Simulation of Heat Release in Premixed Combustion

C.K. Chan*, B. Stewart, and C.W. Leung

***Abstract*— A Lagrangian front-tracking scheme incorporating Contour Advection with Surgery (CAS) is used to simulate turbulent premixed combustion. This paper presents results from calculations of methane/air mixtures and ethylene/air mixtures with equivalence ratios ranging from 0.8 to 1.6 with different turbulence intensities. The positions, thicknesses and half-angles of the turbulent flame zones are compared for each case by plotting contour maps of the time-averaged progress variable <c>. These results are then used to calculate the overall heat release for each equivalence ratio.**

***Index Terms* - Flame surface density, heat release rate, premixed combustion.**

I. Introduction

In the many practical applications of turbulent premixed combustion it is of prime importance to have a quantitative appreciation of the effects that variations in the ambient flow conditions have on the burning characteristics. However numerically modeling the propagation of a premixed flame in a turbulent flow environment remains a challenging task due to the non-linear coupling of mechanical turbulence and the combustion process. The rod-stabilized turbulent premixed V-shaped flame is a common configuration employed for experimentally studying turbulent flames and providing data for comparison with numerical analysis. The current study investigates the burning characteristics of methane (CH_4) and ethylene (C_2H_4) in a turbulent premixed rod-stabilized V-flame at varying freestream equivalence ratios and turbulence intensity levels.

For a flame arrangement that is two-dimensional in nature, the rod-stabilized V-flame is approximated in the simulations as a two-dimensional flame. The theoretical model employed to numerically simulate the flame is the popular reaction sheet model [1]. This model neglects the internal structure of the flame as reaction rates are high and approximates the instantaneous flame zone as an infinitesimally thin front that separates the burnt and unburnt regions. This flame propagates into the oncoming reactant gas mixture via a Lagrangian front-tracking technique known as Contour Advection with Surgery (CAS) [2], [3].

II. Numerical Method

Contour Advection with Surgery (CAS) is a Lagrangian algorithm that provides high-resolution capabilities of a front-tracking scheme without the numerical difficulties normally associated with the Lagrangian approach. A conventional front-tracking method faces numerical challenges when dealing with the growth in complexity of the flame front, having to continually add marker nodes in regions of topological changes. To alleviate these issues, CAS dictates the distribution of the marker nodes that define the front when the front propagates to a new position after each time step. Surgery of the flame front reduces fine-scale complexity of the front below a prescribed threshold scale and limits the growth in the number of marker nodes needed to appropriately define the front.

By utilizing the reaction sheet model, the following assumptions are made:

- the reaction rate is sufficiently high so as to approximate the flame as an infinitesimally thin front; and
- the burnt and unburnt regions have distinct uniform densities; and

The flow is also assumed to be two-dimensional with the mechanism of vorticity production being inviscid.

As described by Chan et al. [4], [5] the total velocity of a fluid particle u in the flow field can be treated as the combination of three independent components, such that

$$u = u_s + u_r + u_p \tag{1}$$

where u_s is the solenoidal component due to the volume expansion across the flame front, u_r is the rotational component due to the vorticity distribution $\omega(x)$, and u_p is the prescribed freestream potential flow.

For the simulation, there are two sources of vorticity. The first source is the injection of small uniform vortices at the domain entrance which governs the freestream turbulence intensity. The other source of is the baroclinic torque caused by the interaction of density and pressure gradients at the flame

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front. To account for this flame-induced vorticity, vortices are injected behind segments during each time-step. The determination of flame induced vorticity is obtained with an expression by Hayes [6] for vorticity jump across the flame front

$$[\omega] = \left(\frac{1}{\rho_b} - \frac{1}{\rho_u}\right)\nabla_t(\rho_u S_u) + \frac{\rho_b - \rho_u}{\rho_u S_u}\left\{D u_t + u_t \nabla_t u_t - u_t u_n \kappa - u_n \nabla_t u_n\right\}, \quad (2)$$

where ρ_u and ρ_b are densities of the unburnt and burnt regions respectively, S_u is the flame speed with respect to the unburnt gas, u_t and u_n are the tangential and normal velocity components at the flame front and κ is the local curvature of the flame. ∇_t is a gradient operator along the flame front and D is the material time derivative taken at a point on the front which moves in the direction normal to the discontinuity.

