

BURNING VELOCITY OF COMBUSTIBLE MIXTURES IN A CLOSED VESSEL

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Abstract. *The burning velocity is an important physico-chemical characteristic of a combustible mixture. There are several experimental and numerical ways to analyze the burning velocity. One of the experimental techniques available consists in measuring by image analysis or estimating from the transient pressure curve the burning speed of the premixed reactant mixture centrally ignited within a sealed constant volume reactor. This work presents a review of the theoretical background of the two methods of measuring burning velocity in closed vessels. Advantages and limitations are discussed in terms of the size of the vessel, accuracy of the available measurement techniques and influence of turbulence. Finally, an experiment with a closed vessel is proposed for the measurement of burning velocity with either the two methods.*

Keywords: *Burning Velocity, Premixed flame speed, Constant volume reactor.*

1. INTRODUCTION

Several physical and chemical processes influence the thermal efficiency, maximum torque, pollutant emissions, driveability and durability of internal combustion engines. The main impact of the thermal processes in thermal efficiency can be divided in aspects related to the volumetric and to the combustion efficiencies. The volumetric efficiency is defined as the ratio of the amount of mass of air actually admitted by an engine and the mass of air that could be admitted in the ambient pressure and temperature in an adiabatic and reversible flow. It is affected by thermodynamic effects, such as those that result from equivalence ratio and internal recirculation of combustion gases, and by transport effects, such as those that originate from fuel evaporation, head loss, inertial and acoustic effects in the admission and exhaust systems and heat transfer. The combustion efficiency, in turn, is defined as the ratio between the amount of energy actually released during combustion and the total amount of energy in the admitted fuel, characterized by its low heating value (LHV). It is affected by ignition, flow and turbulence in the combustion chamber, chemical kinetics and heat transfer.

This work focuses on the propagation of premixed flames in constant volume reactors under conditions of pressure, temperature and equivalence ratio typical of internal combustion engines. In spark ignited, indirect injection engines, turbulence induced by the admission valves and variations in composition induced by mixture stratification affect flame ignition and propagation as much as chemical kinetics. These effects are highly dependent on flow and geometry of induction systems and are hardly reproduced experimentally. The flame speed is a useful parameter describing the effect of fuel air mixture chemical and physical properties on flame propagation and stability and is a parameter widely used in zero-dimensional internal combustion engines modeling and combustion models in the wrinkled flamelet regime. The use of simpler spherical or cylindrical closed reactors and fully premixed gas mixtures allows studying the flame speed without complicated three dimensional geometric effects. The disadvantage when compared to a transparent research engine is the fact that flow and turbulence conditions are reproduced only approximately.

In a typical closed vessel experiment, the fuel air mixture previously dosed fills the vessel homogeneously at a given pressure. After equalization of the initial temperature a flame kernel is initiated by a spark ignition. Under appropriate flammability conditions, the flame kernel grows as a laminar spherical flame. The burned gases expand as a result of an 8 to 10 times temperature increase increasing the average pressure of the vessel. This pressure compresses essentially isentropically the unburned mixture far from the flame front. The flame propagates over this compressed mixture at increasingly higher burning velocities. At higher velocities, flame surface instabilities grow and the flame becomes increasingly wrinkled. This is clearly evidenced by Schlieren and Shadowgraph images of the flame surface. The flame continues to propagate towards the vessel walls until the complete mixture is burned or the flame suffers extinguishment.

The displacement flame speed computed from image is larger than the consumption flame speed, due to the unburned gas flow towards the vessel walls. After accounting for the unburned gas flow, the resulting consumption flame speed is still affected by the flame rate of stretch. For essentially spherical flames the stretch is well defined and the stretch rate decreases as the radius of curvature increases. Then, the flame speed measured can be extrapolated for the zero stretch rate condition returning the unstretched flame speed. This has been measured for methane, propane, hydrogen and natural gas mixtures with air (Checkel and Ting, 1993; Cashdollar et al, 2000; Huang et al., 2006), dimethyl-ether (Huang et al., 2007), and ethanol/air mixtures (Nomura et al., 2003; Liao et al., 2007).

