Modélisation de la Vitesse de Propagation de Flamme Dans Une Chambre de Combustion Sphérique à Volume Constant

PROJET DE FIN D'ÉTUDES

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ABBREVIATIONS

- S_u: Laminar burning velocity
- $x(p)$: Burnt mass fraction at constant pressure
- C_p: Specific heat
- e: Specific internal energy
- h: Specific enthalpy
- m: Mass
- p: Pressure
- S: Entropy
- T: Temperature
- v: Specific volume
- r_b: Radius of the burnt gas
- R: Radius of the spherical vessel

ABSTRACT

In this thesis, multiple burned gas zone model has been used to determine temperature distributions and its relationship between pressure distribution and mass fraction in a constant-volume vessel. The constant-volume spherical vessel has been used for determining distributions of elevated initial temperatures and pressures. Multizone model allows us to find the laminar burning velocity and the intervals of temperature, pressure and equivalence ratios it can be found.

Laminar burning velocity has been found with different methods to compare with multizone model theoretically and experimentally. Various of equations were compared for their accuracy.

1. INTRODUCTION

The burning velocity is the characteristic propagation rate of laminar premixed flames, in order words the burning velocity Su is defined as the velocity at which unburned gases move through the combustion wave in the direction normal to the wave surface. They play essential roles in determining the ignition delay, the thickness of the wall quench layers, the minimum ignition energy. Moreover, a detailed knowledge of laminar pre-mixed flames will provide knowledge to heat release rates, flammability limits, propagation rates, quenching, and emission characteristics. The laminar burning velocity is a function of both fuel/oxidant ratio and temperature and pressure of the system. There are several ways to determine the laminar burning velocity. The most convenient one is the constant-volume bomb method which uses a spherical vessel with central ignition. The aim of using a spherical vessel with central ignition is to generate laminar burning velocities for varying conditions. Fortunately, using a spherical vessel with central ignition with a multizone model provides this to us with a single test.

The fuel is burnt in turbulent combustion mostly. In order to ease the analysis, a set of assumptions is made. These can be classified as uniform pressure, negligible heat loss or gain, no buoyancy, isentropic compression of the unburnt gas, spherical flame front and ideal gas behavior.

The spherical method is widely used for the flammable gases, because it provides experimental accuracy as well as operational simplicity: the burning velocity of a compound together with its temperature and pressure dependence is obtained simultaneously. On the other hand, there is a concern about using spherical vessel method for weakly flammable compounds. For a compound with low burning velocity such as NH3 the buoyancy force may distort the flame front which cannot be regarded as spherical. In other words, it is impossible to use our assumption that the flame front is spherical and smooth.

2. SPHERICAL VESSEL METHOD

The assumptions and mathematical derivations for the pressure and burned and unburned gas temperatures are presented for the single burned gas zone model. The single burned gas zone model was extended to two burned zone and then to multiple zones.The reason of dividing the spherical vessel into multiple zones is the two zone analytical model neglects the burnt temperature gradient. This simplification was shown not to affect the x(p) results within a perfect gas. However, when a both burnt temperature gradient and dissociation are allowed, this may no longer hold true: enhanced dissociation near the core of the vessel may affect the mass averaged burnt temperature, leading to different results for x(p) as well.

In a two zone model, both the burnt and unburnt zones have uniform temperatures and compositions:

$$v_t = x \cdot v_b + (1 + x) \cdot v_u \tag{1}$$

$$e_t = x \cdot e_b + (1 + x) \cdot e_u \tag{2}$$

Having a conversation of specific volume and specific internal energy:

$$x = \frac{p - p_i \cdot (p)}{p_e - p_i \cdot f(p)} \tag{3}$$

Knowing that $f(p)$ in equation(3) is:

$$f(p) = \frac{\gamma_b - 1}{\gamma_u - 1} + \left(\frac{\gamma_u - \gamma_b}{\gamma_u - 1}\right) \cdot \left(\frac{P}{P_i}\right)^{\frac{\gamma_u - 1}{\gamma_u}} \tag{4}$$

In the multi zone model, flame prorogation is seen as the consecutive consumption of unburned mixture within the zones. Before ignition, the mass in the spherical vessel divided into n zones. At the time, when combustion has just began in the bomb, the flame front will consume zone 1 first. As a result, the temperature and hence the pressure of zone 1 will increase by the ideal gas assumption, thereby compressing the rest of the unburned gas and increasing pressure inside the vessel to a higher value. After the consumption of the first zone, consumption of the second zones will take place at a higher pressure than the initial pressure. When the flame front is passing through the nth zone, the combustion of this zone takes place at a temperature of $T_{u,n-1}(> T_i)$ and a constant pressure $P_{u,n-1}(P_i)$. After the flame has consumed the nth zone, it is assumed to be adiabatic. Previous work has shown that when the burning velocities are above $20\frac{cm}{s}$, the effect of buoyancy is less than 0.5 % on the observed burning velocity. Subsequent combustion further compresses the burned gas and the unburned gas. As a result, temperature and density gradients are established in the burned gas region.

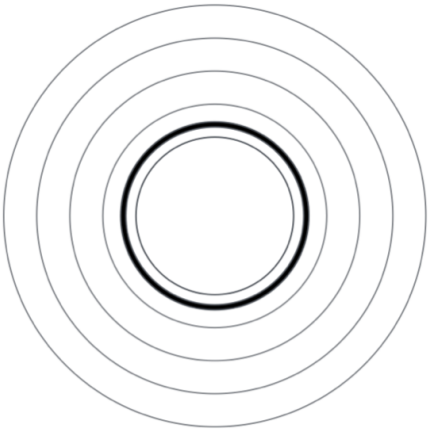

Figure 1: Zone 2 burning

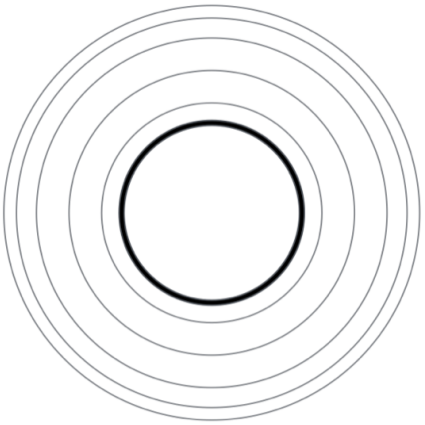

Figure 2: Zone 1 burning

The approach for two zones can be extended to multiple zone model. Neglecting heat loss to the vessel wall:

$$v_t = \sum_{j=1}^{n=1} x_j \cdot v_{bj} + x_n v_{bn} + \left[1 - \sum_{j=1}^{1} x_j\right] \cdot v_u \tag{5}$$

$$e_t = \sum_{j=1}^{n=1} x_j \cdot e_{bj} + x_n e_{bn} + \left[1 - \sum_{j=1}^{1} x_j\right] \cdot e_u \tag{6}$$

