## LAMINAR AND TURBULENT BURNING VELOCITIES OF PREMIXED HYDROCARBON-AIR FLAMES IN CLOSED CUBICAL VESSEL

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### ABSTRACT

Experimental measurements of laminar flame speed using spark-ignited explosions of methane-air mixtures in quiescent conditions in a cubic closed vessel are carried out. Experiments are conducted at initial pressure of 2 bar of stoichiometric methane-air mixture. Numerical simulations to determine the laminar burning velocity of stoichiometric methane-air, and turbulent burning velocity of propane-air mixture which include ignition and flame propagation is carried out using CFD software (CFX 5.7). The effect of pressure, stretch, flame thickness and confinement effects on the burning velocity is analysed. It has been found that when flame thickness in not negligible compared to the radius of curvature of flame and the vessel size, stretch, flame thickness and confinement effects are very important. Accordingly, these effects are taken into account to correct the values of laminar burning velocity obtained by pressure-time history assuming thin flame.

Simulation of turbulent combustion is performed using coherent flamelet model (CFM) [12] and the decay of turbulence during explosions and the effect of changes in pressure on both burning velocity and flow field are taken into account. A few experimental results of Checkel and Thomas [9] have been simulated and compared. The effect of initial values of *rms* turbulent velocity on turbulent burning velocity is analysed. Some of the deficiencies of the models have been brought out and attempts to improve these models are also reported.

### INTRODUCTION

Premixed combustion is of great technological importance having applications that ranges from simple residential cooking stove burner to the industrial gas burners, stationary gas turbine systems for power generation n in industries, and spark ignition engines in transportation industry. The number of such combustion systems is growing rapidly and emission of various pollutants from these devices has become a major concern from the point of view of environmental safety. Current engine designs and operating conditions, therefore, are greatly influenced by the need to control the soot, carbon monoxide and oxides of nitrogen emissions. The combustion process needs to be with high efficiency and low emissions. Therefore more detailed knowledge of premixed turbulent flames is needed to assist such development. Since all physical processes of laminar flames are active in turbulent flames, an understanding of laminar flames is a necessary prerequisite to the study of turbulent flames.

### **MOTIVATION**

A large number of the features of turbulent premixed flames are yet to be understood by the research community. While significant progress to date has been made through experiments, there is, as yet, no satisfactory model have been developed for turbulent combustion phenomena in an engine. The objective of the present paper is to identify the issues of the flame surface density models [10], as a tool to investigate the effects of turbulence on premixed flames.

### LAMINAR BURNING VELOCITY

One of the most important intrinsic properties of any combustible mixture is its laminar burning velocity and its dependence on variables such as pressure, temperature and mixture composition. The burning velocity ( $S_L$ ) is defined as the relative velocity, normal to the flame front, with which the unburnt gas moves into this front and is transformed.

The constant volume combustion method is generally acknowledged as being potentially both versatile and accurate. However, since burning velocity can not be measured directly, many equations for calculating this property from pressure-time records or from flame radius-time records or from both have been proposed [1,2,4,5].

Garforth and Rallis [3], Sharma [5] et al, have used spherical bomb method to find the Laminar burning velocities of Methane-air mixtures. Numerical studies on stretch effects on spherically propagating flames are done by Mishra et al [6]. In recent attempts, an equation for laminar burning velocity of methane-air mixtures from closed vessel gas explosions is fitted by Dahoe et al [7].

#### TURBULENT BURNING VELOCITY

Turbulent flame propagation velocity depends on the character of the flow, as well as on the mixture properties. For an observer traveling with the flame, we can define a turbulent flame speed,  $S_T$ , as the velocity at which unburnt mixture enters the flame zone in a direction normal to the flame. Thus, the turbulent flame speed can be expressed as [8]:

$$S_T = \frac{\dot{m}}{\overline{A}\rho_u} \tag{1}$$

Experimental determinations of turbulent flame speeds are complicated as suitable flame surface area,  $\overline{A}$  should be quantified from thick and frequently curved flame. The ambiguity associated with determining the flame surface area can result in considerable uncertainty in measurement of turbulent burning velocities. Checkel and Thomas [9] have used closed cubical vessel for finding turbulent burning velocity of propane-air mixtures. Veynante and Vervisch [10] have reviewed various models used in turbulent combustion.

The flame is identified as a surface, and the **flame surface density**,  $\Sigma$  is introduced which measures the available flame area  $\delta A$  per unit volume  $\delta V$ . The mean burning rate of *i*th species is then modeled as:

$$\overline{\dot{\omega}} = \dot{\Omega}_i \Sigma \tag{2}$$

The main advantage of this formulation is to decouple the chemical description  $(\dot{\Omega}_i)$  from the flame/turbulence interaction  $(\Sigma)$ . The flame surface density may be estimated either from algebraic relations or as a solution of a balance equation which can be derived using a phenomenological analysis, as was first proposed by Marble and Broadwell for nonpremixed turbulent combustion [12,14] or from geometrical considerations or from a statistical description, leading to an exact, but unclosed, balance equation. Various models are proposed to close these terms and are known as flame surface density models [10,12].