III. SIMULATION PARAMETER

The combination of laminar flame speed, S_L, and the density ratio across the flame front, ρ_u/ρ_b, uniquely defines the fuel type and the equivalence ratio. For a particular turbulence intensity level, the input variables required for the calculations are S_L and ρ_u/ρ_b,. These values for methane and ethylene are obtained from Tseng et al. [7] and are shown in Fig.1 and Fig.2.

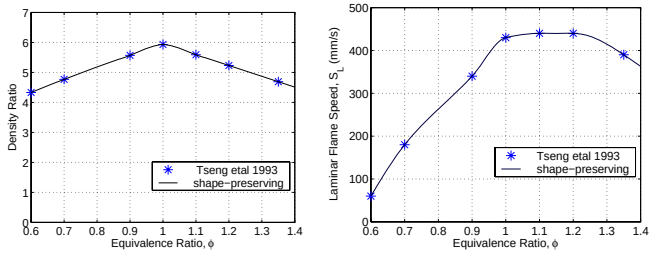


Fig.1 Density ratio and laminar flame speed for CH_4

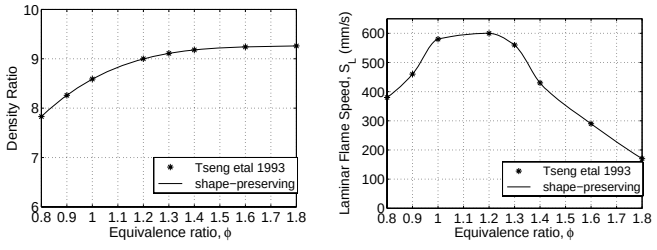


Fig.2 Density ratio and laminar flame speed for C_2H_4

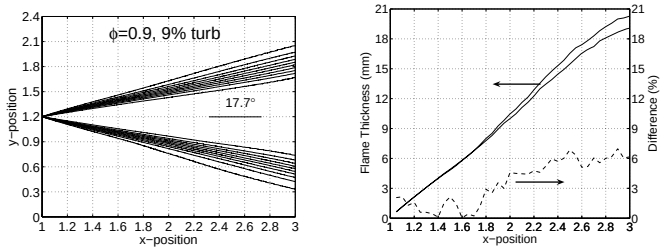
The values for S_L along with all other velocities are normalized by the inflow velocity of 5.5 m/s and all distances are normalized by a distance of 50 mm. In the computation, the distance in the flow direction is kept at 150 mm, while the distance in the transverse direction is varied to accommodate the varying flame angle and flame thickness for different fuel and equivalence ratios. The flame anchor is set at a distance of 50 mm from the inflow boundary at the mid-point of the transverse direction. To simulate freestream turbulence, discrete random vortices are generated across the inflow plane every 10^{th} iteration. These result in four different turbulence intensities of 6%, 9%, 11% and 13%.

IV. RESULTS

A. Turbulent Flame Zone

The turbulent flame zone corresponds to the region within which the flame front fluctuates whilst in a quasi-steady condition. The location of the infinitesimally thin flame front for each time step is recorded by assigning a value of the reaction progress variable, c, to each grid element in the computational domain. This reaction progress variable, c, has either a value of unity in the burnt region or zero in the unburnt region. These instantaneous c values are averaged over all time steps to give a map of the mean reaction progress variable, $\overline{c}$ which signifies the average extent of burning for each grid element in the domain.