$$x = \sum_{n=1}^{N} x_n \tag{7}$$

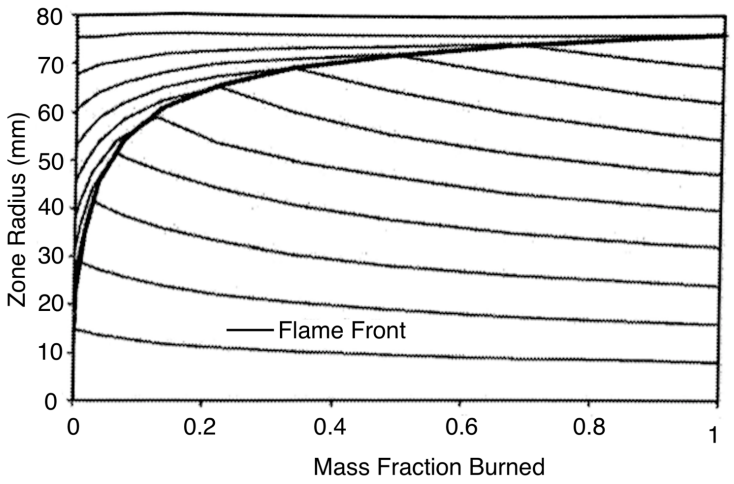

Figura 3: Mass fraction in function of the zone radius

In Figure 3 we are able to see how the radius of each zone varies during the propagation of the flame front. As the flame front travels through the combustion bomb, each zone burns and an increase in the radius of that zone takes place. This is due to the expansion of the products of combustion immediately behind the flame front. When the flame front has passed the zone, recompression of the zones takes

place due to the expansion of the next zone. Due to the recompression, a decrease in the radius and hence the volume of the burned zones takes place. This results in an increase in the temperature of the burned gas zones, which establishes the radial burned gas temperature gradient. As the first burned zone is hotter than the outer zones it can be seen that the zone 1 finishes with a larger radius.

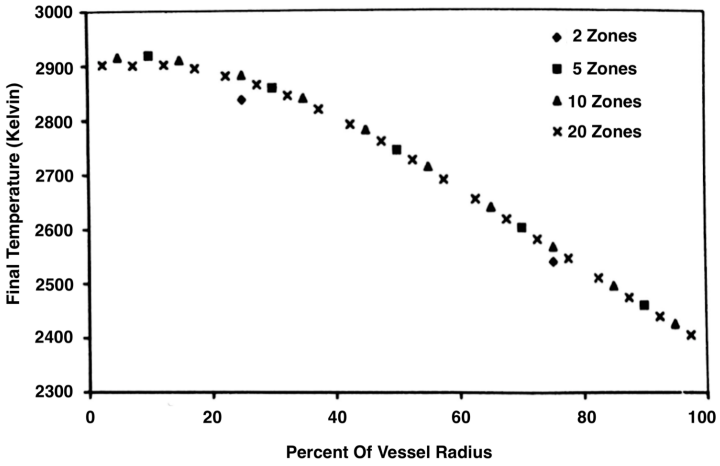

Figura 3: Final variation of temperature with the zones in the equal radius model with initial conditions of 1 bar and 298.1 K for stoichiometric methane-air mixture

3. BURNING VELOCITY MEASUREMENT USING SPHERICAL VESSEL METHOD FOR FLAMMABLE COMPOUNDS

The burning velocity calculations are based on using a spherical closed vessel filled with homogeneous combustible mixture. At time $t = 0$, the mixture is ignited at the center; a spheric flame front is established and begins to propagate outwardly to reach the wall. The following assumptions are used:

- The unburned gas is initially at rest and the gas has a uniform temperature and composition.
- The thickness of the reaction zone is negligible, and the flame front is smooth and spherical.
- The burnt gas fraction x is at local thermodynamic and chemical equilibrium.
- The unburned gas fraction $(1 - x)$ is at local equilibrium but with fixed chemical composition.
- The pressure within the combustion vessel is a function of the time and independent of the flame front.
- The compression for the whole gas is adiabatic and reversible.
- The gas behaves as a semi perfect gas.
- The effects of body forces and of radiative energy transfer can be neglected.
- There is no heat transfer between burned and unburned gas.

From the equation of continuity:

$$\frac{dm_u}{dt} = -A\rho_u S_u \tag{8}$$

Combustion in a constant volume spherical vessel, the mass of unburnt gas at any instant:

$$m_u = \frac{4}{3}\pi[(R^3 - r_b^3)] \tag{9}$$

From the equations (8) and (9) we arrive to:

$$\frac{dm_u}{dt} = \frac{4}{3}\pi\left[(R^3 - r_b^3)\frac{d\rho_u}{dt} - 3 \cdot r_b^2\rho_u\frac{dr_b}{dt}\right] = -A\rho_u S_u \tag{10}$$

From equations (8) and (10) and knowing that $A = 4\pi \cdot r_b$:

$$S_u = \frac{dr_b}{dt} = \frac{R^3 - R_o^3}{3r_b\rho_u} \cdot \frac{d\rho_u}{dt} = S_s - S_g \tag{11}$$

Considering that the compression is adiabatic, $P = Cp^\gamma$:

$$S_u = \frac{dr_b}{dt} - \frac{R^3 - R_B^3}{3R_b^2\gamma_u \cdot P}\frac{dP}{dt} \tag{12}$$

The equation (12) is called: **The unburnt gas equation for the burning velocity of Fiock & Marvin.**

Alternative forms of these equations can be obtained by considering the burnt gas behind the flame front. Combustion in a constant volume vessel:

$$m_u = m_o - m_b \tag{13}$$

$$\frac{dm_u}{dt} = -\frac{dm_b}{dt} \tag{14}$$

From equation (8) and (14), we obtain:

$$S_b = \frac{1}{A\rho_u} \cdot \frac{dm_b}{d} \tag{15}$$

Being S_b a property of the burnt gas.

