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Modelling of Transient Stretched Laminar Flame Speed of Hydrogen-Air Mixtures Using Combustion Kinetics

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Abstract

The calculations of laminar burning velocity are mostly based on empirical correlations obtained from combustion bomb experiments. There is a noticeable scarcity of the fitting parameters in these correlations, especially under increased temperature and pressure conditions. The effects of flame stretch and instabilities further complicate the situation as these effects are not distinguished in some correlations. Furthermore, although combustion products are of great interests in recent computer simulations of combustion, it is difficult to integrate combustion chemistry into the existing correlations. This paper discusses a laminar burning velocity model for hydrogen-air mixtures in a constant volume combustion bomb. The model is based on a one-dimensional three-zone thermodynamic model that calculates the mass transfer and diffusion and the heat transfer between zones. The chemical process involved in the combustion is solved by an in-house chemical kinetics solver with an established reduced hydrogen-oxidation mechanism from literature. The effects of flame stretch and instabilities are simulated using existing experimental data. The calculated laminar burning velocities are compared to existing empirical correlations and experimental data obtained from constant volume combustion bomb tests. The model is able to simulate laminar burning velocities and have the potential to be integrated into IC engine models in the future.

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Keywords: Laminar Flame Speed , Hydrogen, Combustion Kinetics, Thermodynamic Combustion Model

1. Introduction

The calculation of the laminar burning velocities is one of the fundamental components in modelling a variety of combustion systems, such as internal combustion (IC) engines. Some studies were conducted in constant volume combustion experiments and the laminar burning velocity was express as function of bomb pressure history, $u_l = \left(\frac{1}{F_1 P}\right) \left(\frac{r_c}{P}\right) (dP/dt)$ [1]. Others using semi-empirical equations $u_l = u_l^0 (T_u/T_0)^a (P_u/P_0)^b$, where a and b are dependents determined experimentally [2,3,4,5,6,7]. Simulation studies based on bomb pressure history [8,9] showed that $u_l = (dP/dt)(dr_i/dP)(r_i/r_b)^2 (P_i/P)^{1/\gamma_u}$. Due to prerequisite of the experimentally-obtained data, either the exponents a and b , the bomb pressure

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history, or the simulation models can only work when experimental data are available. The aim of this study is to develop a self-sustainable transient laminar burning velocity model that eliminates the need for priori experiments with the capability of providing information on combustion chemistry. This model developed is based on a one-dimensional three-zone thermodynamic model that calculates the mass transfer and diffusion and the heat transfer between zones. The chemical processes involved in the combustion are solved using an in-house chemical kinetics solver with an established reduced hydrogen-oxidation mechanism from literature.

2. Model Development

The propagation of a spherical flame front divides the combustion bomb into three distinctive zones: burnt zone, burning zone and unburnt zone. The unburnt zone is further divided into a number of thin sub-layers. The flame propagation process is seen as the consecutive consumption of these thin unburnt layers. The flame front consumes the unburnt gas at the rate of the flame speed. Following assumptions were applied in the model development:

- homogeneous air-fuel mixture; both burnt and unburnt gases act as perfect gas;
- flow motion is neglected throughout combustion;
- uniform pressure across the bomb during the combustion process;
- flame front maintains its spherical shape;
- unburnt gas is in a chemical-frozen status and is isentropically compressed by the flame;
- starts at ignition kernel, r_{kernel} , of 2mm radius;
- all burnt mixtures are assumed to be in chemical equilibrium state.

The value of the unstretched laminar burning velocity can be calculated as:

$$u_l = \frac{(r_{bomb} - r_{kernel})/n}{\Delta t_{flame}} \quad (1)$$

where r_{bomb} and r_{kernel} are radius of the bomb and the initial ignition kernel respectively, n is the number of calculation steps, and Δt_{flame} is the reaction time of completing in-flame reactions of the step. The choice of n is largely dependent on the bomb size. In this study $r_{bomb}=200$ mm, $n=400$ shows a good best balance between convergence and computational time.