Fig.3 shows a typical case for methane combustion with equivalence ratio at 0.9 and turbulence intensity of 9%. Fig.3(a) highlights the turbulent flame zone for this case. The included half-angle of the flame, θ, defined as the angle between the flame centre-line and the $\overline{c} = 0.5$ contour, is found to be 17.7^0. Fig.3(b) shows the flame zone thickness, t, as measured for each arm of the V-flame in the streamwise direction between the contours of $\overline{c} = 0.05$ and $\overline{c} = 0.95$.



(a) (b)

Fig.3 Flame zone, flame angle and flame thickness for CH_4

Fig.4 shows the corresponding flame angles and flame thickness for an ethylene flame with equivalence ratio of 0.9 and turbulence intensity of 9%. It indicates that both the flame thickness and flame angle for ethylene flames are greater those of methane flames.

For the calculations presented in this paper, 20,000 time steps are used with each time step $\Delta t = 0.005$ second. The thickness of both flame arms are measured as both arms evolve separately with time, and as only a finite number of time steps are used in the calculation, slight discrepancies are expected.

The difference in flame thickness for both arms is shown in Fig.3(b) and Fig.4(b) as a percentage in dashed line. It indicates the level of uncertainty and the maximum difference in flame thickness measured for both arms of the flame is around 6%. For all cases, this measure of uncertainty has a maximum value of around 12 %. By increasing the number of time steps to 100,000, the maximum uncertainty is reduced to around 7-8%, but computational times is significantly increased from around 36 hours to an impractical time of one week. Therefore, as a compromise, 20,000 iterations are used for all calculations.

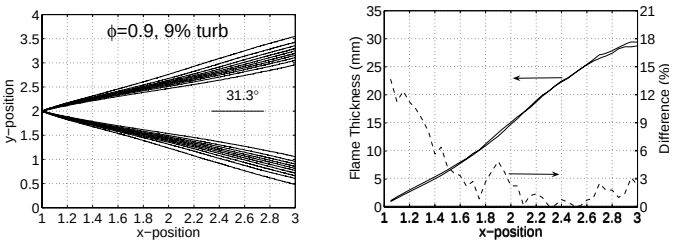
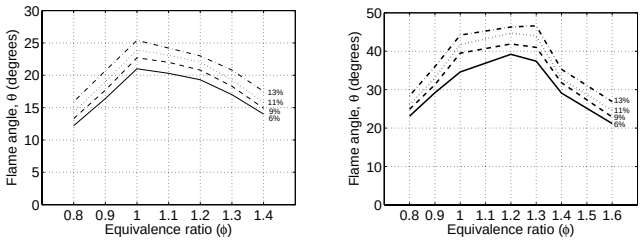


Fig.4 Flame zone, flame angle and flame thickness for C_2H_4

B. Flame Angle

Figures 5 shows of the flame angle, flame, θ, as a function of equivalence ratio, φ for methane and ethylene. For both flames, an increase in turbulence intensity increases the flame angle due to an increase in propagation speed of the flame front. For maximum mean flame angle, it can be seen that methane flames have maximum flame angles at stoichiometric methane mixtures, while for ethylene flames, the maximum flame angle occurs at fuel rich conditions of $\varphi = 1.2-1.3$. This is likely due to differences in flame density ratio characteristics of the two fuels. For methane, the density ratio has a distinct maximum at $\varphi = 1.0$, while for ethylene, density ratio increases asymptotically for the range of equivalence ratios investigated, thus pushing the maximum flame angle for C_2H_4 towards higher equivalence ratios.



