A DYNAMIC SGS MODEL FOR LES OF TURBULENT PREMIXED FLAMES

Sreenivasa Rao Gubba[**,§], Salah S Ibrahim[*] and W Malalasekera[**]

[**]Wolfson School of Mechanical and Manufacturing Engineering
Loughborough University, Loughborough, LE11 3TU, UK

[*]Department of Aeronautical and Automotive Engineering
Loughborough University, Loughborough, LE11 3TU, UK

[§]Correspondence author. Phone: +44 (0) 1509 227520 Email: S.R.Gubba@Lboro.ac.uk

ABSTRACT Numerical simulations are carried out for transient turbulent premixed flames using large eddy simulations (LES) technique. The sub-grid scale (SGS) mean chemical reaction rate is calculated using a simple algebraic relation for flame surface density (FSD), with a dynamic formulation for the model coefficient. The dynamic model is derived based on fractal theory and a flame wrinkling factor and implemented in compressible LES code. The developed model is used to simulate turbulent premixed flames of stoichiometric propane/air mixture in a vented combustion chamber, propagating over built-in solid obstacles. The fractal dimension is dynamically calculated by viewing the flame front as a fractal surface, using the SGS velocity fluctuations and the strained laminar burning velocity. The model predictions are validated against experimental measurements where good agreements are obtained.

1. INTRODUCTION

Combustion plays a vital role in converting energy from one form to another and giving the utmost comfort to the human life. The successfulness of understanding the physics of combustion with the decades of the research is continual, with many open questions to be answered. For example, the chemistry-turbulence interactions, possibilities of flame extinction and re-ignition, the combustion instabilities due to acoustics etc. Combustion being a complex thermo-chemical process, formulates a multifaceted problem when coupled with unsteadiness and turbulence. Transient turbulent premixed propagating flames are encountered in many engineering devices and their optimal design has always faced several difficulties due to the impracticability of the empirical findings in designs. Hence numerical simulations based on the theoretical background is quite encouraged to deal with the combustion modeling in order to improve the understanding.

Numerical simulations of turbulent combustion by large eddy simulations (LES) technique have been established as a potential and reliable technique over the conventional Reynolds averaged Navier-Stokes (RANS) approach in the last two decades. In case of LES, large eddies in the flow field are resolved and the small eddies are modeled by a sub-grid scale (SGS) model. These small

eddies are assumed to be isotropic in nature and modeled by simple algebraic relations and in some instances by empirical models. In LES of turbulent premixed modeling, the main challenges involved are SGS modeling of the turbulence and the chemical reaction rate. Although, LES relies less than RANS on modeling due to the improved involvement of the turbulence by resolving through the dynamic modeling, chemical reaction rate modeling is practically difficult due to the flame thickness, which is less than the grid size to be resolved. Therefore a robust SGS model to account the chemical reaction rate in LES is significantly required.

Several modeling approaches such as flame surface density [Bray 1990 and Pope 1988], flame tracking technique (G-equation) [Williams 1985], probability density function (PDF) [Möller *et al.* 1996] and artificially thickened model [Charlette *et al.* 2002] are successfully adapted from Reynolds Averaged Navier-Stokes (RANS) to LES premixed flames. The flame surface density (FSD) models are well established in accounting the chemical reactions in the context of RANS [Bray 1990 and Pope 1988] and LES [Boger *et al.* 1998 and Kirkpatrick *et al.* 2003], as a function of reaction progress variable and filter width. The present study employs an algebraic flame surface density model to account the mean chemical reaction rate. Flame surface density models are fundamentally based on flamelet concepts, i.e. viewing the reaction rate zone as a collection of thin propagating reaction layers, thinner than the smallest turbulent scales, having laminar flame structure and propagating locally at laminar burning velocity. This approach is based on evaluating the flamelet surface area to volume ratio (flamelet surface density), which can be computed via an algebraic [Kirkpatrick *et al.* 2003] or through a transport equation [Hawkes and Cant 2001]. Computing sub-grid flame surface density by solving a transport equation in LES, though an attractive option, but will result in several unclosed terms which need to be closed by appropriate models and lead to excessive computational times. Algebraic models available are similar to Bray-Moss-Libby (BML) model [Bray *et al.* 1989] in the context of RANS and are simple extensions to LES. The existing simple algebraic model [Boger *et al.* 1998] is capable of predicting turbulent flames, with certain drawbacks such as predicting peak over pressure and the flame arrival time (FAT). One reason might be due to the use of a constant value for model coefficient, which is not universal and generally known to depend on several parameters such as grid resolution, turbulence level and chemistry. Hence in the present study, the model coefficient is modeled dynamically following fractal theory for wrinkled flames.

A laboratory scale premixed combustion chamber established by The University of Sydney combustion group [Kent *et al.* 2005] with built-in solid obstacles is considered as a test case here to validate the model predictions. Repeated solid obstacles are presented to enhance the turbulence levels and to increase flame propagating speed, which eventually lead to stronger interactions between flame and solid obstacles. These interactions 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 paper is organized as follows: Section 2 describes combustion model and development of the dynamic procedure for model coefficient. Section 3 presents the laboratory scale test case used for model validation. Section 4 describes numerical procedures used in LES calculations and the computational domain. Validation of LES predictions and their comparisons with experimental measurements are presented and discussed in Section 5. Conclusions of the present investigation are summarized in Section 6.