For a spherical flame front:

$$m_b = \frac{4}{3}\pi r_b^3 \bar{\rho}_b \tag{16}$$

The mean density allows us to obtain non-uniform properties of the gas behind the flame front due to recompression:

$$\bar{\rho_b} = \frac{3}{r_b^3}\int_0^{r_b} \rho_b \cdot r^2 dr \tag{17}$$

From the equations (16) and (17) we get:

$$\frac{dm_b}{dt} = \frac{4}{3}\pi\left[r_b^3\frac{d\bar{\rho}_b}{dt} + 3\cdot r_b^2 \cdot \bar{\rho}_b \frac{d\bar{\rho}_b}{dt}\right] \tag{18}$$

From equations (15) and (18):

$$S_b = \frac{\bar{\rho}_b}{\rho_u}\frac{dr_b}{dt} + \frac{r_b}{3\rho_u}\frac{d\bar{\rho}_b}{dt} \tag{19}$$

Considering adiabatic compression $P = C'\bar{\rho}_b{}^{\gamma b}$ we arrive to:

$$\frac{d\bar{\rho_b}}{dt} = \frac{\bar{\rho_b}}{\gamma_b P}\frac{dP}{dt} \tag{20}$$

$$S_b = \frac{\bar{\rho_b}}{\rho_u}\left[\frac{dr_b}{dt} + \frac{r_b}{3\gamma_b P}\frac{dP}{dt}\right] \tag{21}$$

The burnt equations for the burning velocity

Substituting we obtain:

$$r_b = R \cdot \left[\frac{\frac{\rho_u}{\rho_o} - 1}{\frac{\rho_u}{\rho_o} - \alpha}\right]^{\frac{1}{3}} \tag{22}$$

The calculated values of r_b are nearly always less than the observed radius. This difference suggests the existence of a reaction zone of significant thickness, particularly during the early stages when the spatial velocity is high. Values based on the low range pressure record one constantly nearer the observed radius than values from the high range record. The discrepancy between the calculated and observed flame radius suggests a lock of equilibrium in the burnt gas, probably confined to a reaction zone adjacent to the flame front. With the equations derive, on estimate of the degree of lack of equilibrium is possible.

Consider the parameter α which is defined as the ratio of the mean density of the burnt gas to the density of the unburnt mixture before ignition:

$$\alpha = \frac{\bar{\rho_b}}{\rho_o} = \frac{\bar{\rho_b}}{m_u}\frac{T_o}{\bar{T_b}}\frac{P}{P_o} \tag{23}$$

Using the observed maximum pressure, P_e, m_e and T_e, corresponding to final conditions in the burnt gas at the flame front, may be calculated assuming equilibrium conditions. An approximate value of ? may be calculated:

$$\alpha_e = \frac{m_e}{m_o}\frac{T_o}{T_e}\frac{P_e}{P_o} \tag{24}$$

In all cases ?e is less than unity. Since the total mass of gas in the vessel remains constant, the mean density of the products when the flame has reached the bomb wall must equal the initial density of the unburnt mixture:

$$\rho_b = \alpha\rho_o \tag{25}$$

Hence α_e should have a value of value of unity at the end of the process. The discrepancy must therefore be attributed to P_e and $\frac{m_e}{T_e}$ being too low.

- Consider P_e: an error could arise from:

- Incorrect calibration of the pressure measuring system
- Inadequate transient response of the pressure transducer

Use of the correct value would lower α_e still further.

- Consider $\frac{m_e}{T_e}$ instead of mean value of $\frac{m_e}{T_e}$:
  - The temperature at the flame front is less than that at the centre of the vessel. Thus T_e is less than mean value of T_e.
  - The difference between me and mean value of me is small compared with the difference between Te than mean value of T_e.
    Hence the use of mean temperatures to calculate α_e would yield even lower values than those obtained by using flame front temperatures.
    The only term left to account for the discrepancy between the deserved and expected values of: α_e is the temperature of the burnt gas. It appears that the calculated equilibrium value of flame front temperature is too high. There are two factors which may account for the calculated value of T_b being too high:
  - Combustion may not occur adiabatically due to heat loss. But, the quantity of heat loss by radiation up to the time the flame reaches the bomb wall is negligible. Conductive heat loss, due to buoyancy, is likely to be longer for slow burning mixtures, and should lead to lower values of α_e for the rich and lean mixtures tested. Therefore, heat loss can not explain discrepancy.
  - The assumption that equilibrium is attained immediately behind the flame front may not be justified: insufficient time may be available for the reactions to go to completion. If this is so then at any air/fuel ratio the thickness of such a reaction zone should increase with flame speed.

The lowest value of α_e coincides with the greatest observed spatial velocity. Thus if a non-equilibrium condition exists at the end of the precess ($\alpha_e < 1$); on even greater departure from equilibrium probably exits over the initial stages since the spatial velocity is then higher.

Using the alternative approximate expression for α:

$$\alpha = \frac{m_b}{m_e}\frac{T_e}{T_b}\frac{P}{P_e} \tag{26}$$

which must yield the correct value of α_e (unity).

All previous burning velocity equations have been based on the assumption that chemical equilibrium exists in the burnt gas. In the burning velocity equation any such lack of equilibrium is partly allowed for by using the dimensionless density ratio ? calculated from the above equation.

t msec	r_b in	dr_b/dt in./sec	P Low	lb/in^2 abs. High	$dP/\mathbf{dt}$ Low	lb/in^2 msec High	T_U R	M_b	T_b R	α
0	0.0823	—	12.09	12.09	—	—	531.9	29.01	4622	0.1248
1	0.4767	391	12.11	12.09	0.054	—	531.9	29.01	4622	0.1248
2	0.8699	395	12.27	12.15	0.328	0.215	532.6	29.01	4623	0.1255
3	1.2623	388	12.65	12.57	0.912	0.660	537.5	29.01	4626	0.1297
4	1.6437	371	14.20	13.58	1.808	1.428	548.8	28.99	4635	0.1399
5	1.9949	325	16.69	15.56	—	2.667	569.3	28.98	4650	0.1598
6	2.2948	281	—	19.17	—	4.667	602.3	28.96	4667	0.1960
7	2.5556	237	—	25.23	—	7.674	648.6	28.93	4694	0.2563
8	2.7730	202	—	35.84	—	12.121	713.0	28.89	4727	0.3611
9	2.9599	172	—	57.03	—	28.205	808.1	28.86	4761	0.5689
10	3.1080	121	—	87.50	—	24.937	907.0	28.83	4779	0.8679

Tabla 1: Abridged observations and results for stoichiometric acetylene−air mixture

In the Table (1) we have:

- Mixture composition:7,72 per cent acetylene in dry air (by volume)
- Spark: gap 0,040 in; max. voltage=6 kV; max energy=18 mJ
- Vessel radius: 3,153 in
- Initial conditions $P_0 = 12{,}09 lb/in^2$ abs; $T_e = 71{,}9^o F$
- Molecular weight of unburnt mixture: 28.63
- Observed maximum pressure: $P_e = 100{,}9 lb/in^2$ abs
- Properties of burnt gas at P_e: $M_e = 28{,}82$; $T_e = 4786 * R$

4. BURNING VELOCITY MEASUREMENT FOR FLUORINATED COMPOUNDS USING THE SPHERICAL VESSEL METHOD

The burning velocity:

$$S_u = \frac{R}{3}\left[1-(1-x)\cdot\left(\frac{P_0}{P}\right)^{\frac{1}{\gamma_u}}\right]^{\frac{-2}{3}}\cdot\left(\frac{P_0}{P}\right)^{\frac{1}{\gamma_u}}\frac{dx}{dt} \tag{27}$$

In order to use this equation, we have to obtain the relationship of P with x, γ_u, r_f, and burned and unburned gas temperatures T_u and T_b by equilibrium calculation at a constant volume condition. Here γ_u was obtained from the averaged value at the initial gas temperature T_0 and the instantaneous unburned gas temperature T_u. Then, these relationships were applied to the experimentally measured pressure P, and finally obtained S_u by solving the equation (27).