Traditional experiments performed by Metghalchi (1982), Bradley et al. (1996), Bradley et al. (1998) and Aung et al. (1997) performed experiments for hydrogen, methane, iso-octane, n-heptane, methanol, indolene mixtures with air at different equivalence ratios, initial pressures and temperatures in a CVR for initially quiescent premixed mixtures. They showed the potential of the method and presented the first modeling to interpret the experimental results. From the literature in recent years, Checkel and Ting (1993) analyzed the combustion of propane and methane mixtures with air in a CVR for different equivalence ratios and initial turbulence, generated by a perforated plate. The turbulent fluctuations produced by the plate are altered by the flame propagation. The results show a linear dependence between flame speed and turbulence intensity. The linear coefficient, however, grew linearly with the flame radius, more strongly when initial turbulence had smaller integral length. Cashdolar et al. (2000) presented a flammability limits study for the combustion of methane, propane, hydrogen and deuterium mixtures with air in 20 L and 120 L spherical CVR. They measured lower and upper flammability limits, rates of pressure rise and maximum pressures as related to explosion hazards in premixed mixtures. Song and Sunwoo (2000) studied the initial flame kernel development as a function of spark energy for indolene-air mixtures. They developed a theoretical model for kernel ignition and growth and compared to measurements in CVR. Nomura et al. (2003) studied the flame propagation in CVR for fully premixed mixtures and fuel droplets dispersed in air, for ethanol. Results showed the effect of the liquid fuel in the flame speed. The flame speed and maximum pressure increased for low equivalence ratio and decreased for higher equivalence ratio (above and below stoichiometry). This effect was also shown to be dependent on droplet size. Smallbone et al. (2006) measured the flame velocity of premixed hydrogen air mixtures in a fan agitated constant volume reactor for different pressures and equivalence ratios. They analyzed the turbulent flame velocities for different initial turbulent intensities. Chen and Ju (2007) modeled the flame propagation in normal and elevate pressures in constant pressure and constant volume reactors. The results show the strong dependence of flame measured displacement speed on compression speed of the unburned gas and flame stretch. They then propose correction functions to be applied over measurements. Huang et al. (2006) measured flame velocities for natural gas and hydrogen mixtures with air for different hydrogen fractions and fuel equivalence ratios. Correlations were proposed for the unstretched flame speeds. Huang et al. (2007) measured flame speed in CVR for dimethyl-ether/air mixtures at different pressures and equivalence ratios. Liao et al. (2007) measured the flame speed of premixed ethanol-air mixtures in a CVR and proposed correlations as a function of equivalence ratio and unburned pressure and temperature.

Extending the initial results and measurement methods of Metghalchi (1982), Bradley et al. (1996), Bradley et al. (1998), Gu et al. (2000), Rahim et al. (2001) presented measurements for cylindrical and spherical vessels for methane/air and methane/oxygen/argon mixtures for different temperatures, pressures, equivalence ratios and diluent concentrations. Parsinejad (2005) presented measurements in the same vessels for JP-8, JP-10 and reformed fuels at high temperatures and pressures, extending the previous results. Rahim et al. (2008) reanalyzed the thermodynamic models used to predict flame speeds and proposed new corrections to be applied over the measured values. These measurement and modeling efforts will be analyzed in more detail in the following.

The objective of this work is to analyze the flame propagation in initially quiescent premixed fuel/air mixtures in a constant volume reactor. This is an ongoing research. Here, we present the modeling needed to analyze the experimental results, discuss the limitations of the different methods and present a design of an experimental facility capable of achieving the expected results.

2. FLAME MODELLING IN CONSTANT VOLUME REACTORS

In a constant volume reactor, the average flame surface grows essentially as a spherical wave. The flame surface is defined as the sharp interface separating the burned from the unburned gases. Figure 1 presents a rendering of the flame surface for a given elapsed time during flame propagation towards to the unburned gases. The flames of interest here are the deflagration waves that do not find suitable conditions, due to limitations in pressure, temperature and available space, for transition to detonation. The deflagration waves present smaller gradients of pressure across the flame front and smaller characteristic speeds.

Different speeds may be defined for a propagating deflagration wave. The rate of propagation of the flame front, as measured by optical methods, is related to the time change of a flame surface coordinate related to a frame of reference at rest in respect to the laboratory. This is the displacing flame speed and can be calculated as

$$S_d = dr/dt \quad (1)$$

where S_d is the displacing flame speed and r is the flame radius as detected by image treatment.

For plane flame propagation in a flowing mixture, this flame speed is equal to the consumption flame speed, and is called the burning velocity. Mallard and Le Chatelier established in the 19th century, the first theory on the consumption flame speed. They identified two heat transfer zones controlling flame propagation, as rendered in Fig. 2(a). From a heat transfer analysis, they proposed that the consumption flame speed scales with the thermal diffusivity of the gas mixture α and the thermal thickness of the premixed front δ following

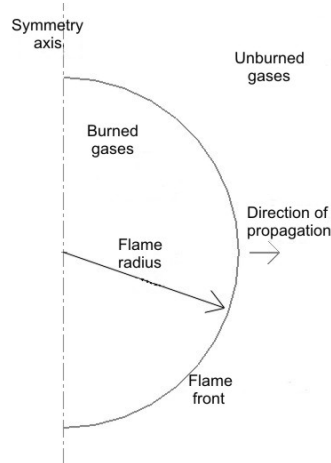


Figure 1. Rendering of the propagation of a spherical flame. The flame is considered with negligible thickness.