2. COMBUSTION MODELLING

2.1 The Reaction Rate Model: Modelling reaction rate in turbulent premixed flames is very challenging due to its non-linear relation with chemical and thermodynamic states, and often

characterized by propagating thin reaction layers thinner than the smallest turbulent scales. The major difficulty in the modelling of reaction rate is due to the sharp variation of thermo chemical variables through the laminar flame profile, which is typically very thin [Veynante and Poinsot 1997]. This issue is strongly affected by turbulence, which causes flame wrinkling and thereby forming the most complex three way thermo-chemical-turbulence interactions. However, assuming single step irreversible chemistry and the Zeldovich instability (thermal diffusion), i.e. unit Lewis number will reduce complexity of the whole system. The chemical status is described by defining the reaction progress variable c from zero to one in unburned mixture and products respectively, based on fuel mass fraction. Mathematically it can be derived as, $1 - Y_{fu}/Y_{fu}^0$. 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:

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

In 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 $\dot{\omega}_c$ is the chemical 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 of the equation (1) is filtered reaction rate, which is required to be model by sub-grid scale model.

The SGS mean chemical reaction rate is modelled by following the flamelet approach, by viewing reaction zone as a collection of thin propagating layers, having structure of laminar flames. One major advantage of this approach is decoupling of chemistry from flame-turbulence interactions by describing mean flame surface density. Therefore, the mean chemical reaction rate per unit volume, can be modelled as $\overline{\dot{\omega}}_c = R\overline{\Sigma}$. Here R is the mean reaction per unit surface area and $\overline{\Sigma}$ is the flame surface density, which is to be modelled in the framework of LES. In present work, a simple algebraic model given in equation (3) for flame surface density derived from DNS analysis based on flamelet concept [Boger *et al.* 1998] is employed with dynamic procedure for model coefficient.

$$\overline{\dot{\omega}}_c = \rho_u u_L \overline{\Sigma} \tag{2}$$

where ρ_u is the density of unburned mixture, u_L is the laminar burning velocity, and $\overline{\Sigma}$ is the flame surface density. Flame surface density can be modelled as:

$$\overline{\Sigma} = 4\beta\frac{\tilde{c}(1-\tilde{c})}{\overline{\Delta}} = 4\alpha\Xi\frac{\tilde{c}(1-\tilde{c})}{\overline{\Delta}} \tag{3}$$

where $\tilde{c}$ is the Favre-filtered mean reaction progress variable, $\overline{\Delta}$ is the filter width, Ξ is flame wrinkling factor and β and α are model coefficients. From the DNS analysis [Boger *et al.* 1998], values of α and β are derived considering unity flame wrinkling factor, as:

$$\beta = \alpha\Xi = \sqrt{\frac{6.0}{\pi}}\Xi = 1.382 \tag{4}$$

A range of values for the model coefficient β, in RANS and LES can be found in literature ranging from 1.0 to 2.6. In most of the studies, model coefficient has been tuned in order to get the qualitative agreement with experimental values. From previous studies of propane/air turbulent premixed flames [Ibrahim *et al.* 2007], it is identified that the model coefficient β is dependent on several parameters, such as chemistry, turbulence level, grid resolution and flame wrinkling factor. Choosing a constant value for β resembles the Eddy-Break-Up (EBU) model in RANS, which is inappropriate and alters the solution based on model coefficient. Hence, there is a requirement of

dynamic modelling or self-scaling of the model coefficient based local flame characteristics. From equation (3) it can be seen that the model coefficient is of multiplicative nature and deriving it using Germano identity [Germano *et al.* 1991] fails as shown below.

2.1.1 Determination of the multiplication coefficientβ. The basic idea is to derive model coefficient from filtered reaction progress variable at test filter by applying Germano identity to equation (2). However, following the work of Charlette *et al.* [2002], we identified that the model coefficient in equation (3) is of multiplicative in nature and fails for the application of Germano identity [Germano *et al.* 1991]. Considering the equation (2) and (3) for mean SGS chemical reaction rate and defining γ as a ratio of test filter to grid filter, i.e. $\hat{\bar{\Delta}}/\bar{\Delta}$, such that the test filter $\hat{\bar{\Delta}}$ is greater than grid filter $\bar{\Delta}$. Applying test filter to flame surface density (equation 2) using the Germano identity [Germano *et al.* 1991] leads to:

$$\left\langle \widehat{4\rho_u u_L \beta \frac{\tilde{c}(1-\tilde{c})}{\bar{\Delta}}} \right\rangle = \left\langle 4\rho_u u_L \beta \frac{\hat{\tilde{c}}(1-\hat{\tilde{c}})}{\hat{\bar{\Delta}}} \right\rangle \tag{5}$$

If one assumes that β is model coefficient in the volume over which averaging has been performed, then the above equation can in principle be solved for β. The above equation reduces to

$$4\rho_u u_L \beta \left\langle \widehat{\frac{\tilde{c}(1-\tilde{c})}{\bar{\Delta}}} \right\rangle = 4\rho_u u_L \beta \left\langle \frac{\hat{\tilde{c}}(1-\hat{\tilde{c}})}{\hat{\bar{\Delta}}} \right\rangle \tag{6}$$

As it is immediately apparent, β cancels from each side of equation (6) and the Germano identity becomes ineffective in helping us to determine β.