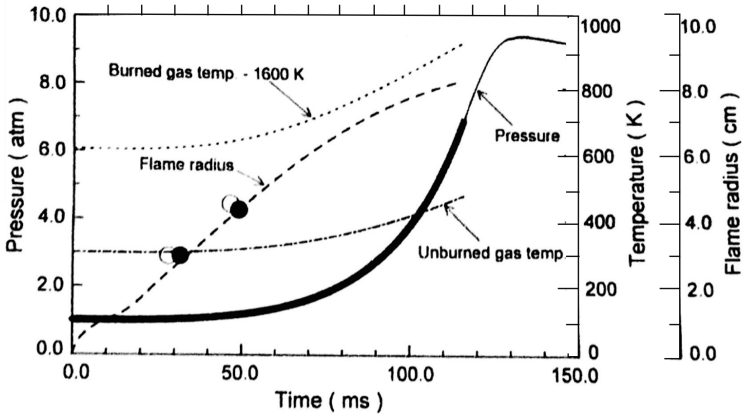

Figura 4: The experimental result for HFC143/air mixture. $\phi = 0{,}94$,$T_0 = 300K$, and $P_0 = 1{,}0atm$. The solid curve is the measured pressure. The broken dotted, and dotted-broken curves are calculated values of r_f, T_b and T_u. The filled and open circles are the arrival time at ion probes in the lower and upper part of the vessel.

The consistency between the calculated r_f and the measured arrival time indicates that the spherical vessel method is valid in this case.

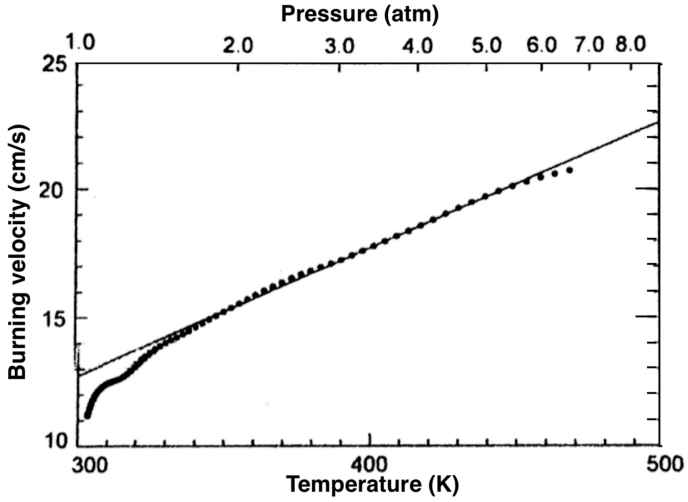

Figura 5: Burning velocity of HFC$-143/air$ mixture. $\phi = 0{,}94$, $T_0 = 300K$, and $P_0 = 1{,}0atm$. The dotted curve is the experimentally obtained burning velocity. The solid curve is the result of the fitting by equation (27) in the text

Figure (5) shows temperature and pressure dependence of the burning velocity of HFC−143/air mixture.

The obtained burning velocity S_u has been fitted to:

$$S_u = S_{u_0} \left(\frac{T}{T_s}\right)^{\alpha} \cdot \left(\frac{P}{P_s}\right)^{\beta} \tag{28}$$

$T_s = 298K$, $P_s = 1atm$, S_{u0} is the burning velocity at T_s and P_s and α and β indicate coefficients of temperature and pressure dependence.

To assess the accuracy of the spherical vessel method, the burning velocities of CH_4 and C_3H_8 were measured:

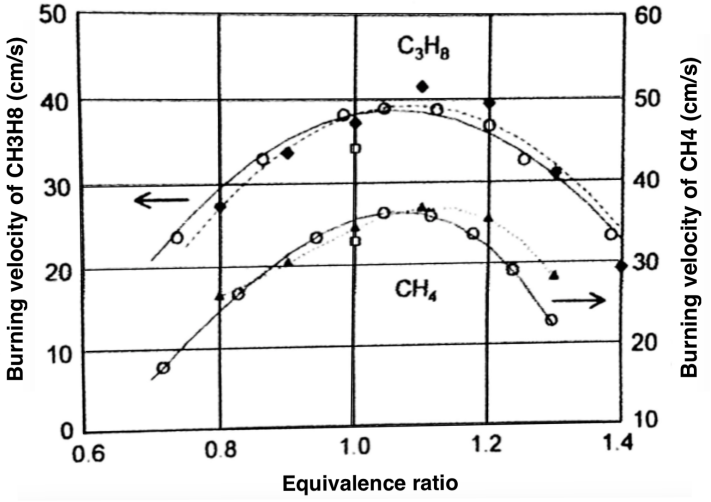

Figura 6: Burning velocity of CH_4 and C_3H_8 as functions of equivalence ratio. Open circle and solid curve are the present results: open square is by Hill and Hung [12]; filled diamond and broken curve are by Metghalchiand Lecl [10]; filled triangle and dotted curve are bylijima and Takeno [11]. All the data are obtained by the SV method.

Composition	S_{uo}				α		β	
	$S_{u,0,max}$	s_1	s_2	ϕ_{max}	α_1	α_2	b_1	b_2
HFC−32	6.7	−22.3	6.99	1.08	1.97	0.47	−0.055	-0.29
HFC−143	13.1	−38.3	17.8	1.05	1.87	−0.47	−0.17	0.072
HFC−143a	7.1	−39.5	52.5	1.02	2.32	−2.00	−0.18	−0,074
HFC−152a	23.6	−93,9	−49,2	1.09	1.89	−0,41	−0,22	0.022
CH_4	36.5	−217	−180	1.07	1.88	−0,095	−0,36	−0,13
C_3H_8	38.7	−138	5.8	1.06	1.89	−1,46	−0,27	0.54

Tabla 2: Dependence of burning velocity on temperature, pressure and ϕ

- α and β are coefficients for temperature and pressure dependence

Property	Method	HFC−32	HFC−143	HFC−143a	HFC−152a	CH_4	C_3H_8	Reference
Burning velocity (cm s^{-1})	SV	6.7[a]	13.1[a]	7,1[a]	23,6[a]	36.5[a]	38,7[a]	This work
	SV					36,9[c]		[10]
	SV					32,9[b]	34.2[b]	[11]
	SV					32,9[b]	34,2[b]	[12]
	Tube	6,7[d]		6,7[d]	23,0[d]	37,0[d]	39,0[d]	[8]
	Calculation	6,7[b]				40.7[b]		[2]
	Range[e](%)	16.0−22.0	7,5−13,0	9,0−12,0	6,0−10,0			This work
Flammability limits LFL−UFL(%)		13.3−29.3	6.2−22.6	7.4−17.0	4.35−17.5	4.9−15.8	2.1−9.5	[4]

Tabla 3: Burning velocities and flammability limits for compound−air mixtures

- [a] Maximum burning velocity at 298 K and 1 atm.
- [b] Burning velocity at $\phi = 1{,}298$ K and 1 atm.
- [c] Maximum burning velocity at 291 K and 1 atm.
- [d] Maximum burning velocity at 296 K and 1 atm.
- [e] The range of concentration where ignition was successfully done.