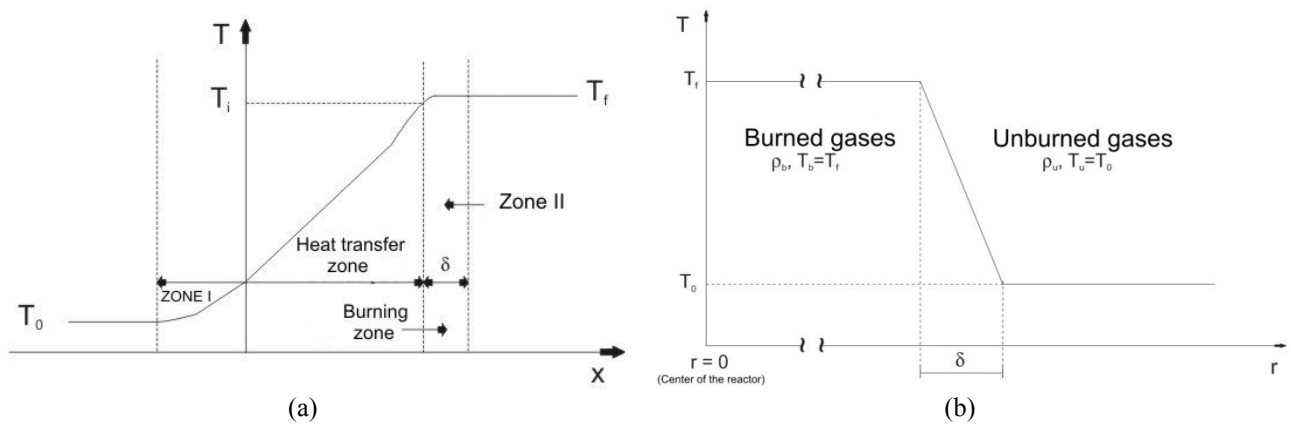


Figure 2. (a) Heat transfer controlling regions proposed by Mallard-Le Chatelier's model and (b) simplification of the flame front structure as a simple one length-scale model. T_0 is the temperature of unburned gases, T_f is the temperature of burned gases and T_i is the temperature of ignition of the mixture.

$$S_B \approx \alpha / \delta \quad (2)$$

The relation between the displacement flame speed and the consumption flame speed for a propagating mixture in a closed vessel can be developed based on Mallard-Le Chatelier's model. Figure 2(b) presents a simpler model of the flame structure as a simple one length-scale boundary layer. The burned gases are at a temperature above that of the reactants. Heat transferred to the unburned gases causes an expansion of the reactants in front of the interface between zones I and II. This expansion results in a relative velocity of the gases immediately in front of the interface. The consumption burning speed (or burning velocity, Glassman, 1996) is related to the mass consumption speed of the unreacted mixture, i.e.,

$$\dot{m}_{consumed} = \rho_u A_u S_B \quad (3)$$

In steady state, the mass flow that arrives at the flame zone with thickness δ from the reactants side must balance the mass flow leaving the flame surface in the products side, i.e.,

$$\dot{m}_{reactantsconsumed} = \dot{m}_{productsformed} = \rho_b A_b S_d \quad (4)$$

For a very thin flame sheet, $A_u = A_b$, and then

$$S_B = S_d \frac{\rho_b}{\rho_u} \quad (5)$$

The assumption of thin flame sheet may not hold for dilute mixtures or fast diffusing fuels. Then, Equation (5) leads to errors and a correction factor should be used. Bradley (1998) proposed a correction factor for methane and air mixtures as function of flame thickness, flame radius and the densities of burned and unburned gases.

The burning velocity is directly related to the rate of energy release and that is a key factor for internal combustion engines. There are basically two main methods for measuring the burning velocity: The thermodynamic methods that uses the pressure rise in the reactor and the optical methods that measure the displacement velocity of the flame front by image analysis.

3. EXPERIMENTAL METHODS FOR FLAME PROPAGATION MEASUREMENTS

Both the thermodynamic and the optical methods have been used as complementary strategies for measurement of the burning velocity. In the following, both methods are reviewed as they have been applied by different groups.