2.1.2 Modelling β using wrinkling flame factor. In order to overcome the above failure, model coefficient can be modelled as wrinkling flame factor as observed in the equation (3) by choosing unity for *α*. Defining the flame wrinkling factor Ξ in the equation (3), as a ratio of flame surface density to its projection in the normal direction of the flame propagation [Knikker *et al.* 2004] and identifying flame surface as a fractal surface between inner and outer cut-off scales leads to:

$$\Xi = \left[\frac{\bar{\Delta}}{\delta_c} \right]^{D-2} \tag{7}$$

This approach has been implemented successfully in the thickened flame modeling [Charlette *et al.* 2002]. In the above equation, $\bar{\Delta}$ is outer cut off scale, δ_c is the inner cut-off scale and *D* is the fractal dimension. The critical assumption involved in choosing such an expression for wrinkling flame factor is that vortices of all sizes between outer and inner cut-off scales contribute to the wrinkling of the flame surfaces. In general, outer cut-off length represents the largest eddies of integral length scales and the inner cut-off length represents eddies of the size Kolmogorov length scales. In LES, filter width, Δ is generally considered as outer cut-off scale and for inner cut-off scale there are several expressions available in the literature related to Gibson scale or Kolmogorov scale or laminar flame thickness. In the present study, we considered inner cut-off scale as three times of the laminar flame thickness following Knikker *et al.* [2004]. Hence, β is calculated as:

$$\beta = \alpha \Xi = \left[\frac{\bar{\Delta}}{\delta_c} \right]^{D-2} \tag{8}$$

2.1.3 Modelling of the fractal dimension. Several experimental and numerical studies have been conducted in past to identify the fractal dimensions of turbulent premixed flames. Majority of the studies related to turbulent premixed flames have been used the appropriate values for fractal

dimension as an input parameter, based on the turbulence levels and flame wrinkling. These values are ranging [Gülder *et al.* 2000] from 2.2 to 2.5 as found in literature. However, present study is carried out using an empirical model parameterised by North and Santavicca [1990] to calculate fractal dimension of the turbulent propagating flame following fractal theory, by employing dynamic formalism. This relation is based on the local velocity fluctuations and the laminar burning velocity for turbulent flames given in equation (9). This model allows one to automatically clip the fractal dimension in between the chosen lower and upper limits for a particular flame. For the present investigation, laminar fractal dimension D_L and the turbulent fractal dimension D_T are taken as 2.19 and 2.35 respectively, following the analysis of wrinkling length scales of propane/air flames of Patel and Ibrahim [1999]. Recently Fureby [2005] implemented this empirical model in LES calculations successfully by replacing *u'* with SGS velocity fluctuations, u'_Δ as shown in equation (10), to determine the fractal dimension for propane/air turbulent flames. The local fractal dimension is dynamically determined for every realisation, by calculating SGS velocity fluctuations from the flow strain rate tensor.

$$D = \frac{D_L}{\left(\dfrac{u'}{u_L}+1\right)} + \frac{D_T}{\left(\dfrac{u_L}{u'}+1\right)} \tag{9}$$

$$D = \frac{D_L}{\left(\dfrac{u'_\Delta}{u_L}+1\right)} + \frac{D_T}{\left(\dfrac{u_L}{u'_\Delta}+1\right)} \tag{10}$$
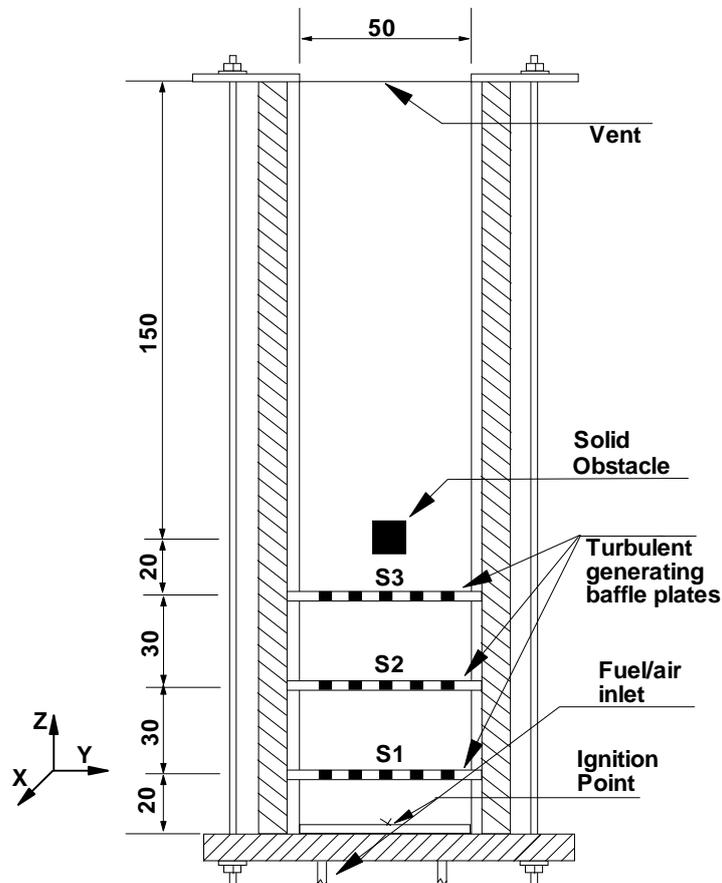
Figure 1. Schematic diagram of the premixed combustion chamber. All dimensions are in mm.

2.2 Turbulence Modelling: In LES, it is usual practice to model the SGS contributions of turbulence in Favre-filtered momentum equation, using classical Smagorinsky procedure. The momentum flux $\tau_{ij} = \bar{\rho}\left(\tilde{u}_i\tilde{u}_j - \widetilde{u_iu_j}\right)$ is computed using Smagorinsky eddy viscosity model [1963], which yields the SGS turbulent eddy viscosity as:

$$\tau_{ij} - \frac{1}{3}\delta_{ij}\tau_{kk} = -2\bar{\mu}_{\mathrm{SGS}}\left(\tilde{S}_{ij} - \frac{1}{3}\delta_{ij}\tilde{S}_{kk}\right) \tag{11}$$

Here, the eddy viscosity μ_{SGS} is modelled as a function of the filter size and strain rate $\tilde{S}_{ij}$.

$$\mu_{\mathrm{SGS}} = \bar{\rho}\left(C_s\bar{\Delta}\right)^2\left|\tilde{S}\right| \tag{12}$$

In the above equation, $\left|\tilde{S}\right| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$ and C_s is the dimensionless Smagorinsky coefficient. The Smagorinsky coefficient is evaluated using instantaneous flow conditions using the dynamic procedure of Germano *et al.* [1991] for compressible flows [Moin *et al.* 1991].