Direct measurement of flame propagation showed that a flame with a larger burning velocity is less affectedly buoyancy than those with smaller burning velocity. For HFC−143 concentration that is far from stoichiometric, the flame shapes were distorted by buoyancy. For the concentrations that were used for the measurements, the burning velocity was obtained with good accuracy and buoyancy effects were negligible. Thus the spherical vessel method is appropriate for determining the burning velocity even for weakly flammable HFCs.

5. CONCLUSION

- A temperature difference exists between the first and the last burned gas zones.
- The relationship between the pressure rise and the burned mass fraction is nonlinear.
- The burned gas temperature profile has an effect on the end pressure for flammable compounds.
- The multi zone burning velocity technique has been successfully used for the determination of the laminar burning velocities of the flammable compounds.
- The spherical vessel method is appropriate for determining the burning velocity even for weakly flammable HFCs.

6. BIBLIOGRAPHY

- Impact of dissociation and end pressure on determination of laminar burning velocities in constant volume combustion (C.C.M. Luijiten, E. Doosje, J.A. van Oijen, L.P.H. de Goey, 2009)
- www.elsevier.com/locate7ijts
- Mathematical Solutions for Explosions in Spherical Vessels (Derek Bradley and Alan mitcheson, 1976)
- Measurements of the laminar burning velocity for mixtures of methanol and air from a constant -volume vessel using a multizone model (Khizer Saeed, C.R. Stone, December 2003)
- Burning velocity measurement of fluorinated compounds by the spherical-vessel method (Kenji Takizawa, Akifumi Takashashi, Kabuki Tokuhashi, Shigeo Kondo, Akira Sekiya, June 2004)
- Equations for the Determination of Burning Velocity in a Spherical Constant Volume Vessel (C. J. Rallis and G. E. B. Tremeer, October 1962)
- Course of subject of Combustion of ITU (Istanbul)
- Course of subject of Combustion of UPV (Valencia)

A.

Measurements of The Laminar Burning Velocity For Mixtures of Methanol and Air From A contant-Volume Vessel Using A Multizone Model

Abstract

- A multiple burned gas zone model has been used to determine the temperature distribution within the burned gas and the relationship between the pressure rise and the mass fraction burned in a constant-volume vessel.
- A constant-volume spherical vessel has been used for measuring burning notes for liquid fuels at elevated initial temperatures and pressures
- Using the multizone model the laminar burning velocity has been found for mistures of methanol-air with initial temperatures of 293.15K and 425K, initial pressures of 0.5 bar, 1.0 bar, 2.0 bar and 3.5 bar, and equivalence ratios of 0.8 to 1.6.
- The laminar burning velocities were fitted to a seven-term equation to describe the effects of stoichiometry, pressure and temperature.

Introductiont

- Laminar premixed flames have a characteristic propagation rate, called the burning velocity. The burning velocity S_u is more precisely defined as the velocity at which unburned gases move through the combustion wave in the direction normal to the wave surface.
- Laminar burning velocities play essential roles in determining the ignition delay (affects the rande of equivalence ratios over which an engine can be operated), the thickness of the wall quench loyers and the minimum ignition energy
- A detailed knowledge of laminar pre-mixed flames will provide knowledge to heat release rates, flammability limits, propagation rates, quenching, and emission characteristics.
- There are two methods for determining a laminar burning velocity : stationary and nonstationary (the counterflow-burner method and the constant-volume method).
- The counterflow-burner tecnique is convenient for both liquid and gaseous fuels, qith good control of mixture composition. it is best suited for the pressures and temperatures close to ambient.
- The constant-volume bomb method uses a spherical vessel with certain ignition and relies on measurements taken after the early stages of flame propagation, during which there is a significant pressure rise.
- The laminar burning velocity is a function of not only the fuel/oxidant ratio but also the temperature and pressure of the system and the presence of any diluents in the misture.

Modeling

- The single-burned-zone model was extended to two burned zones and then to multiple zones.The mass in the spherical vessel can be divided into the multiple-zones in a number of ways. The two ways used here are equal mass zones (EQM) or equal radial zones (EQR). In the multizone model, flame propagation is seen as the consecutive consumption of unburned mixture within the zones. Before ignition, the mass in the spherical vessel divided into n zones. At the time, when combustion has just begun in the bomb, the flame front will consume zone 1 first. As a result, the temperature and hence pressure of zone 1 will increase, thereby compressing the rest of the unburned gas and increasing the pressure inside the vessel to a higher value. After

the consumption of the first zone, consumption of the second zones will take place at a higher pressure than the initial pressure, When the flame front is passing through the nth zone, the combustion of this zone takes place at a temperature of $T_{u,n-1}$ ($> T_i$) and a constant pressure $P_{u,n-1}$ ($> P_i$)

- After the flame has consumed the nth zone, it is assumed to be adiabatic
- Subsequent combustion further compresses the burned gas and the unburned gas.Temperature and density gradients are established in the burned gas region. In each zone will be at different temperatures, they each have a different composition. Equilibrium will be solved for $CO, CO_2, H_2O, H_2, H, OH, O, N_2, NO, O_2$ at each temperature.
- These equilibrium calculations are solved by minimizing the Gibbs energy

Model result

When the combustion ends in a spherical vessel, the radial temperature distributions for EQR model are shown.
To obtain accurate results and to reduce the run time of simulation, it was decided to use 10 zones and 200 steps for all the investigations.
When the flame front has passed the zone, recompression of the zones take place due to the expansion of the next zone. Due to the recompression, a decrease in the radius and hence the volume of the burned zones takes place. This results in an increase in the temperature of the burned gas zones, which establishes the radial burned gas temperature of the burned gas zones, which establishes the radial burned gas temperature gradient. As the first burned zone is hotter the outer zones, zone 1 finishes with a larger radius
The pressure variation with the mass fraction obtained in this study is nonlinear.
The maximum error in the pressure with the varying mass fraction is for stoichiometric combustion.