(a) methane (b) ethylene

Fig.5 Flame angle for different fuel/air mixtures

C. Burning Rate and Heat Release

To calculate the overall burning rate, an expression by Bray [8] for the local consumption rate of reactant, $\overline{w}$ at a point in a turbulent flame zone is used where

$$\overline{w} = \rho_r S_L I_0 \Sigma, \tag{3}$$

where ρ_r is the density of the unburnt reactant, S_L, is the laminar flame speed, I_0 is the flamelet stretch correction term and Σ denotes the flame surface density which is defined as the flame surface area per unit volume. For the two-dimensional V-flame studied in this paper, flame surface density is redefined as the ratio of the average flame length to flame zone area. In terms of mean reaction progress variable, the flame surface density is expressed as

$$\Sigma(\overline{c}) = \frac{\Delta L(\overline{c})}{\Delta A(\overline{c})}, \tag{4}$$

where ΔL and ΔA are the flame length and flame zone area respectively for an incremental change in $\overline{c}$. As shown by Tang et al. [9], by denoting η as the integration path through the flame zone, Eq.4 can be integrated across the thickness of the flame to yield the mean consumption rate of reactant per unit length of flame, $\overline{C}$ as

$$\overline{C} = \rho_r S_L I_0 \int_{0.05}^{0.95} \Sigma \, d\eta \tag{5}$$

where the integration bounds $\overline{c} = 0.05$ and $\overline{c} = 0.95$ stand for boundaries of reactants and products respectively. For relatively low turbulence, the stretch correction term I_0 is taken as unity as suggested by Shepherd and Cheng [10].

The mean consumption rate, $\overline{C}$ represents the average mass consumption rate of reactant per second per unit length of flame. To obtain the mean burning rate of fuel, $\overline{W}$, the consumption rate must be multiplied by the mass-fraction of fuel in the reactant, m_f yielding

$$\overline{W} = \overline{C} m_f \tag{6}$$

Finally, the average overall rate of heat release from combustion, $\overline{Q}$ (Watts per meter), is obtained as

$$\overline{Q} = \overline{W} \cdot \Delta E \tag{7}$$

where ΔE is the heat of combustion per kilogram of fuel.

Fig.6 shows the mean consumption rate obtained for a methane flame between $x = 2.0$ and $x = 2.5$, as a function of the equivalence ratio. As consumption rate is essentially the mass-flow rate of reactant through the flame and, accordingly, the trend for $\overline{C}$ closely resembles that of the laminar flame

speed as shown in Fig.1. The consumption rate rises rapidly as equivalence ratio of the reactant gas approaches 1.0, then remains relatively steady until $\varphi = 1.2$ before starting to decrease as the equivalence ratio continues to increase. In addition, the increase in flame speed that results from the increase in turbulence intensity leads to an increase in $\overline{C}$ at higher turbulence levels.

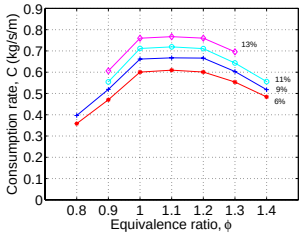


Fig.6 Mean consumption rate of premixed CH_4 reactant

The mean burning rate of methane (kilograms of CH_4 per second per meter) obtained for each simulation is shown in Fig.7. As the reactant has a higher mass-fraction of fuel at higher equivalence ratios, the maximum burning rate occurs at about $\varphi = 1.2$ which is higher than that for the consumption rate. As shown by Eq.7, the rate of heat release is obtained as the product of burning rate, W, and the heat of combustion, ΔE, which for methane is approximately 55.6 MJ/kg.

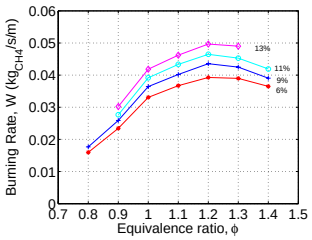


Fig.7 Mean burning rate of methane

The resulting heat release is shown in Fig.8, which illustrates that the maximum rate of energy release for the turbulent combustion of methane in an open V-flame occurs at an equivalence ratio of about 1.2. The mean consumption rates obtained from simulations of various ethylene flames are shown in Fig.9 to be similar to those of methane flames. However, in contrast to the results for the methane flame where the incremental increases in the turbulence level resulted in uniform increases in $\overline{C}$ for all equivalence ratios, the ethylene flame results show that increases in the turbulence level have a diminishing effect on the consumption rate for cases where $\overline{C}$ is at or near its maximum; i.e. $\varphi = 1.2 - 1.3$. This suggests that further increase in turbulence intensity for the more fluctuating ethylene flames would have little effect on the maximum consumption rate.