3.1. Thermodynamic method

Metghalchi (1982), Rahim et al. (2001, 2008) and Parsinejad (2005) used the thermodynamic method to measure the burning flame speed of methane, iso-octane, n-heptane, methanol, indolene and hydrogen mixtures with air at different equivalence ratios, initial pressures and temperatures in a CVR for initially quiescent premixed mixtures. The method originally developed by Metghalchi (1982) and extended by Rahim et al. (2001) will be discussed.

Rahim et al. (2001) used two constant volume reactors, one cylindrical with optical access and the other spherical without optical access. The spherical reactor had diameter of 15.24 cm and the cylindrical reactor had inner diameter and length of 13.34cm. The cylindrical reactor was used for studies of the evolution of surface instabilities. The two optics accesses allowed imaging by Schlieren. The spherical reactor was subjected only to pressure rise measurement. Conservation of energy and mass in the constant volume reactor provides

$$\frac{E}{m} - \frac{A}{m_0} \int_0^{\delta} p d\delta' = \int_0^x e_b dx' + \int_x^1 e_u dx' \quad (6)$$

$$\frac{V}{m} - \frac{A\delta}{m} = \int_0^x v_b dx' + \int_x^1 v_u dx' \quad (7)$$

where m , E and V are the mass, the energy content and volume of the reactants at the initial conditions, A is the inner area of the reactor, p is the pressure in the reactor, e and v are the specific energy and volume, the subscripts b and u are related to the burned and unburned gases respectively, x is the mass fraction of burned gases and δ is a thermal boundary layer next to wall. This boundary layer is responsible for heat loss and is used to correct the values calculated at latter times.

Since both specific energy and volume are functions of temperature there are three unknowns: the temperature and mass fraction of burned gases and the pressure. The pressure is obtained from the experiments and is considered constant spatially inside of the reactor (since the energy associated with sound waves is much smaller than the internal energy of the combustion mixture, sound waves are not taken into account). For essentially adiabatic and reversible conditions, both the burned and unburned gases are isentropically compressed during the combustion. The equations are then resolved using the shell's method. In this method, the burned gases are sliced into shells whose thickness is inversely proportional to the combustion duration. A 2-D Newton-Raphson method is then used to solve the equations. From the mass fraction and temperature of burned gases the burning velocity is calculated by

$$S_B = m\dot{x}v_u / A_f \quad (8)$$

where \dot{x} is the rate of variation of the mass fraction of the burned gases and A_f is the area of the surface of the flame. This area is calculated from the volume of the burned gas as

$$V_b = xv_b m = \frac{4}{3} \pi r_f^3 \quad (9)$$

Note that since the value of V_b is related to the burned gases, therefore, both A_f and r_f are related to the unburned gas side. In the thin flame sheet model it does not matter from which side r_f is measured. However, when the flame is modeled as having a thickness equal to δ , this method could lead to errors. Parsinejad (2005) presented a work where the flame thickness and other heat loss corrections were considered.

For the effect of flame stretch rate on flame speed Rahim et al. (2001) used the Clavin's expression, given by

$$S_n = S_B + \ell \alpha \quad (10)$$

where S_n is the unstretched burning velocity, ℓ is a characteristic length called the *Markstein Length* and α is the rate of stretch of the flame surface given by

$$\alpha = \frac{1}{A_f} \frac{dA_f}{dt} \quad (11)$$

Bradley (1996) presented a theoretical and computational work addressing the effect of stretching on the flame velocity. However, stretching effects are most relevant only for small radii. In the small radii regime, the pressure increase is also small, is heavily affected by experimental uncertainties, and the thermodynamic method based on the pressure curve results in large errors.

3.1. Optical method

Bradley and co-workers published experimental and theoretical works addressing optical measurements of burning speed. They use a spherical reactor with optical accesses for the Schlieren method.

Basically, from the image analysis, the variation of radius with time is determined. Then, Eq. (1) is used to determine the flame displacement speed. However, the radius measured by Schlieren cannot be used directly. The flame front evidenced by Schlieren method corresponds to the value of maximum spatial variation of the gas density. Since the density is directly related to the temperature, this corresponds to the inflection point in the temperature rise along the premixed flame. For most hydrocarbons at low initial temperature, this point corresponds to the isotherm of approximately 700 K. The equations used by Bradley and co-workers are based on an isotherm that is about 5 K above the reactants temperature. Since there is a displacement between these two isotherms, a correction factor transforming the Schlieren radius to the flame radius is proposed as

$$r_f = r_{sch} + 1,95 \delta_l \left(\frac{\rho_u}{\rho_b} \right)^{0,5} \quad (12)$$