Experimental Apparatus

The apparatus consists of the combustion vessel and the heating system, ignition circuit gaseous and liquid fuel handling system and data acquisition system.
The spherical test vessel is provided with central ignition electrodes and it can withstand a pressure of 34 bar.
The combustion vessel is placed inside an over. It is fitted with a fan, a temperature controller and an air baffle plate.
Gaseous fuel air mixtures are prepared by sing their partial pressures. For liquid fuel-air mixture preparation, a calibrated amount of liquid fuel is injected.
The methanol was injected through a calibrated injector, and there were then two independent checks on the air-fuel ratio (AFR). The pressure and the temperature in the vessel were measured before and after addition of the fuel.
Previous work has shown that when the burning velocities are above 20 $\frac{cm}{s}$ the effect of buoyancy is less than 0.5 % on the observed burning velocity

Burning Velocity Calculation

The use of multizone model for the determination of the laminar burning velocity is explained below.
The burning velocity calculation are based on using spherical closed vessel filled with homogeneous combustible mixture. At time t=0, the mixture is ignited at the center; a spheric flame front is established and begins to propagate out —— to reach teh wall. The following assumptions are used:

- The unburned gas is initially at rest and the gas has uniform temperature and composition
- The thickness of the reaction zone is negligible, and the flame front is smooth and spherical

- The unburned fas fraction x is at local thermodynamic and chemical equilibrium
- The unburned gas fraction (1-x) is at local equilibrium but with fixed chemical composition.
- The pressure within the combustion vessel is a function of time and independent of the flame front.
- The compression for the whole gas is adiabatic and reversible.
- The gas behaves as a semiperfect gas.
- The effects of body forces and of radiactive energy transfer can be neggleted.
- The is no heat transfer between the burned and unburned gas.

Consider on elemental shall thickness dr_i at radius r_i. If the burned gas had not expanded, then an element dr_i would be the thickness of a shell at the temperature T_i and pressure P_i. Its volume:

$$4\pi r_i^2 dr_i$$

By expansion we have $r_i \to r_b$, $P_i \to P$, $T_i \to T_u$. Then we have its volume:

$$4\pi r_i^2 dr_i \left(\frac{T_u P_i}{T_i P}\right)$$

Since the thickness of the shell is equal to $S_u dt$, its volume:

$$4\pi r_b^2 S_u dt$$

Being S_u the burning velocity. However, the unburned gas is assumed to be undergoing isentropic compression;

$$T_u = T_i \left(\frac{P}{P_i}\right)^{\frac{\gamma_u - 1}{\gamma_u}} \tag{29}$$

We obtain for the burning velocity:

$$S_u = \left(\frac{dr_i}{dt}\right)\left(\frac{r_i}{r_b}\right)^2 \left(\frac{P_i}{P}\right)^{\frac{1}{\gamma_u}}$$

For a constant volume vessel a differential form of the energy conservation equation is given as:

$$m\frac{de}{dt} - \frac{dQ}{dt} = 0 \tag{30}$$

The conservations of volume and internal energy are given by:

$$\upsilon = \frac{V}{M} = x\upsilon_b(P, T_b) + (1-x)\upsilon_u(P, S_{u,0})$$

$$e = \frac{E}{M} = xe_b(P, T_b) + (1-x)e_u(P, S_{u,0})$$

These differential equations are extended to the multiple burned gas zones for the multizone analysis;

$$\frac{dP}{dt} = \frac{B}{C+D}$$

$$\frac{dT_U}{dt} = \frac{\upsilon_u}{C_{pu}} \frac{\partial ln\upsilon_u}{\partial lnT}\left(\frac{B}{C+D}\right)$$

$$\frac{dT_b}{dt} = -(1-x)\frac{\upsilon_u}{T_u}\frac{\partial ln\upsilon_u}{\partial lnT_u}\frac{T_b}{x\upsilon_b}\frac{\partial lnT_b}{\partial ln\upsilon_b}.\frac{\upsilon_u}{C_{pu}}\frac{\partial ln\upsilon_u}{\partial lnT_u}\frac{\partial ln\upsilon_u}{\partial lnT_u}\left(\frac{B}{C+D}\right) - \tag{31}$$

$$-\frac{T_b}{x\upsilon_b}\frac{\partial ln T_b}{\partial ln \upsilon_b}\left(x\frac{\upsilon_b}{P}\frac{\partial ln \upsilon_b}{\partial ln P}+(1-x)\frac{\upsilon_u}{P}\frac{\partial ln \upsilon_b}{\partial ln P}\right)\left(\frac{B}{C+D}\right)-$$
$$-\frac{T_b}{x\upsilon_b}\frac{\partial ln T_b}{\partial ln \upsilon_b}(\upsilon_b-\upsilon_u)\frac{dx}{dt}$$

Where:

$$B=\left((\upsilon_b-\upsilon_u)+\frac{\upsilon_b}{C_{p,b}T_b}(h_b-h_u)\right)\frac{dx}{dt}$$
$$C=x\left(\frac{\upsilon_b^2}{C_{p,b}T_b}\left(\frac{\partial ln \upsilon_b}{\partial ln T_b}\right)^2+\frac{\upsilon_b}{P}\frac{\partial ln \upsilon_b}{\partial ln P}\right)$$
$$D=(1-x)\frac{\upsilon_u^2}{C_{p,u}T_u}\left(\frac{\partial ln \upsilon_u}{\partial ln T_u}\right)^2+\frac{\upsilon_u}{P}\frac{\partial ln \upsilon_u}{\partial ln P}$$

For the multizone analysis, the above equations are extended to N zones. Burned gas volume and radius are calculated from the following equations:

$$\upsilon_b=V-m_i(n-1)\left(\frac{R_uT_u}{P}\right)$$

and

$$r_b=R\left(V-m_i(n-1)\left(\frac{R_uT_u}{P}\right)\right)$$

The burning velocity by using multizone modal is:

$$S_u=\left(\frac{dp}{dt}\right)\left(\frac{dr_i}{dp}\right)\left(\frac{r_i}{r_b}\right)^2\left(\frac{P_I}{P}\right)^{\frac{1}{\gamma_u}}$$

Being

$$\left(\frac{dp}{dt}\right)\rightarrow Experimental\ data$$
$$\left(\frac{dr_i}{dp}\right)\rightarrow BOMB\ program$$

Conclusion

- A 10-zone model with 200 steps gives adequate accurate results
- A temperature difference exits between the first and the last burned gas-zones
- The relationship between the pressure rise and the mass fraction burned is nonlinear
- The burned gas temperature profile has an effect on the end pressure for methane
- The multizone burning velocity technique has been succesfully used for the determination of the laminar burning velocities of methanol-air mistures at varying equivalence ratios, temperatures and pressures
- Cellular flames have been found to exist in the test runs

B. Mathematical Solutions for Explosions in Spherical Vessels

Equations, assumptions and previous solutions for central ignition of premixed gases in closed spherical vessels are reviewed.Three new categories of solution are presented:

1. -Approximate Computer Solution (Case 1)
2. -The Dimensionless Universal Expression (Case 2) *-Does not require computer and has a good accuracy*
3. -The Complet Computer Solution (Case 3)-*The most accurated*

Introduction

A simple model is presented which is amenable to computer simulation and this is used to derive pressure-time curves in dimensionless form which are universally applicable for all explosions. From these curves, it is seen that corresponding dimensional curves are very sensitives to the value of burning velocity. Both temperature and pressure of the unburnt gas are changing during the explosion and data are required for the associated changes in burning velocity. With the availability of such data it has been worthwhile develop a much none accurate computer model based upon finite difference techniques and less restrictive assumptions than formaly used.