In-flame reactions are characterized as high reaction rate and rapid energy release, while post-flame reactions are relatively slow and release less energy. The reaction time of completing in-flame reactions of the step considers the high reaction rate only. H radical is a sensible indicator of in-flame and post-flame reactions [10]. Fig.1 shows its mole fraction Y_H and change rate \dot{Y}_H within a calculation time step where the rate is divided by 10^5 . The sharp increase indicates fast production. The following sharp decrease shows sharp consumption, eventually overwhelms the production when the rate becomes negative. As \dot{Y}_H increases towards a constant value close to zero, it indicates the end of fast chemical reactions. In this study, the end of in-flame reactions is defined as the point when $\Delta Y_H / \dot{Y}_H \leq 10^{-3}$. The hydrogen combustion kinetics used in this work consists of 11 species and 19 reversible elementary reactions [11]. Fig.2 shows the calculated unstretched laminar burning velocities using Eq.1 in comparison

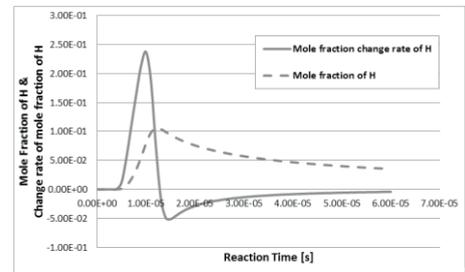


Fig.1 Variations of H radical mole fraction Y_H and its change rate \dot{Y}_H

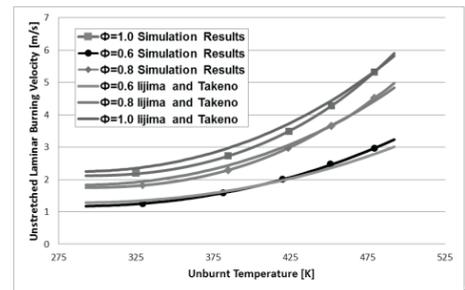


Fig.2 Comparisons of simulated unstretched laminar burning velocities and numerical correlations (Iijima & Takeno, 1986).

with literature results [12]. In all cases, the burning velocities increase with increasing temperature and become more sensitive to temperature increase at higher temperature region. These phenomena are expected as the unstretched laminar burning velocities are kinetically-controlled.

The unstretched laminar flame speed can be obtained by adding the burnt gases expansion velocity S_b to the unstretched laminar burning velocity:

$$S_u = u_l + S_b = u_l \cdot \kappa_{exp} \tag{2}$$

where S_u represents the unstretched laminar flame speed, κ_{exp} is the expansion coefficient given as:

$$\kappa_{exp} = \frac{\rho_u/\rho_b}{((\rho_u/\rho_b)-1)X_b+1} \tag{3}$$

where ρ_u and ρ_b are densities of the unburnt and the burnt mixtures, and X_b is the mass fraction burnt. The gas properties of unburnt and burnt air-fuel mixtures were obtained from energy conservation principles. Fig.3 shows the calculated density ratios, ρ_u/ρ_b , at different temperatures and pressure.

The transient stretched laminar flame speed S_f is obtained from relationship with unstretched laminar flame speed S_u , the flame stretch rate κ , and the Markstein length of the burnt mixture L_b , often described as:

$$S_f = S_u - L_b\kappa \tag{4}$$

where the total stretch rate of a stable, outwardly propagating spherical flame is given as $\kappa = 2S_f/r_f$. Verhelst [13] proposed values of L_b for higher temperature and pressure by using the regression methodology developed by Bradley [14]. These values were used in this study.