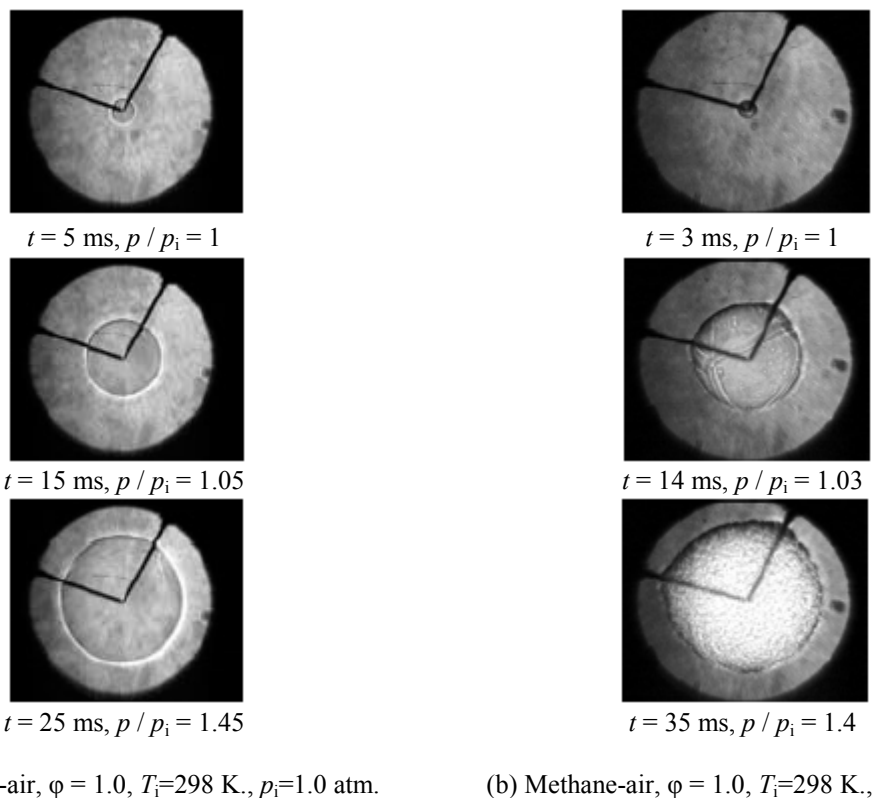
where r_{sch} is the flame radius measured by the Schlieren method and δ_l is the flame thickness. We note that the flame velocity is then evaluated in the unburned gases side.

From the corrected flame radius, the displacement flame velocity is evaluated. Then, the consumption flame speed is determined from Eq. (5) using a correction that accounts for the flame thickness. The correction proposed by Bradley and co-workers for a stoichiometric mixture of methane and air at 300 K and 1 atm is

$$S = 1 + 1,2 \left[\frac{\delta_l}{r_u} \left(\frac{\rho_u}{\rho_b} \right)^{2,2} \right] - 0,15 \left[\frac{\delta_l}{r_u} \left(\frac{\rho_u}{\rho_b} \right)^{2,2} \right]^2 \quad (13)$$

This correction is based on a proposed premixed flame structure typical of methane air stoichiometric flames. Although it can be used as an approximation for other hydrocarbon fuels, this extension is not warranted.

For the correction due to stretch effects, Clavin's expression was not used, but rather, they developed a composed correction factor, influenced by curvature effects and by hydrodynamics factors. Another important aspect regarding Bradley and co-worker's model is about the locus of evaluation of the burning properties. The places where the properties are evaluated affect the value of the calculated burning speeds. Further information can be obtained in Bradley (1996).



(a) Methane-air, $\phi = 1.0$, $T_i=298$ K., $p_i=1.0$ atm.

(b) Methane-air, $\phi = 1.0$, $T_i=298$ K., $p_i=5.0$ atm.

Figure 3: Shadowgraphs showing flame propagation in a constant volume cylindrical reactor for stoichiometric methane-air mixtures at three elapsed times at $\phi = 1.0$, $T_i=298$ K and (a) $p_i=1.0$ atm, and (b) $p_i=5$ atm (adapted from Rahim et al., 2008).