The Basic Equations

- It is assumed that central ignition occurs in a rigid sphere and that a laminar flame that is smooth and spherical propagates outwards without any significant movement due to natural convection.
- The unburnt gas is isotropic
- Mass conservation gives:

$$m_o = m_u + m_b$$
$$\frac{dm_u}{dt} = -\frac{dm_b}{dt}$$

- The burnt gas fraction is:

$$n = \frac{m_b}{m_o}$$

- From the definition of burning velocity S_u:

$$\frac{dm_u}{dt} = -4\pi r_b^2 \rho_u s_u$$

Being r_b the radio of the inner boundary and $\rho_u$the density of unburnt gas.

- Volume conservation:

$$V_o = V_b + V_u$$

- The equation of state:

$$PV = mR_gT$$
$$\frac{d}{dt}[(R^3 - r_b^3)\rho_u] = 3r_b^2\rho_u S_u$$

Where ρ_b is the mean density of the gas within the radius r_b

Simplified Analyses

· The unburnt gas is compressed isentropically:

$$(P\rho_u)^{\gamma_u} = constant$$

Fiock and Marvin result:

$$S_u = \frac{dr_b}{dt} - \frac{(R^3 - r_b^3)}{3r_b^2\gamma_u P}.\frac{dP}{dt}$$

· The fractional pressure rise is proportional to the fractional mass burnt

$$\frac{P - P_o}{P_e - P_o} = \frac{M_b}{M_o} = n$$

Being e: the condition when the explosion is completed.

Case 1:The Approximate Computer Solution:

Pressure-time curves were obtained by increasing "nïn elemental steps from 0 to 1. The computation procedure will be appreciated from the following equations:

$$P = n(P_e - P_o) + P_o$$

$$T_u = T_o \left(\frac{P}{P_o}\right)^{\frac{\gamma_u - 1}{u}}$$

$$M_u = M_o(1 - n)$$

$$\frac{4}{3}\pi r_b^3 = \frac{4}{3}\pi R^3 - \frac{m_U R_{gu} T_u}{P}$$

$$\rho_u = \frac{3m_u}{4\pi(R^3 - r_b^3)}$$

$$dt = -\frac{dm_u}{4_b^2 \rho_u S_u}$$

Case 2:The Dimensionless Universal Expression:

This attempts to obtain the maximum generality in the pressure time relationship.

$$\frac{dP}{dt} = \frac{3S_u\rho_u}{R\rho_o}(P_e - P_o)\left[1 - \left(\frac{P_o}{P}\right)^{\frac{1}{\gamma_u}} \frac{P_e - P}{P_e - P_o}\right]^{\frac{2}{3}}$$

Equation derived by Benson and Burgoyne. Dimensionless pressures and times are defined in terms of conditions at the end of the explosion:

$$\bar{P} = \frac{P}{P_e}; \bar{P}_o = \frac{P_o}{P_e}; \bar{t} = \frac{t}{t_e}$$

A mean flame speed, S_u, is defined by:

$$S_m = \frac{R}{t_e}$$

In nondimensional form the first equation becomes:

$$\frac{d\bar{P}}{d\bar{t}} = \frac{3S_u}{S_m}(1 - \bar{P}_o)\left(\frac{\bar{P}}{\bar{P}_o}\right)^{\frac{1}{\gamma_u}}\left[1 - \frac{1 - \bar{P}}{1 - \bar{P}_o}\left(\frac{\bar{P}_o}{P}\right)^{\frac{1}{\gamma_u}}\right]^{\frac{2}{3}}$$

$$\frac{dP}{dt} = \frac{dn}{dt}(P_a - P_o)$$

$$\frac{dn}{dt} = \frac{3S_u}{r_b}\left[n - 1 + \left(\frac{P}{P_o}\right)^{\frac{1}{\gamma_u}}\right]$$

Substituting:

$$S_s = S_u\left[1 + \frac{1}{\gamma_u \bar{P}}\left(\frac{R^3}{r_b^3} - 1\right)\left(\bar{P} - 1 + (1 - \bar{P}_o)\left(\frac{\bar{P}}{\bar{P}_o}\right)^{\frac{1}{\gamma_u}}\right]\right.$$

Where $S_s = \frac{dr_b}{dt}$

$$\left(\frac{r_b}{R}\right)^3 = 1 - \left(\frac{1 - \bar{P}}{1 - \bar{P}_o}\right)\left(\frac{\bar{P}_o}{\bar{P}}\right)^{\frac{1}{\gamma_u}}$$

$$\frac{dr_o}{dt} = S_s = S_u f(\bar{P})$$

$$\int_0^{te} dt = \int_0^R \frac{dr_b}{S_u f(\bar{P})}$$

If S_u is assumed to be constant through the explosion:

$$\frac{t_e S_u}{R} = \frac{S_u}{S_m} = \int_0^1 \frac{d\left(\frac{r_b}{R}\right)}{f(\bar{P})}$$

The problem presented by the fact that S_u is not constant but varies during the compression process accompanying combustion might be circumvented by the selection of an appropiat mean value of S_u for the whole explosion.

Other Approximate Solutions

The simplicity of the Case 1 and Case 2 solutions rests upon the assumed equality of the fractional pressure rise and the fractional mass brunt. An alternative route involves a knowledge of the changes in the mean density of the burnt gas,ρ_b. This is not easy because of the non uniformity of the burnt gas temperature the gas burnt first attains a temperature higher than that burnt later. An assumption of the global isentropic compression low$(P\rho_b)^{-\gamma_b}$ = constant. The temperature of the burnt gas was assumed to be that at the center of the vessel. The equations of mass and volume conservation, the perfect gas equation of state, and an assumed equality of the burnt and unburnt gas constants give rise to:

$$\frac{dP}{dt} = \frac{3\gamma_u S_u r_b^2 P\left(\frac{\rho_u}{\rho_b} - 1\right)}{R^3\left[1 + \left(\frac{r_b}{R}\right)^3\left(\frac{\gamma_u}{\gamma_b} - 1\right)\right]}$$

and

$$S_s = \frac{\rho_u}{\rho_b} S_u - \frac{r_b}{3\gamma_b P}\frac{dP}{dt}$$

Solutions of these equations were obtained numerically and presented in graphical form with P, T_u, r_b, S_s and n plotted against t.