3. TEST CASE

The experimental test case used in present work for model validation is that reported by The University of Sydney combustion group [Kent *et al.* 2005]. Schematic diagram of the laboratory scale premixed test rig with built-in repeated solid obstacles is illustrated in Figure 1. The chamber is of 50 mm square cross section with a length of 250 mm and having a total volume of 0.625 L. This chamber is of particular interest because of its smaller volume and its capability to hold a propagating flame in strong turbulence environment, generated due to the repeated solid obstacles at different downstream locations from the bottom ignition end. Totally it has three baffle plates at 20, 50 and 80 mm respectively from the ignition point and a solid square obstacle of 12 mm in cross section, which is centrally located at 96 mm from the ignition point running through out the chamber, causing significant disruption to the flow. Each baffle plate is of 50 x 50 mm aluminum frame constructed from 3 mm thick sheet. This consists of five 4 mm wide bars each with a 5 mm wide space spreading them through out the chamber, rendering a blockage ratio of 40%. The baffle plates are aligned at 90 degrees to the solid obstacle in the chamber. Experimental data for flame structure and generated over-pressure, recently published by Kent *et al.* [2005] are used here for model validation.

4. LES SIMULATIONS

The models described in section 2 are implemented in an in-house, compressible version of LES code PUFFIN [Kirkpatrick *et al.* 2003], originally developed by Kirkpatrick [2002]. LES simulations are performed for initially stagnant propane/air mixture of equivalence ratio 1.0, propagating past obstacles upon ignition, thereby generating turbulence. The LES code solves fully compressible, strongly coupled, Favre-filtered flow equations, written in a boundary fitted co-ordinates 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 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, QUICK [Leonard 1979] and SHARP [Leonard 1987] 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 Wengle [1991] is 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. Ignition is modelled by setting the reaction progress variable to 0.5 with in the radius of 4 mm at the bottom centre of chamber.

The governing equations, discretized by finite volume method, 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.

4.1 Computational Domain: The computational domain has dimensions of 50 x 50 x 250 mm (combustion chamber) where the combustion takes place and the flame propagates over baffles and solid obstacle surrounded by solid wall boundary conditions. This domain is adequately extended to 325 mm in x, y and 250 mm in z direction with the far-field boundary conditions. LES simulations are carried out for 3-D, non-uniform, Cartesian co-ordinate system for a compressible flow, having low Mach number. Sub-grid scale chemical reaction rate is calculated using models described in section 2 and LES predictions are compared against experimental measurements. In order to examine the solution dependence on grid resolution, simulations are performed for three grid resolutions with coarse (0.25 million), medium (0.55 million) and fine (2.7 million) grids.

5. RESULTS AND DISCUSSION

Results from LES simulations using a constant and dynamic model coefficient in flame surface density equation are compared against the experimental measurements and discussed in this section. Grid dependency tests have been carried with three different grids described in the above section (not shown in this paper) and identified that beyond fine grid resolution, the LES solution is grid independent. Hence all the results presented in this paper are for fine grid (90x90x336) resolutions. For the initial analysis, time histories of over pressure measured near closed ignition end is considered and shown in Figure 2a. Solid line in Figure 2a represents the dynamic model coefficient and dash double dotted line represents a constant model coefficient, compared together with dashed line representing experiments. It is evident from Figure 2a that, both the simulations predicted similar pressure trend and rate of pressure rise. Slightly higher peak over pressure i.e. 114 mbar at 11.0 ms is predicted by the dynamic model coefficient compared with 110 mbar at 11.05 ms using a constant value for β. However, both LES simulations slightly under predicted the peak over pressure inside chamber against experimental measurement of 138 mbar at 10.3 ms. One reason for the under prediction of peak pressure might be due to the simple algebraic model used in present study. Employing a dynamic model or solving a transport equation for FSD could improve the pressure predictions.

Flame characteristics such as flame position, speed and structure are extracted from experimental video images in order to validate the numerical predictions. In present study, we considered a bin size of 0.5 ms to evaluate these characteristics, as used in experiments to explore the recorded measurements. Figure 2b shows the flame position from both LES simulations against experimental flame position. In case of LES, flame position is defined as the leading edge of the flame, where reaction progress variable is 0.5 i.e. extreme edge of the flam front from the ignition end in axial

direction. Evidently, Figure 2b shows a very good overlapping of LES predictions with experiments, which confirms the excellent agreement. Calculated time histories of flame speed are presented with experimental flame speed in Figure 2c. Figure 2d presents flame speed against flame position for numerical predictions and experimental measurements. Figure 2c and 2d are confirming the excellent agreement (based on time scale) at any stage of the flame propagation, while encountering the solid obstacles. For example, at time 11 ms experiments recorded 55 m/s where as LES has predicted ~ 57m/s. However, based on the peak over pressure reference, the flame characteristics are slightly different due to the peak pressure time incidence as shown in Table 1. This difference is expected due to the simple algebraic model used in present simulations. It is quite encouraging that, using a dynamic model coefficient is predicting almost all the same trend as predicted by LES simulation with model constant, except slightly higher peak over pressure. However, to confirm the influence of model coefficient on numerical predictions, further analysis is carried and presented below.