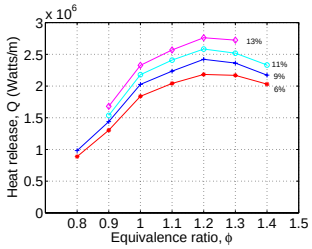


Fig.8 Mean heat release rate for a CH_4 flame

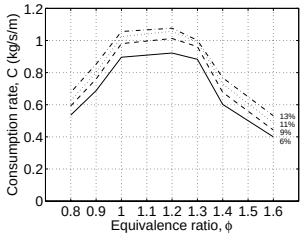


Fig.9 Mean consumption rate of premixed C_2H_4 reactant

Due to the higher flame speeds, the reactant consumption rate for the ethylene flames are around 40-50% higher than for the methane flames. It can be seen from Fig.10 that for each turbulence level, the maximum value for $\overline{W}$ is achieved at $\varphi = 1.3$, which is slightly higher than the W_{max} at $\varphi = 1.2$ for methane. For the lower turbulence cases of 6% and 9%, the ethylene flames consume around 75-80 % more fuel per second than for a comparable methane flame. For the higher turbulence levels of 11% and13%, this increase in the burning rate of fuel reduces to 60-65%. After considering the heat of combustion of C_2H_4, at about 49.6 MJ/kg, the overall rate of heat release is shown in Fig.11. It ca be seen that the maximum rates of heat release for the turbulence intensity investigated in this paper is between 3.5 to 4 MW/m. These values for an ethylene flame are around 50-60% higher than can be achieved from a comparable methane flame of 2.2 to 2.7 MW/m.

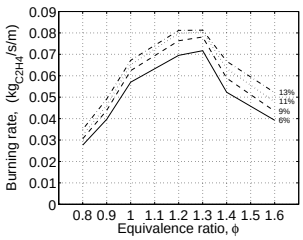


Fig.10 Mean burning rate of ethylene

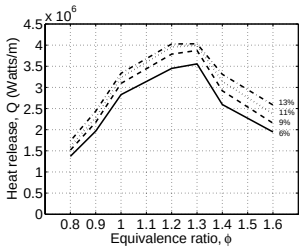


Fig.11 Mean heat release rate for a C_2H_4 flame

V. CONCLUSIONS

Numerical simulation of two-dimensional premixed methane and ethylene V-flames are conducted to investigate the effects of equivalence ratio and turbulence intensity on heat release rate. The equivalence ratios under investigation in this paper range from $\varphi = 0.8-1.4$ for methane and $\varphi = 0.8-1.6$ for ethylene. Turbulence level varies from 6% to 13%.

For a methane flame, the maximum heat release rate for a given turbulence intensity, is shown to be when equivalence ratio of the reactant mixture is 1.2. For ethylene, this maximum occurs at a slightly richer fuel/air mixture of $\varphi = 1.3$. The general effect of increasing turbulence is to increase the speed of the mean turbulent flame zone relative to the oncoming freestream flow. This leads to an increase in the total amount of fuel burnt per second, and ultimately the rate of energy release. As turbulence is gradually increased for the methane flame, steady and consistent increases in the heat release rate are found over the range of equivalence ratios under investigation. However, for ethylene, the change in the maximum heat release rate associated with a change in the turbulence level is found to diminish at higher turbulence intensity. This suggests that further increase in the turbulence level beyond 13% would not increase the maximum heat release rate substantially for an ethylene flame.

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