3. Model Validation

A spherical stainless steel combustion bomb with 400mm inner diameter, as shown in Fig.4, was employed. It has an optical access through a pair of orthogonal quartz windows of 100 mm diameter. The optical system is arranged into a Z-shaped, the two primary mirrors have diameter of 100 mm and focal length of 100 cm. The slit has an adjustment range of 0-3 mm and the blade can be adjusted in the range of 0-10 mm. The mixture is spark ignited at centre of the chamber. After the induction of fuel and air is completed, sufficient time is allowed for the mixture motion to decay. Flame images, as shown in Fig.5, are recorded by a TRI Phantom v7.3 camera capable of a maximum speed of 200,000 frames per second.

The instantaneous flame speed is calculated as:

$$S_f = \Delta r_f / dt_{camera} \tag{5}$$

where Δr_f is the flame radius increase between two consecutive flame images and dt_{camera} is the time interval between two images. Fig.8 shows the comparisons of the calculated transient stretched laminar

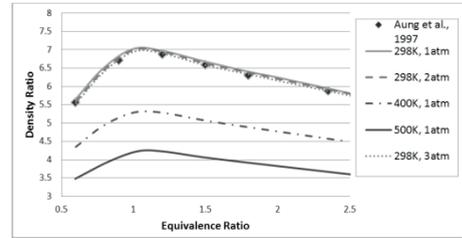


Fig.3 Calculated density ratios of unburnt and burnt mixtures at 298±3K and 1bar

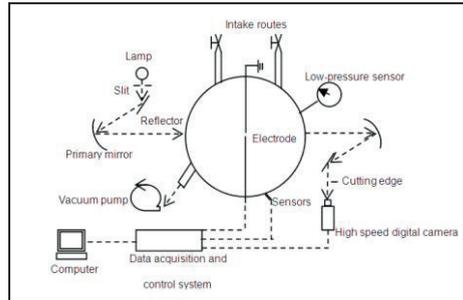


Fig.4 Experimental apparatus for constant volume combustion

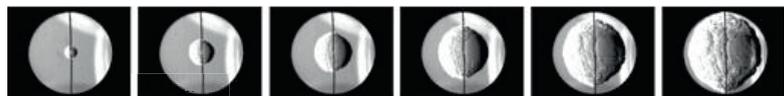


Fig.5 H₂-Air flame at $\Phi=0.6$, 298K and 1bar. Measured flame radii are: 5.8, 12.1, 17.8, 23.9, 30.0 and 35.0mm

flame speeds and the experimental results, normalised by the bomb radius $r_n = r_f/r_{bomb}$. The calculated flame speeds match the measured flame speeds well in most of the flame propagation processes. The flame speed of very lean mixture ($\Phi=0.6$) maintains an almost constant value throughout the combustion with a large initial speed reduction due to large stretching rates. Stoichiometric flame experiences a rapid initial flame speed increase as a result of decaying flame stretch and strengthening combustion. Following the initial increase the flame speed maintains a nearly constant value from 20% to 55% bomb radius. The flame surface becomes completely cellular when the flame radius reaches the size of about 60% bomb radius and a steep increase in flame speed is triggered by the cellular structures.

Conclusions

H radical is used to define the end of the in-flame reactions. Based on the unstretched laminar burning velocity model, unstretched flame speed and stretched flame speed models have been developed using established theories and experimental data. The model reproduced the effect of flame stretch well. The predicted flame speed has been validated against experimental results and good agreement has been achieved. Flame speed has been found to increase with increased fuel-air equivalence ratio (from 0.6 to 1.0), temperature and pressure.

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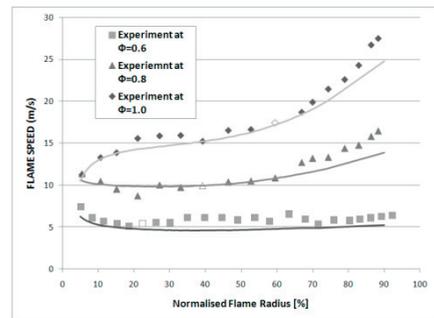


Fig. 6 Comparisons of transient stretched laminar flame speeds. Solid lines represent corresponding simulation results.