Figure 3 shows time histories of the model coefficient β, for both the LES simulations. The value of the model coefficient is extracted from numerical data at leading edge of the propagating flame front, where flame position is defined. The solid line in Figure 3 represents model coefficient calculated by dynamic formalism and thin dashed line represents constant value i.e. 1.2 used in simulations. It is noteworthy at this stage that, the model coefficient calculated by the wrinkling flame factor, is almost all close to the constant value used (1.2) before the peak over pressure occurrence ($t < 11$ms). After the peak over pressure, it is noticed that the model coefficient has reached a maximum value of about 1.6, which is due to the dynamic modelling. It can also be noticed that, the model coefficient has suddenly jumped at around 11ms from 1.2 to 1.25, which has caused to account slightly higher SGS chemical reaction rate, due to which a little higher peak pressure has predicted.

Figure 3 also shows the fractal dimension D represented by a dash dot line showing on the right hand scale, calculated using the empirical model in Equation (10). These values are also extracted at leading edge of the flame and representing wrinkled nature of flame at various instants of time. The values of fractal dimensions are confirming the dynamic nature of the flame wrinkling due to the local turbulence, which has captured properly at various instants. A sudden jump of fractal dimension from 2.25 to 2.35 at around 8 ms can be noticed, where flame protrudes through third baffle plate and encounters square solid obstacle. However, there is no much impact noticed due to this jump on model coefficient, as lower cut-off scale is acting as a damping function.

Figure 4 shows accounted chemical reaction rate plotted against reaction progress variable by both models at peak over pressure reference. The scattered data shown in symbols (dots) is from dynamic modelling of the model constant and dashed line represents averaged reaction rate from FSD using a model constant for β. The reason for showing averaged reaction rate instead of scattered data in later case is just to distinguish the reaction rates from both models. It can be noticed that, a slightly higher chemical reaction rate (~210 kg/s) has captured at reaction progress variable 0.5, which is used to define flame position in the combustion chamber.

Table 1
LES predictions and experimental measurements based on peak over pressure reference.

