for the SGS reaction rate, simulations are performed for coarse (0.25 million), medium (0.55 million) and fine (2.7 million) grid resolutions in order to examine the grid dependency of the results obtained.

4 EXPERIMENTAL TEST CASE

The experimental test case used here for model validation is that reported by the combustion group at the University of Sydney^{8, 28}. The test rig consists of a laboratory scale premixed combustion chamber with built-in repeated solid obstructions as shown in figure 1. Experimental data for the flame structure and generated over-pressure have recently been published^{8, 28} are used here for model validation. The chamber has a square cross section of 50 mm and a length of 250 mm. It has a total volume of 0.625 L. Three baffle plates and a square obstacle are placed at different downstream location from the bottom ignition end. Each baffle plate is of 50 x 50 mm aluminium frame constructed from 3 mm thick sheet. This consists of five 4 mm wide bars each with a 5 mm wide space separating them, rendering a blockage ratio of 40%. The baffle plates are aligned at 90 degrees to the solid obstacle in the configuration and located at 20, 50 and 80 mm respectively from the ignition point. A solid square obstacle of 12 mm in cross section is centrally located at 96 mm from the ignition

point running through out the chamber cross section which causes significant disruption to the flow.

5 RESULTS AND DISCUSSIONS

LES results for turbulent propagating premixed flame in a confined chamber, shown in figure 1, are presented for two SGS reaction rate models, namely the FSD and DFSD, and compared with experimental measurements. LES predictions of time traces of the over pressure from the SGS-DFSD for various grid resolutions stated above are shown together with experimental measurements in figure 2. It is evident from these results that, the fine grid results are in good comparison with experimental measurements in capturing the over pressure trend. Grid dependency tests have been conducted for LES simulations using the FSD (not shown here) and identified that beyond the fine grid resolution, results are grid independent. Therefore, results reported in the following sections are from the fine grid simulations for both the FSD and DFSD reaction rate models.

Figure 3 (a), (b), (c) shows a comparison of time traces of the over pressure, flame position, flame speed and 3 (d) shows flame speed with flame position for LES simulations of both the models with experimental measurements. Peak over pressure predictions from DFSD model is slightly under-predicted but it has captured the additional reaction rate when compared to FSD model. Additional reaction rate is due to the involvement of the unresolved flame surface density. The peak over pressure as shown in figure 3 (a) from the LES of the dynamic flame surface density model is 118.24 mbar at 11.42 ms and from flame surface density model 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. Flame propagation speed, position and structure after ignition and until the flame exits the chamber are in excellent agreement with the experimental measurements for both the FSD and DFSD models.

Calculated SGS reaction rate are presented in figure 4 at different times after ignition and compared with the corresponding experimental high speed video images. The calculated reaction rate images from both the FSD and DFSD models clearly matches with experimental images. The overall flame structure and speed as well as the mechanism by which the flame approach the solid obstructions, jetting through the gap around the obstacle and reconnection downstream from the solid obstacle are all very well predicted. It has been found that both models successfully predict the essential features of flame/flow interactions, however results from the DFSD model, shown in figure 4(c), are in better agreements with experimental measurements compared with those obtained using the FSD model shown in figure 4(b). This

better results with the use of the DFSD model is due to the contributions of unresolved flame surface density to the mean rate of chemical reaction.

It is evident from figure 4(c) that, the DFSD model is able to predict the regions of the locations of the sub-grid scale contribution of the flame surface density. To get more details out of this, resolved and unresolved flame surface density contributions to the reaction rate from the DFSD simulation are presented in figure 5. Reaction rate contours of DFSD model at 11.0 ms after ignition are shown in figure 5 (a). Corresponding resolved and unresolved contributions of the flame surface density are shown in figures 5(b) and 5 (c). Resolved flame surface density contribution to the reaction rate by DFSD model is the same as that of the FSD model as both models are based on the flamelet concept. It can be identified from figure 5(c), that the unresolved flame surface density contribution is accurately predicted by the dynamic formalism. Additional or unresolved contributions of flame surface density shown in 5 (c) is evidently increasing the global mean reaction rate and seems to be fairly calculated.

Overall, the numerical predictions from DFSD model are quite encouraging and substantiate the good representation of the flame position, speed, structure, and the interactions between the flame, flow and solid obstructions. However, the magnitude and timing of occurrence of the peak over pressure are slightly under-predicted. This may be due to some errors associated with the calculations of the fractal dimension, especially at early stages of flame propagation and the assumption of lower cut-off scale employed. Further investigation in this direction is planned by the current authors to assess the predictability of this model over a wide range of flow configurations.