The mean consumption rate per unit volume at a point in the flow may be determined as the product of flame surface density at that point and the volume consumption rate per unit of flame area, obtained from the analysis of local strained laminar flamelets. Thus the mean burning rate of a i <sup>th</sup> species in an unstretched laminar flamelet regime is given as,

$$\overline{\dot{\omega}} = \rho_u Y_{u,i} S_L \Sigma \tag{3}$$

Recent models [10] estimate  $\Sigma$  by deriving an unclosed conservation equation and then proposing models for unclosed terms.

The conservation equation for flame surface density,  $\boldsymbol{\Sigma}$  can be written as:

$$\frac{\partial \rho \Sigma}{\partial t} + \nabla \cdot (\rho U \Sigma)$$

$$= \rho \nabla \cdot (\frac{\nu_t}{\sigma_{\Sigma}} \nabla \Sigma) + \rho S - \rho D - (\nabla \cdot U) \rho \Sigma$$
(4)

where S is the production rate of flame surface density ( $\Sigma$ ) due to mean flow field, turbulent fluctuations etc. D is the consumption of flame surface density ( $\Sigma$ ).  $\sigma_{\Sigma}$  is flame surface turbulent Schmidt number. The different closures are summarized in [10,12]. Chen et al [13] performed direct numerical simulations of 2-D unsteady premixed methane/air flames to determine the correlation of flame-speed with stretch over a wide range of curvatures and strain rates generated by intense 2-D turbulence.

The production term, S of CFM-1 model [12] is given by the average rate of strain. This is given as :

$$S = \Sigma \alpha \sqrt{\frac{\varepsilon}{15\nu}}$$
(5)

It is essentially the same form as used in the Checkel and Thomas[9]. In CFM-2 model [12], the average rate of strain is given proportional to u' and production term is given as [12]:

$$S = \alpha \frac{u'}{l_{lc}} \Sigma \tag{6}$$

where  $l_{tc}$  is arbitrary length scale introduced for dimensional consistency and it may be combined with  $\alpha$  as a single arbitrary tuning constant.



FIG. 1 CLOSED CUBICAL VESSEL FOR DETERMINATION OF BURNING VELOCITY

Destruction term D is given as [12];

$$D = \beta \frac{S_L}{\frac{\overline{Y}}{Y_0} \left(1 - \frac{\overline{Y}}{Y_0}\right)} \Sigma^2 \tag{7}$$

where  $\beta$  is model tuning constant.

### **EXPERIMENTAL TECHNIQUE**

Fig.1 shows the experimental setup containing the cubical vessel of 80 mm inside length. Spark plug electrodes are fitted on two opposite faces of the vessel, with 1 mm gap between them maintaining at the centre of hollow cubical vessel. 0-70 bar (gauge) strain gauge pressure transducer (Make: Ajay sensors, Bangalore) is connected to an adjacent face of a cubical vessel. Analog pressure signal is processed by a signal conditioning card (Strain gauge module, DBK 43a, Make: IOTech, US) and finally converted to digital values by an ADC card (Daqboard 2000, Make: IOTech, US). DasyLab software is used to log the pressure-time history during combustion. Usually pressure transducers are not exposed to the temperature above 400 K. As the temperature of the flame and combustion products are of the order of 2500 K, pressure sensor is safely connected through a capillary passage in the cube wall. Stoichiometric methane air mixture is filled in to the cubical vessel through connected needle valves using partial pressure values. Pressure-time data is acquired at 2 kHz frequency for initial quiescent mixture at 2 bar pressure and temperature 300 K.

# SIMULATION OF LAMINAR BURNING VELOCITY

Numerical simulations to determine the laminar burning velocity from closed vessel gas explosions which include ignition and flame propagation are carried out using CFD software (CFX 5.7). Quiescent stoichiometric methane-air mixture at initial 2 bar pressure and temperature 300 K is taken in the solution domain of 125 mm<sup>3</sup> cubical box and the behavior of pressure in the vessel as a function of time is obtained. A structured uniform mesh with element size 0.1 mm (number of elements=125000) has been found to be consistent with the flow features that is needed to be captured.