	Model Coefficient (β)	Peak over pressure (mbar)	Time (ms)	Flame Position (cm)	Flame Speed (m/s)
LES	Constant	110.0	11.05	17.2	77
	Dynamic	114.0	11.00	16.5	75
Experiment	-N/A-	138.0	10.30	12.0	54
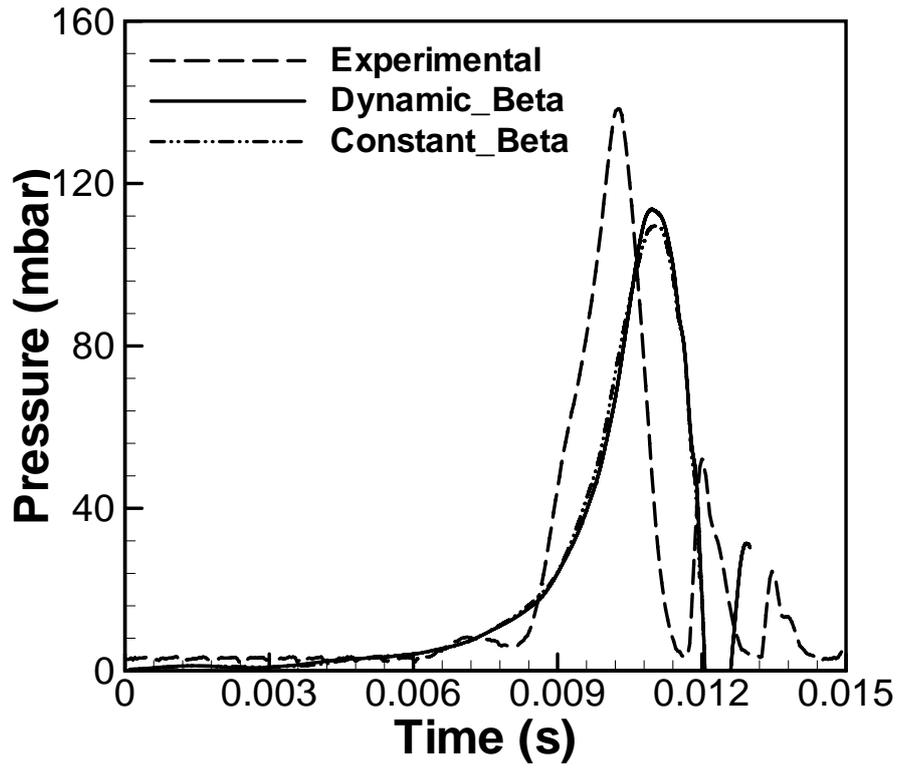
Figure 2a. Comparisons between experimental and numerical results for the pressure-time history.
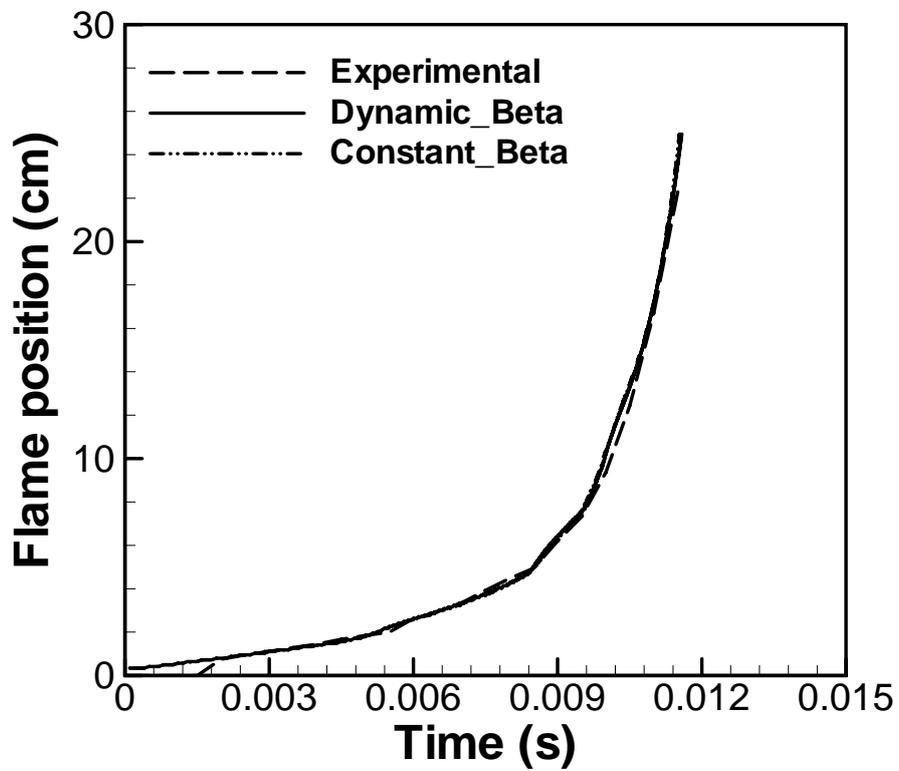
Figure 2b. Comparisons between LES simulations and experimental results for the flame front location at different times after ignition.
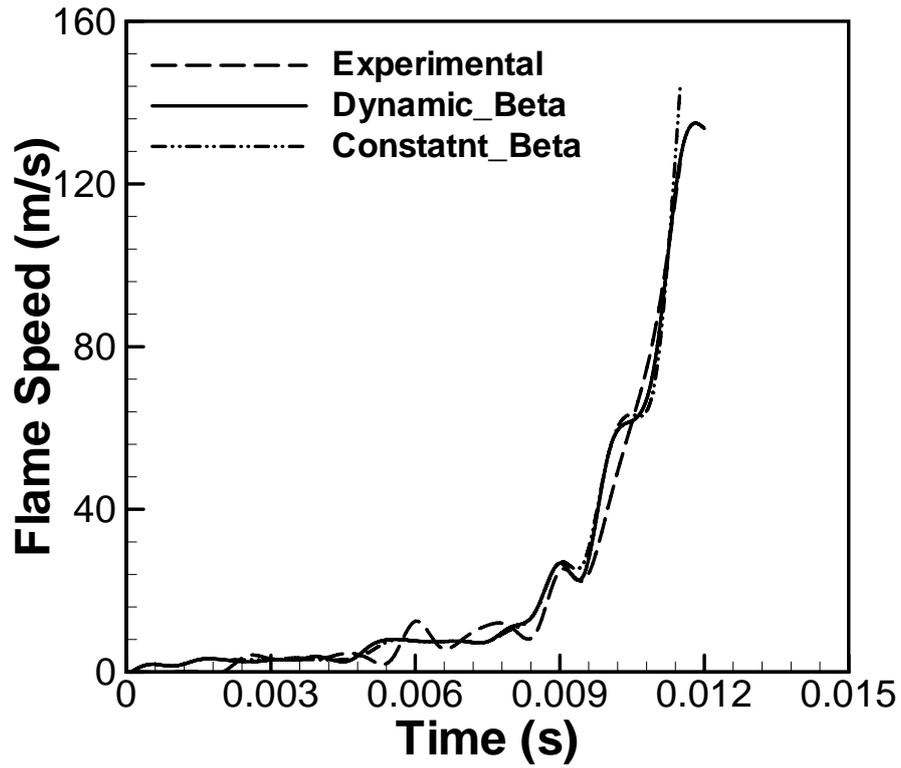
Figure 2c. Comparisons between LES simulations and experimental results for the flame speed at different times after ignition.