6 CONCLUSIONS

LES simulations of propagating turbulent premixed propane/air flame is reported using two SGS reaction rate models, namely a dynamic DFSD and the conventional FSD models. A newly formulated DFSD model, based on the flamelet concept, is implemented in an LES code and numerical predictions are compared with results from the FSD model and both models are validated against experimental measurements. It can be concluded that the DFSD model, reported in this paper, has remarkably predicted the sub-grid reaction rate and the overall features of the turbulent propagating flame. A further analysis is planned by the current authors to identify a more accurate dynamic determination of the fractal dimension and the lower cut-off scale, which are expected to improve the quality of the results.

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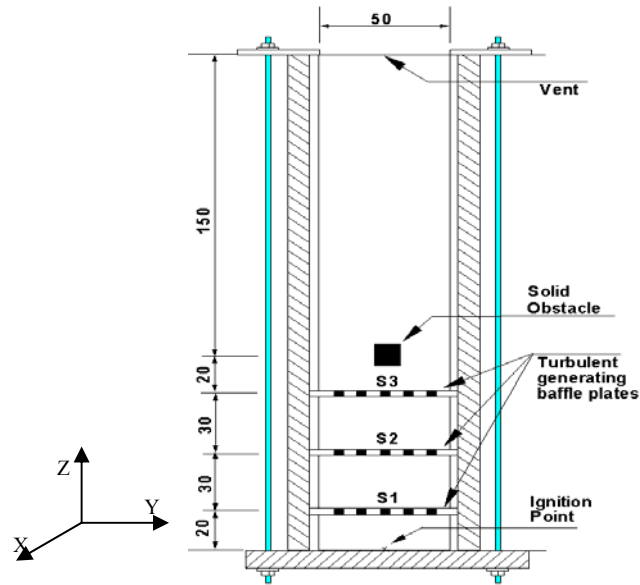


Figure 1: Schematic diagram of the premixed combustion chamber. All dimensions are in mm.

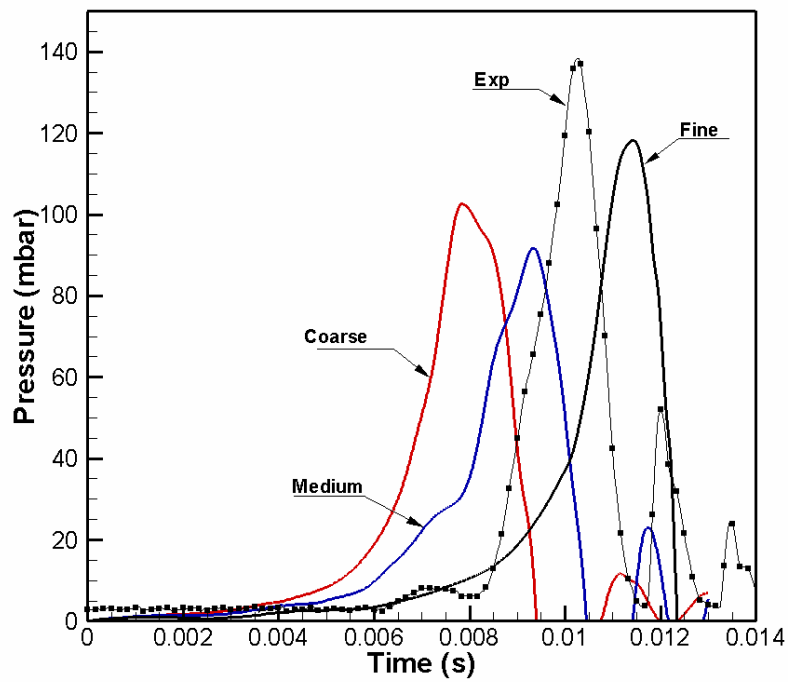


Figure 2: Time traces of the over pressure from LES of DFSD model for various grids employed are compared with experimental measurements.