A point heat source is applied for 1 ms time duration to simulate spark. Heat source value is adjusted to 50 mJ s<sup>-1</sup> such that sustainable combustion is initiated in the domain. Finite rate chemistry model is used for simplicity of modeling chemical source term  $\dot{\omega}_i$  for quiescent mixture combustion. The viscosities and thermal conductivities are calculated from power law equation [11] to account for the change with temperature. Thin, thick flame and stretch effect equations [4,6] are used to determine the laminar burning velocity from pressure-time history. Fig.2 shows the evolution of temperature profiles as the flame progresses in the domain. Initially temperature is raised to 6,500 K due to point heat source. It is required for initiating sustainable combustion in the domain. However, in fig.2, temperature profiles show that there is no residual effect of initial high temperature after about 3 ms when temperature becomes adiabatic flame temperature.

Fig.3 shows the concentration profiles of reactants and products at an instant of time (7 ms). All these profiles show that the flame is not infinitely thin as is assumed but have a finite thickness.



FIG. 2 EVOLUTION OF TEMPERATURE PROFILE



AND PRODUCTS

Fig.4 shows simulated pressure-time history as the combustion progresses in the domain. In experiments, the pressure is seen to decrease after achieving a

maximum because of heat loss to the walls. However, since the walls are adiabatic in the simulations, a decrease in pressure after maximum is not seen.

Fig. 5 shows burning velocity plotted against the pressure using thin and thick flame equations. Thickness of the flame is more important when it is comparable with the radius of curvature of flame and vessel size, as in the present case. However, still the burning velocities are quite less than the experimental values. This is found to be due to the stretch effect.



FIG. 4 EXPLOSION PRESSURE-TIME HISTORY IN THE DOMAIN (INITIALLY 2 BAR, 300 K)



FIG. 5 LAMINAR BURNING VELOCITY FROM THIN [2] AND THICK-FLAME [4] EQUATIONS

Fig.6 shows the comparison of burning velocity with and without stretch. The burning velocity after

eliminating stretch, match with the burning velocity calculated from thick flame equation at high pressure. At low pressure, the mismatch in velocities may be due to the fact that ignition is not modeled properly. In the present case, ignition is carried out only by giving high temperature to the gases so that reaction could sustain. However, in actual case, at ignition, the reaction rate depends more on radical concentration than the temperature.



FIG. 6 BURNING VELOCITY WITH STRETCH EFFECT

Fig. 7 shows the plot of velocity of gases in the domain along the radius of flame at time t=8 ms. It shows that there are movements of gases behind the flame front i.e. burnt gases are not stationary as in case of constant pressure combustion. The maximum unburnt gas velocity adjacent to the flame front has been used to calculate the laminar burning velocity with respect to unburnt gases. This is due to confinement effect which creates the gas movement behind the flame front. Fig.8 shows the plot of spatial velocity and laminar burning velocity of flame with respect to unburnt gas. The spatial velocity is calculated by noting the flame front radius,  $r_f$  values at

regular time intervals and thus calculating  $\dot{r}_f$ . The flame front is identified at location at which temperature is  $(T_o + T_{ad})/2$ . The laminar burning velocity of flame with respect to unburnt gas is then calculated as:

$$S_u = S_s - S_{ug} \tag{8}$$

and laminar burning velocity of flame with respect to burnt gas is calculated as:

$$S_b = S_s - S_{bg} \tag{9}$$

where  $S_{ug}$  and  $S_{bg}$  are unburnt and burnt gas velocity adjacent to the flame front.



FIG. 7 VELOCITY OF GASES ALONG THE RADIUS OF FLAME



FIG. 8 BURNING VELOCITY WITH RESPECT TO BURNT AND UNBURNT GAS

# SIMULATION OF TURBULENT BURNING VELOCITY

Numerical simulations to determine the turbulent burning velocity, from closed vessel stoichiometric propane-air explosions, are carried out using CFX 5.7 software by including user FORTRAN code for coherent flamelet models [CFM] [12]. Two flame surface density models CFM1 and CFM2 [10, 12], are used to simulate the turbulent flame propagation.

The experimental conditions of Checkel and Thomas [9] which has been simulated are presented in Table 1. Computational field consists of a box with dimensions 60X60X60 mm<sup>3</sup>. Grids with different element size has been tested and a grid with element size 3 mm (number of elements=8000) has been found to be consistent with the flow features that is needed to be captured. The reason for taking coarse grid compared to the laminar case is that the turbulent flames are many times thicker than the laminar flame thickness. *rms* turbulent velocity is denoted by u'.