Figure 3 presents shadowgraphs showing flame propagation in a constant volume cylindrical reactor for stoichiometric methane-air mixtures at three elapsed times at $\phi = 1.0$, $T_i=298$ K for $p_i=1.0$ atm [Fig. 3(a)] and $p_i = 5$ atm [Fig. 3(b)] (adapted from Rahim et al., 2008). In the third picture in Fig. 3(a) we note that the flame has covered much of the viewing window but the pressure has increased only 45%. The total pressure increase observed in that experiment is about 7 atm. Therefore, the majority of the pressure increase occurs for high flame radius, where stretch ceases to be dominant. We note also that, even for an initially quiescent mixture, for higher pressure the flame develops surface instabilities, initially in the form of surface cracks (at 14 ms) and latter as a cellular surface (at 35 ms). The wrinkling is associated to the development of surface Darrieus-Landau instabilities which are locally reduced or reinforced by a Lewis number effect.

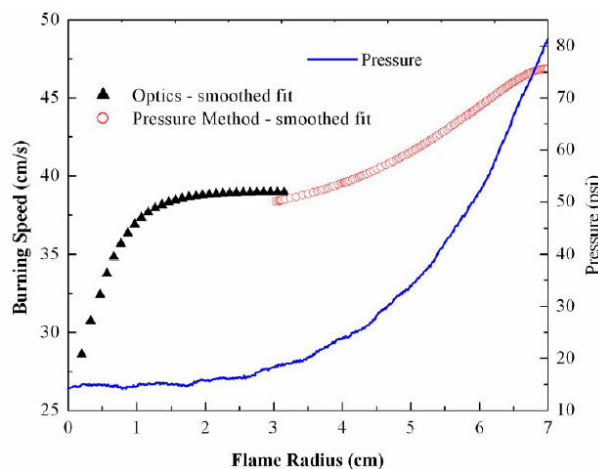


Figure 4: Complementary use of image analysis and pressure profile thermodynamic methods to measure flame speeds (methane-air flames, $\phi = 1.0$, 298 K, 101 kPa, from Parsinejad, 2005).

These instabilities appear once a critical rate of stretch is exceeded. This critical rate of stretch depends on the fuel, equivalence ratio and pressure. When the Lewis number is larger than one the instability is partially suppressed and the flame remains smooth for larger rates of stretch. In methane-air flames at $\phi = 0.8$, $Le = 1.01$ and this behavior prevails. In hydrogen-air mixtures, however, $Le = 0.57$ and then instability develops at a smaller rate of stretch (Bradley, 1996; Smallbone et al., 2006). Although the flame speed is lower at higher pressures, the wrinkling results in a larger velocity when compared to a smooth flame in the same conditions, due, largely, to the increase in the flame surface area. The analysis that follows will focus on smooth surface flames.

Figure 4 presents the flame speeds computed from pressure profile and from image analysis for the same methane-air flame at $\phi = 1.0$, 298 K and 100 kPa (from Parsinejad, 2005). We note that for smaller flame radius, the optical method is more accurate and the pressure increase is still too low to be used. Then, for higher flame radius the image is affected by distortions and the pressure profile method becomes more reliable. Therefore, both the thermodynamic and the optical methods have been used as complementary strategies for measurement of the burning velocity.

Based on the thermodynamic analysis presented above, a simplified model is applied as a first assessment of the burning speed in constant volume reactors. This is presented and applied below for a simple methane-air flame.

4. A SIMPLER THERMODYNAMIC METHOD

The model proposed is based on equations of volume and energy conservation. No account is made of heat loss and boundary layer effects. The burning velocity is calculated using Eqs. (10) and (11). Using the ideal gas law, the conservation of volume can be stated as

$$V = V_b + V_u \quad (14)$$

$$m = m_b + m_u \quad (15)$$

$$\frac{V}{m} = \frac{V_b}{m_b} + \frac{V_u}{m_u} = \frac{V_b}{m_b} \frac{m_b}{m} + \frac{V_u}{m_u} \frac{m_u}{m} \quad (16)$$

$$v = v_b x_b + v_u x_u \quad (17)$$

$$v = \frac{R_{g,b} T_b}{p} x_b + \frac{R_{g,u} T_u}{p} x_u \quad (18)$$

where R_g is the universal gas constant and the subscripts b and u are related to the burned and unburned gases respectively.

For the conservation of energy, assuming constant properties, the internal energy is expressed as

$$u = u_f^o + \int c_v dT \quad (19)$$

where the internal energy of formation at standard state is

$$u_f^o = h_f^0 - p_0 v_0 = h_f^0 - R_g T_0 \quad (20)$$

Then the equation of conservation of energy is written as

$$u = x_b h_{f,b}^0 + x_u h_{f,u}^0 - R_g T^0 + x_b \int_{T_0}^{T_b} c_{v,b} dT + x_u \int_{T_0}^{T_u} c_{v,u} dT \quad (21)$$

With the equations (18) and (21), equation for the isentropic compression of unburned gases, the sum of the mass fraction of burned and unburned gases and a pressure function of the time the temperature and mass fraction of burned gases can be obtained.