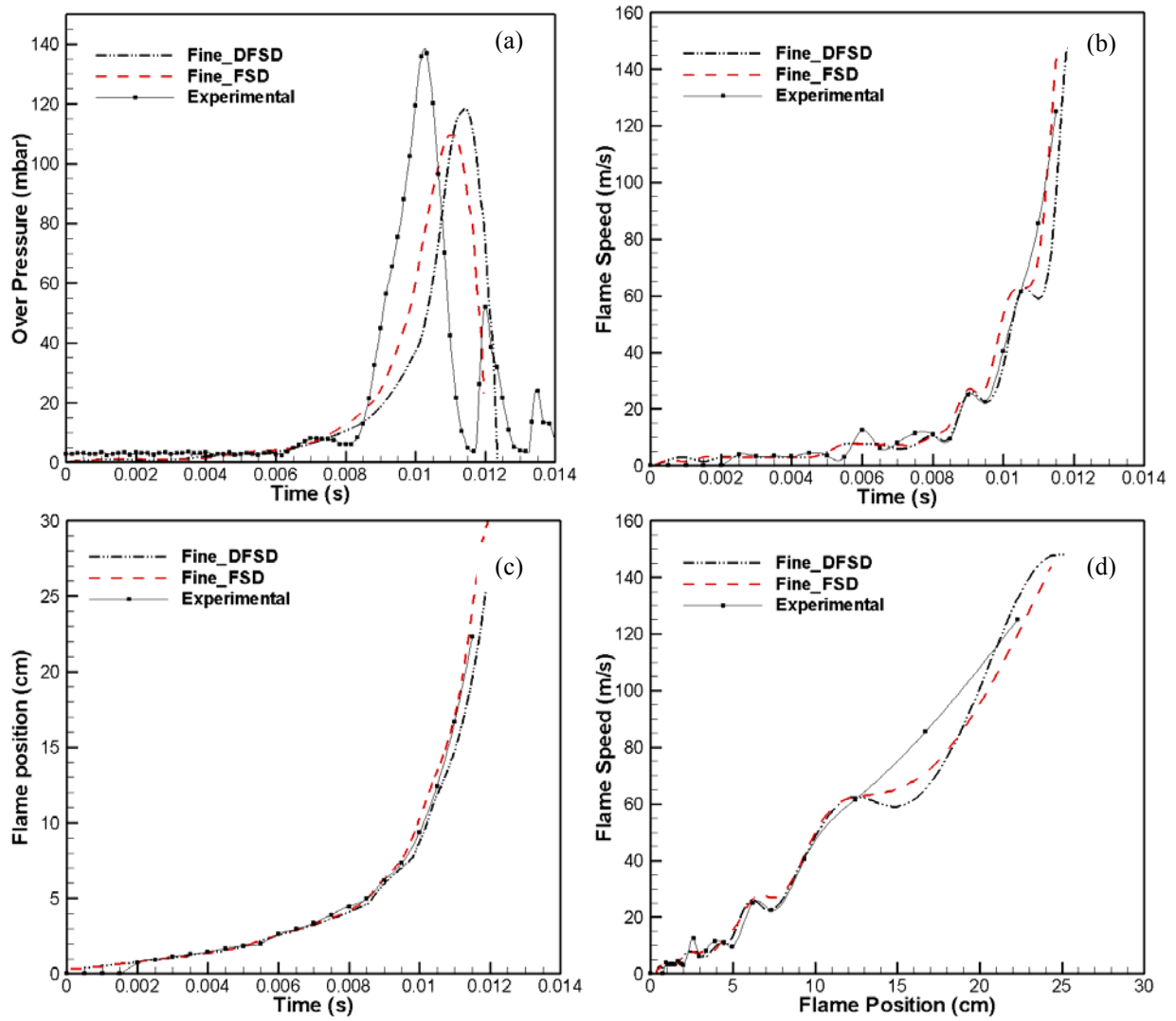


Figure 3: Time traces of LES simulations from FSD and DFSD models are compared with experimental measurements (a) Peak over pressure (b) Flame speed (c) Flame position (d) Flame speed is plotted against flame position.