TABLE 1: EXPERIMENTAL RESULTS AT 1 ATM,EQUIVALENCE RATIO UNITY [9]

Condi- tion No.	u' (m/s)	Rate of Strain (s <sup>-1</sup> )	t <sub>p</sub> (ms)	$S_T/S_L at t_p$
2	2.32	12044	10.1	4.24
3	3.46	19048	9.3	4.71
4	4.32	25011	8.4	5.15

An arbitrary initial profile of flame surface density is given in the domain to get the initial flame kernel which is assumed to be formed after the spark. Turbulent burning velocity values reported by of Checkel and Thomas [9] are compared with those obtained by using CFM1 and CFM2 model in Fig.9. The slope of the curve of  $S_T/S_L$  versus u' of CFM1 model is more than the experimental curve while that of CFM2 model is approximately same as that of experiments. This is due to the fact that in CFM1 model, the rate of strain is proportional to  $\sqrt{\varepsilon/\nu}$  i.e.  $u'^{1.5}/l_L^{0.5}$  while that in CFM2 model, the rate of strain is proportional to  $u'/l_{tc}$ .



FIG. 9 TURBULENT BURNING VELOCITY VS *u*' OF CHECKEL AND THOMAS [9], CFM1 AND CFM2 MODELS [12]

Fig. 10 compares the time for pressure to reach 2.2 times its initial value with u'. Both the models are not predicting the time correctly. However, CFM1 predicts

time closer to experimental value than CFM2 model. Since the slope of  $S_T/S_L$  versus u' for CFM2 model is same as experimental values, the constant  $\alpha$  of CFM2 model is increased from 10 to 15 to match the experimental results of [9] and the simulation results are obtained are shown in Fig.11 and Fig.12.



FIG. 10  $t_p$  VS u' FOR CHECKEL AND THOMAS [9], CFM1 AND CFM2 MODEL [12]





 $S_T/S_L$  values are close to experimental results for  $3^{rd}$  and  $4^{th}$  conditions mentioned in Table 1. However, for  $2^{nd}$  condition, there is considerable variation from experimental values. This may be due to increase in the value of constant  $\alpha$  causes a decrease in the flame thickness. Hence, element size needs to

capture the flow features also to be decreased. Here, element size used is 3 mm and this needs to be decreased.



FIG. 12  $t_p$  VS u' OF CHECKEL AND THOMAS [9], CFM1 AND CFM2 MODEL [12]

### CONCLUSIONS

The effects of factors, other than pressure and temperature, which are particularly important in context of spherical expanding flames, have been explored. Flame thickness has been found to be an important factor when it is not negligible in comparison to radius of curvature of flame and vessel size. In context of spherical flames, stretch effect is very important and it has been taken into account. Confinement effect i.e. gas movement in burned region is shown due to the closed vessel. Corrected laminar burning velocity after taking into account all these effects is found to be satisfactory. However, simulation of laminar burning should be carried out with mesh adaptation technique which reduces number of elements without losing accuracy of results.

Studies on turbulent burning velocity show the inadequacy of models to predict burning velocity at different turbulence levels. Comparison of calculated

 $t_p$  with experimental values brings out an important

phenomenon of flame kernel development phase during which flame evolves from an arbitrary distribution of flame surface to a propagating flame front. Comparison of calculated  $S_T/S_L$  with experimental values have

been satisfactory for some conditions. However,  $t_p$ 

seems to be better parameter for comparison because  $S_T/S_L$  is a local factor and needs the state to be specified at which it is measured. Turbulent flame thickness has been found to be much larger than laminar flame thickness.

### **FUTURE WORK**

- An exhaustive set of experimental values are needed to have a meaningful insight into the behavior of St with turbulence parameters.
- Simulations with various integral length scales are needed to examine its influence.
- Grid size has to be changed in order to take into account the varying turbulent flame thickness with varying turbulent intensity.
- A complete understanding of flame kernel development phase is required.
- The effect of various forms of mean stretch factor available in literature has to be explored.
- And above all, a model has to be developed which can predict turbulent burning velocity in various turbulence levels as well as in all conditions like whether turbulence is decaying or frozen.

#### NOMENCLATURE

- $S_L$  Laminar burning velocity (ms<sup>-1</sup>]
- $S_{T}$  Turbulent burning velocity (ms<sup>-1</sup>]
- *t<sub>p</sub>* Time required for a pressure rise of 2.2 times above initial pressure, (mili seconds, ms)
- u' rms turbulent velocity (ms<sup>-1</sup>)
- $\overline{Y}$  Average mass fraction of species
- $Y_0$  Initial mass fraction of species
- lpha , eta Model tuning constants
- $\Sigma$  Flame surface density (m<sup>-1</sup>)
- $\dot{\omega}_i$  Mass of species produced or consumed per unit volume per unit time (kg m<sup>-3</sup>s<sup>-1</sup>)
- *E* − Dissipation rate of turbulent K.E (m<sup>2</sup>s<sup>-3</sup>)
- V Kinematic viscosity (m<sup>2</sup>s<sup>-1</sup>)
- $V_t$  Turbulent kinematic viscosity (m<sup>2</sup>s<sup>-1</sup>)
- $\sigma_{\scriptscriptstyle \Sigma}$  Turbulent Schmidt number of flame surface

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