5. RESULTS AND DISCUSSIONS

The system of equation above was solved using the software *EES – Engineering Equation Solver 6.833-3D* and a code in FORTRAN language. In the FORTRAN code the Newton-Raphson method was used as a numerical solver. The properties of burned and unburned gases were obtained from polynomial obtained in the CEA/NASA website for the FORTRAN code. The burned and unburned gases were considered in thermal and chemical equilibrium and the burned gases are assumed formed by water vapor, nitrogen and carbon dioxide. The pressure versus time curve measured by Parsinejad (2005) for a stoichiometric methane/air flame was used as input. Figure 5 presents the pressure profile measured by Parsinejad (2005) for a stoichiometric methane/air flame at 298 K, 100 kPa.

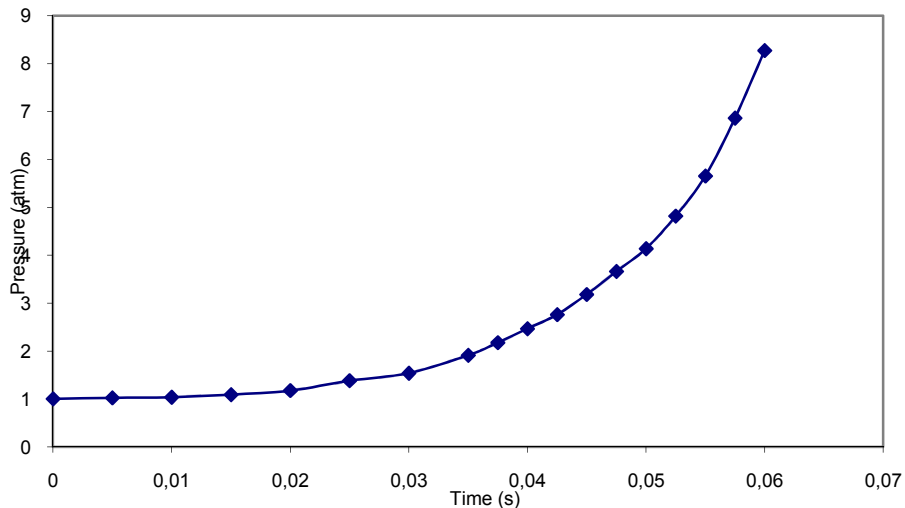


Figure 5: Pressure profile measured by Parsinejad (2005) for a stoichiometric methane/air flame at 298 K, 101 kPa.

Figure 6 presents the measurements and values predicted by ChemKin using GRIMEch 3.0 for methane-air mixtures at different fractions of diluents (86 % N₂ and 14 % CO₂) from Rahim et al. (2008). The curve for 0% diluents corresponds to the data in Figure 3(a). As expected from the literature, the flame speed remains around 40 cm/s and GRIMEch 3.0 provides a good prediction.

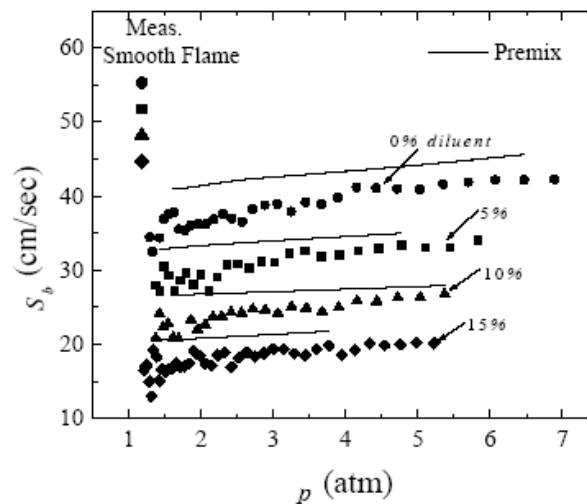


Figure 6: Measurements and values predicted by ChemKin using GRIMEch 3.0 for methane-air mixtures at different fractions of diluents (86 % N₂ and 14 % CO₂). The curve for 0% diluents corresponds to the data in Figure 3(a).

Figure 7 presents the results of flame consumption speed, the burning velocity, calculated by the proposed FORTRAN code. For comparison, the results were superimposed to Fig. 6. The model, described in section 4, approximates the results of Rahim et al. (2008) for pressures above 2 atm.