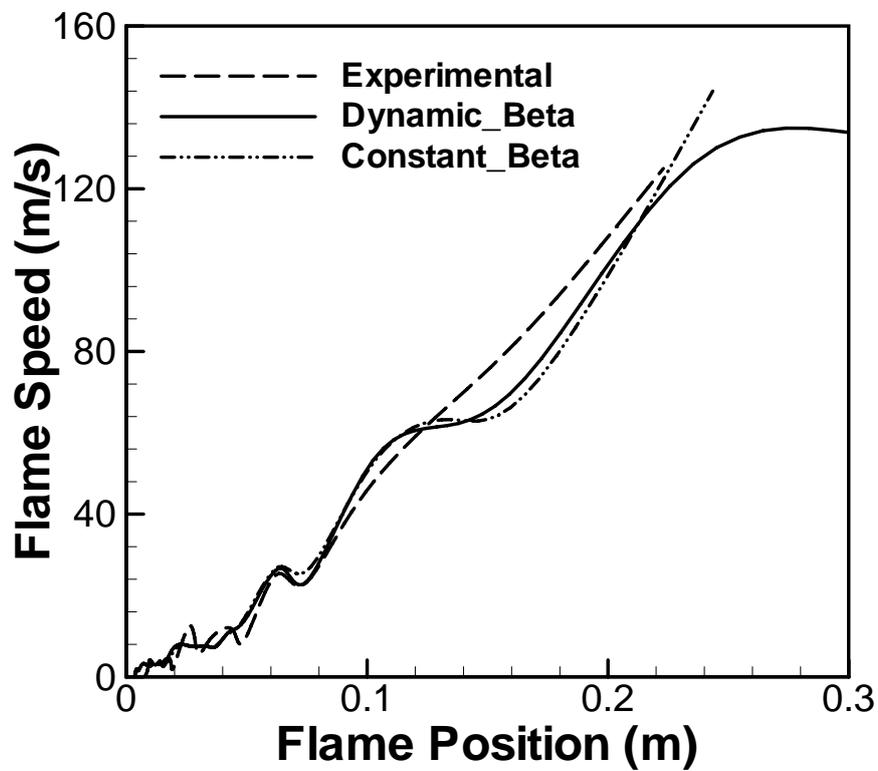
Figure 2d. Comparison between LES simulations and experimental data for the variation of the flame speed with flame position.
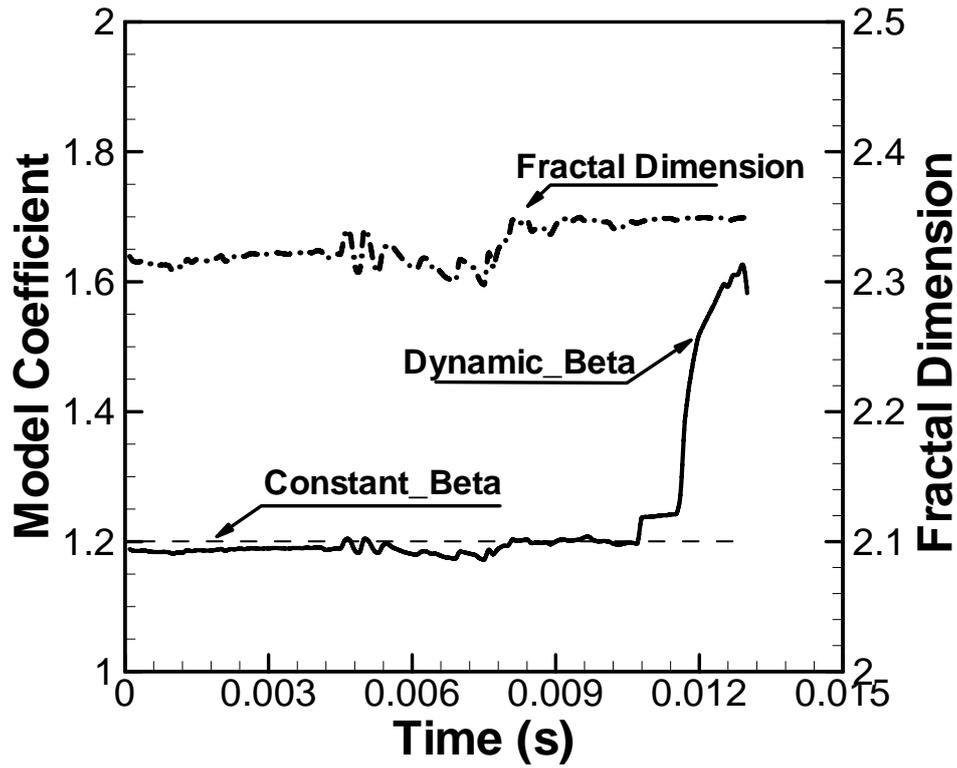
Figure 3. The time series of the model coefficient using dynamic procedure and the fractal dimension at the leading edge of the propagating flame.
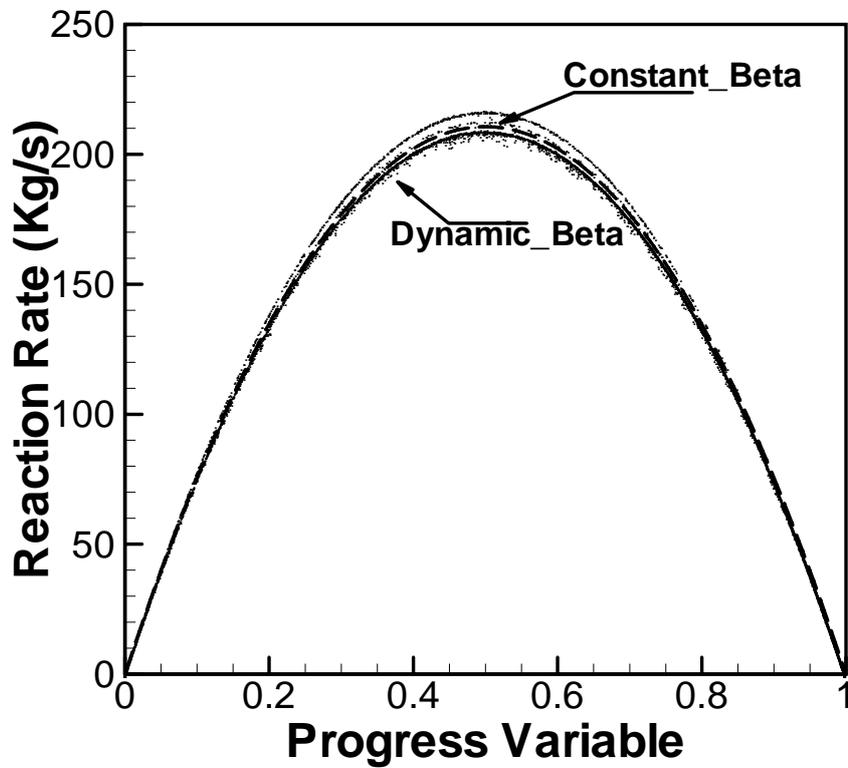
Figure 4. Variation of the reaction rate with the reaction progress variable, calculated by the FSD model at peak pressure.
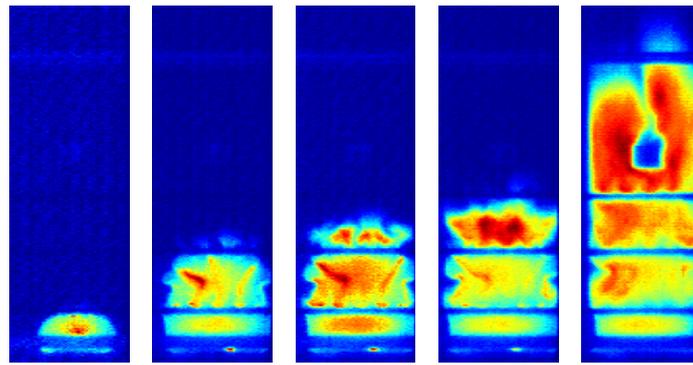
(a)
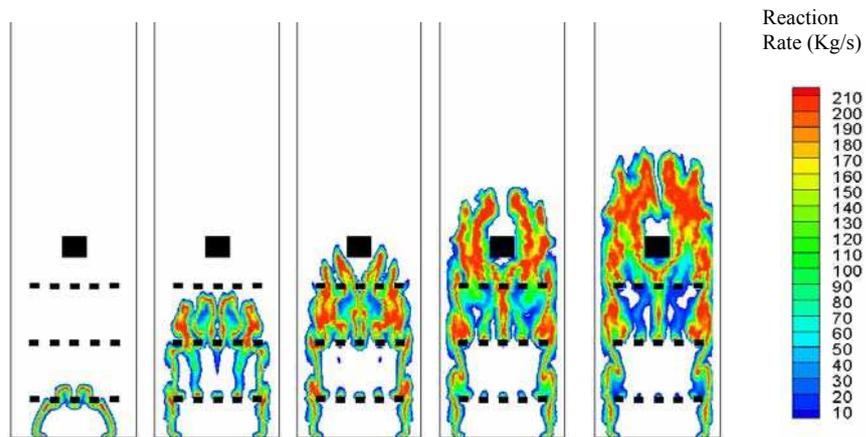
(b)
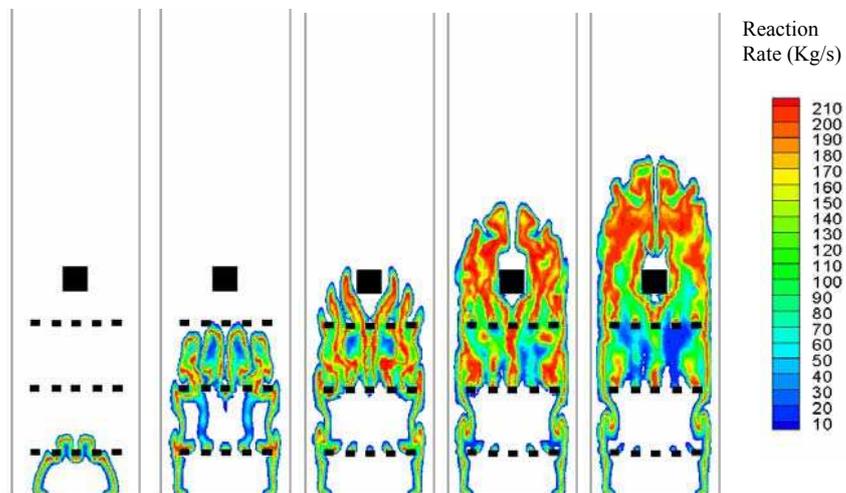
(c)