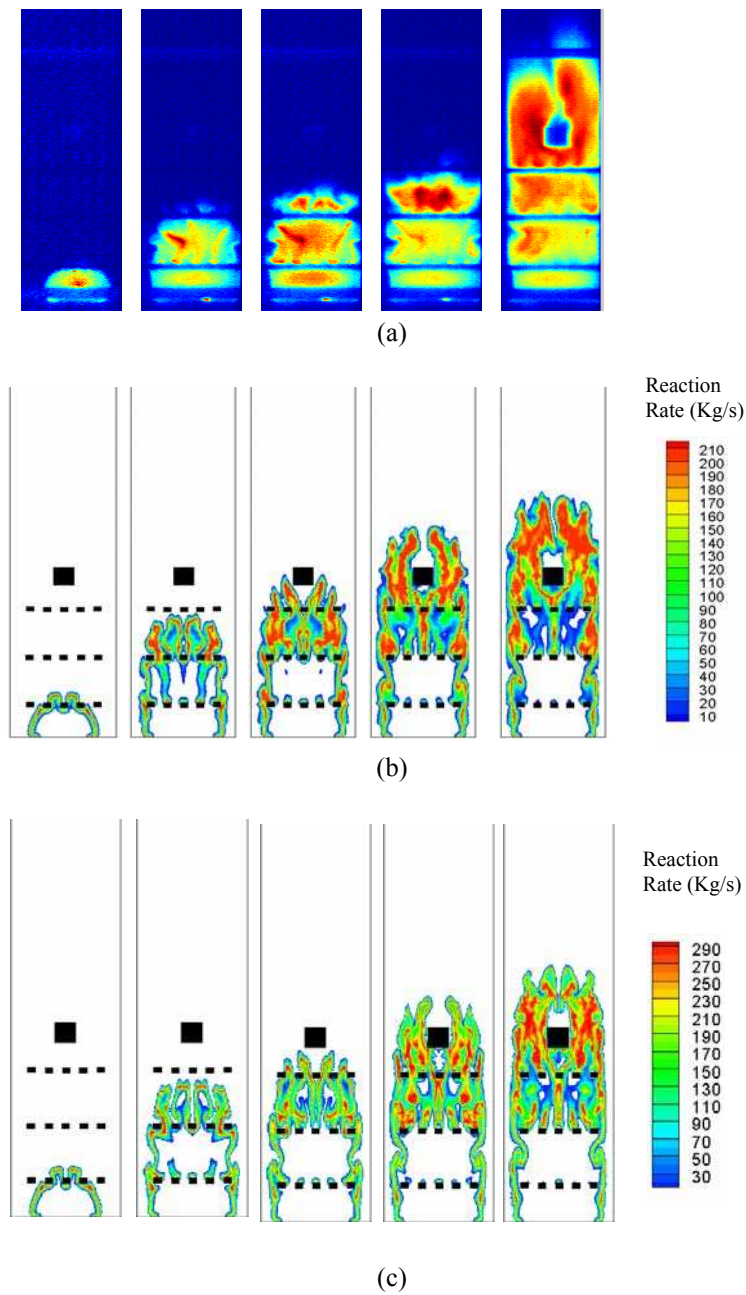
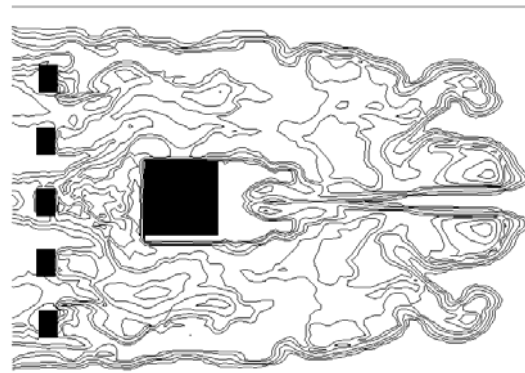
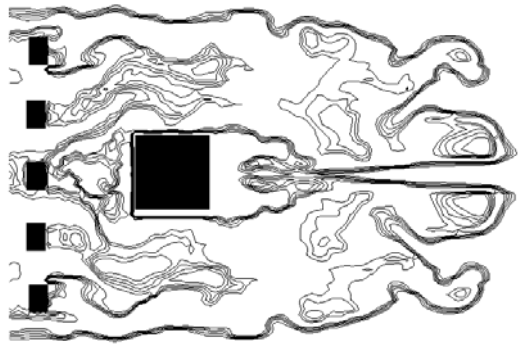


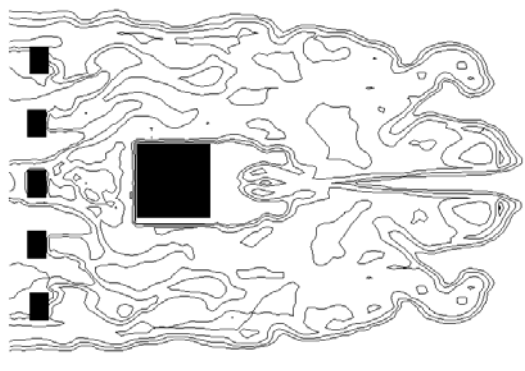
Figure 4: Sequence of images to show flame structure at different times after ignition. Reaction rate contours generated from LES predictions are presented against high speed recorded video images of experiments. (a) Experimental images at 6, 9.5, 10, 10.5 and 11.0 ms (b) Numerical snap shots of reaction rate from FSD model at 6, 9.5, 10.0, 10.5, and 10.8 ms and (c) Numerical snap shots of reaction rate from DFSD model at 6, 9.5, 10.0, 10.5, and 10.8 ms.



(a)



(b)



(c)

Figure 5: Turbulent premixed flame after 11.0 ms of ignition from numerical simulations using DFSD model. For better visualisation, flame front after the square obstacle is considered (a) reaction rate contour image (b) contributions of the resolved flame surface density shown in equation 5 (c) contribution of the unresolved flame surface density modelled by dynamic formalism.