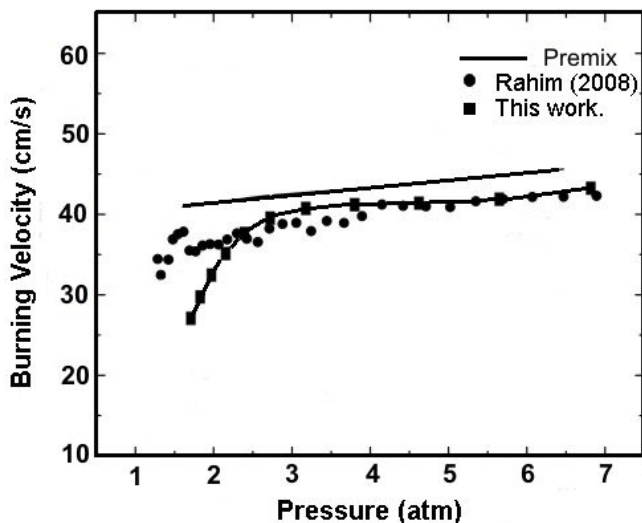
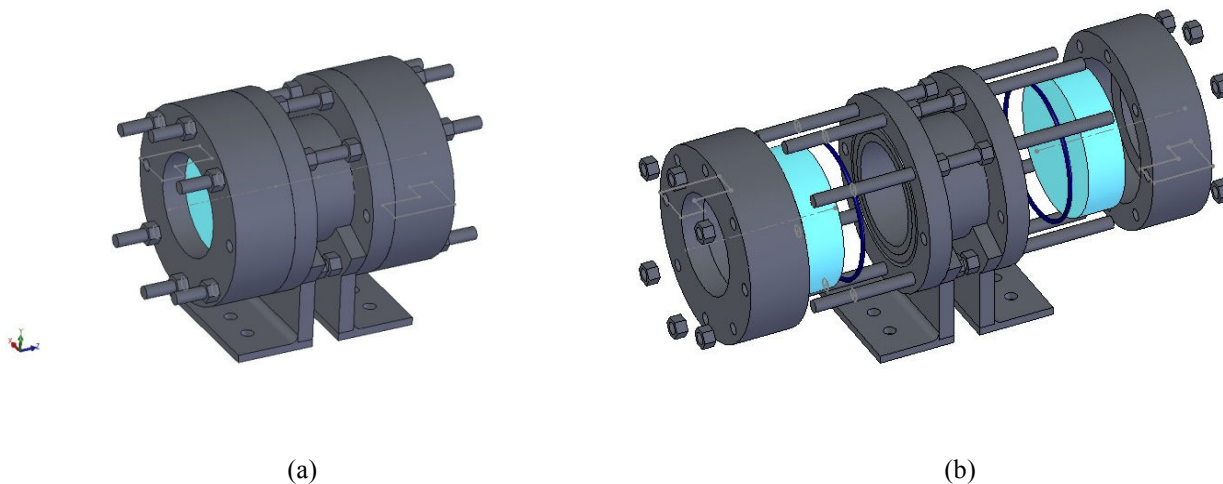


Figure 7. Burning velocity as a function of the pressure inside the reactor calculated using model described in the section 4 compared to the results calculated by Rahim et al. (2008) from the same pressure curve. Results for a stoichiometric mixture of methane and air initially at 300 K and 1 atm superimposed to the figure 6.

5. PROPOSED EXPERIMENT

Based on the analysis above, an experiment using a cylindrical constant volume reactor is proposed. The reactor is formed by two cylinders connected by a flanged hinge. Fuels are fed tangentially in the flanged region and both ends of the reactor have quartz windows, for image analysis. The fuel may be fed in high speed generating internal turbulence. This turbulence may be allowed to damp before ignition, or may be used as a way to impose and initial turbulent field. In this case, characterization of the turbulence is needed before the combustion experiments are performed. The analysis of the results will follow largely Parsinejad (2005) and Rahim et al. (2008), including the models of Bradley and co-workers for the flame thickness and heat loss effects.



Figure

Figure 8. Twice party reactor for low pressure experiments. (a) Mounted reactor and (b) exploded view.

6. CONCLUSION

The propagation of premixed flames in constant volume reactors was discussed. A thermodynamic model based on the pressure profile and optical methods to measure the flame velocity were discussed in context of experiments performed for methane-air mixtures available in the literature. A thermodynamic model was then developed for the prediction of the flame velocity from the pressure profile and the results compared well to results available in the literature. From the analysis, an experiment with a cylindrical reactor is proposed as a continuation of the present study.

7. ACKNOWLEDGEMENTS

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