Figure 5. Sequence of images showing the flame structure at 6.0, 9.5, 10.0, 10.5 and 11.0 ms after ignition. (a) Experimental images (b) Numerical snap shots of reaction rate using a constant value for β (c) Numerical snap shots of reaction rate using dynamic formalism for β.

Snapshots of the turbulent premixed flame at various instants after ignition, from numerical data and high speed video images are shown in Figure 5 for flame structure. Numerical images are extracted from the reaction rate data at 6.0, 9.5, 10.0, 10.5 and 11.0 ms, significantly showing the flame interactions with baffle plates and square obstacle. At the same time scales, experimental snapshot are extracted from high speed videos. It is worth noting at this stage, that video images are taken from the front end of combustion chamber. However, numerical images are extracted from the central plane of the chamber in *x*-direction shown in Figure 1. Using both models for model coefficient, numerical images are capable of predicting exact recirculation zones and entrapment of the unburned mixture around solid obstacles. Over all, using dynamic modelling for model coefficient did predicted the global features of flame characteristics at various stages well with in very good agreement. It can also be concluded that, using a constant value for model coefficient, based on the specific fuel and turbulence levels is not a bad choice for preliminary investigations. However it should be noticed that, the cost of the solution in terms of days is 32 and 34 by a Viglen computer having Xeon® processor, approximately requiring 3 GB of RAM.

6. CONCLUSIONS

Large eddy simulations (LES) of turbulent premixed propagating flames are carried out using two sub-grid-scale (SGS) models in the flame surface density equation. The first model is used by choosing an appropriate constant value for model coefficient. The second is based on dynamic formalism for model coefficient. In the first case, model coefficient was taken as 1.2 from previous parametric studies and later on, model coefficient was modelled as wrinkling flame factor between outer and inner cut-off scales, by assuming wrinkled flame surface as fractal surface. The outer and inner cut-off scales are taken as filter width and three times of laminar flame width respectively. Fractal dimension has been dynamically modelled by an empirical relation using SGS velocity fluctuations and laminar burning velocity.

A laboratory scale premixed combustion chamber with built-in solid obstacles is used for model validation. A stagnant, stoichiometric propane/air mixture, propagating over solid obstacles after ignition is numerically simulated and compared against experimental measurements. The following observations are made during present study:

- LES predictions of over pressure, flame position and flame speed, using both models are in good agreement with experimental measurements. Dynamic evaluation of the model coefficient has predicted slightly higher peak pressure. However, both LES simulations found to slightly under-predicted the peak pressure.
- Results for the flame structure from both LES models are in good agreement with high speed recorded video images from experiments.
- The reaction rate calculated using dynamic model is slightly higher than that calculated by the constant coefficient value model.

Over all, results are very encouraging and confirming the applicability of the dynamic modelling of turbulent premixed combustion using LES technique.

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