- Assumption 1: $\gamma_b = \gamma_u = \gamma$
- Assumption 2: isothermal compression with $T_u = T_o$, $\gamma_b = \gamma_u = 1$

The analysis later were modified to take turbulence into account by the introduction of a constant,α, such that the turbulent burning velocity was α times the laminar burning velocity.

Influence of Temperature and Pressure Changes on Burning Velocity

All solutions indicate their sensitivity to the numerical value of burning velocity. ITt is therefore necessary to know with some accuracy not only the initial value of burning velocity, but also the changes in it that occur during an explosion, as a result of the compression of the unburnt gas. Perlee considered the burning velocity of stoichimetric methane-air and combined the pressure dependence with their own temperature dependance to give:

$$S_u = \left(\frac{T_u}{t_o}\right)^2 \left(32{,}9 - 6{,}78 ln\left(\frac{p}{p_2}\right)\right) cmsec^1$$

Better agreement with experiment;

$$S_U = \left(S_{uo} - \beta_1 ln\left(\frac{p}{p_0}\right)\right)\left(\frac{T_u}{T_o}\right)^{\beta_2} cmsec^{-}1$$

Where S_{uo} the burning velocity at the initial conditions, β_1 β_2 where constants chosen to give the best agreement with experiment. Noggy used:

$$S_u = S_{uo}\left(\frac{T_u}{T_o}\right)^2\left(\frac{P_o}{P}\right)^\beta$$

For a variety of mixtures, in which β was zero for the isothermal and 0.25 for the adiabatic model. S_{uo} was chosen to give good agreement with experiment. Babkin and Kazachanko have carried out the most comprehensive experimental investigation of the influence of temperature and pressure during the period of constant pressure methane-air burning in a bomb explosion.

$$S_u = \frac{\rho_b}{\rho_u}S_s$$

It was assumed that the maximum temperature of the burnt gas was the ideal temperature.

Accurate Analysis

In recent years computer based analysis have been developed with emphasis on chemical kinetic effects relevant to exhaust emissions. The present mark is less concerned with kinetics and more concerned with deriving accurate pressure-time solutions.

Case 3: The Complete Computer Solution

Flame propagation is seen as the consumption of unburnt gas in small mass decrements dm_u. This mass does not become burnt gas instantaneously, but first passes through a reaction zone of finite thickness. The basic statement is that of conservation of total volume, which is made up the three volumes of unburnt, reacting and burnt gas. Consider the consumption of the nth elemental unburnt mass decrement, dm_n. This moves into the reaction zone with a temperature $T_{u,n-1}$, burns at the constant pressure P_{n-1}, and a proportion of the gas attains the ideal equilibrium temperature $T_{f,n}$ for these conditions.This reaction must increase the pressure and in the model this is assumed to follow the constant pressure combustion and to be isentropic.The pressure throughout the vessel becomes P_n and the uniform unburnt gas temperature becomes $T_{u,n}$. At this stage the radius of the inner boundary of the unburnt gas is $r_{b,n}$;

$$m_{u,n} = M_o - \sum i = 1^{i=n} dm_{u,i}$$

and

$$V_{u,n} = \frac{m_{u,n}R_{gu}T_{u,n}}{P_n}$$

Knowing that $R_{g,u}$ = constant. The flame thickness, S_n between the temperatures $T_{u,n-1}$ and $\mathrm{T}_{f,n} can be calculated and the volume, \mathrm{V}_{f,n}$, associated with this flame thickness is found from;

$$V_{f,n} = \frac{4\pi}{3}[r_{b,n}^3 - (r_{b,n} - \rho_n)^3]$$

where

$$r_{b,n} = \left(R^3 - \frac{3}{4\pi}V_{u,n}\right)^{\frac{1}{3}}$$

The gas must be within the flame thickness before it is burnt, $dm_{b,n}$;

$$dm?b, n = dm_{u,n} - (m_{f,n} - m_{f,n-1})$$

where $m_{f,n}$ and $m_{f,n-1}$ are masses within the flame thickness. The isentropic compression immediately following constant pressure combustion raises the freshly gas from a temperature $T_{f,n}$ to $T_{b,n}$. Thus the volume of burnt gas produced during the decremental charge is:

$$V_{b,n} = \frac{[dm_{u,n} - (m_{f,n} - m_{f,n-1})]R_{gb,n}T_{b,n}}{P_n}$$

The total volume of burnt gas up to the nth decrement is;

$$V_{\frac{1}{P_n}} \sum i=1^{i=n} [dm_{u,i} - (m_{f,i} - m_{f,i-1})] R_{gbi,n} T_{bi,n}$$

$$M_{f,o} = 0$$

Volume conservation gives:

$$V_o = V_{u,n} + V_{f,n} + V_{b,n}$$

$$dt = \frac{-dm}{4\pi r_b^2 \rho_u S_u}$$

Equilibrium temperatures were computed from the JANAF. The presence of elevn chemical species was assumed in the methane-air explosions investigated, namely, CO, CO_2, H_2, H_2O OH N_2 N NO O O_2 and from their concentrations could be obtained the burnt gas constant, R_{gb}. Equilibrium constants were evaluated from values of Gibbs function.Enthalpies and entropies for each species were conveniently obtained from sets of polynomials derived from the JANAF data.

$$h_j^\circ = A_j T^4 + B_J T^3 + C_J T^2 + d_j T + E_J$$

and

$$s_j = A_j T^3 + B_j T^2 + C_j T + D_J ln T F_j$$

h_j° and s_j° : specific values

Conclusions

- The basic equations and associated assumptions for flame propagation in spherical vessel have been reviewed.
- The fractional pressure rise is proportional to the fractional mass burnt
- The simplest solution to apply is that of Dimensionless Universal Expression
- The Complete Computer Solution is good agreement with accurate experimental values of the pressure time relationships.

C. Equations for the Determination of Burning Velocity In A Spherical Constant Volume Vessel

Introduction

Since burning velocities can not be measured directly, equations for calculating this property must be derived. It would appear that the various equations proposed have never been satisfactorily compared, either theoretically or by applying them to the results of a particular set of experiments.

Derivation of Burning Velocity Equations

From the continuity equation

$$\frac{dm_u}{dt} = A\rho_u S_u$$

S_u the normal velocity with which the unburnt gas crosses normal perpendicular to the flame front Combustion in a constant volume spherical vessel the mass of unburnt gas at any instant;

$$m_u = \frac{4}{3}\pi \left[(R^3 - r_b^3)\frac{d\rho_u}{dt} - 3r_b\rho_u \bar{d} r_b dt \right]$$

R: radius of the spherical vessel r_b: radius of the burnt gas Using these equations we find:

$$\frac{dm_u}{dt} = \frac{4}{3}\pi \left[(R^3 - r_b^3)\frac{d\rho_u}{dt} - 3r_b^2\rho_u \frac{dr_b}{dt} \right]$$

$$S_u = \frac{dr_b}{dt} = \frac{(R^3 - R_o^3)}{3r_b\rho_u}\frac{d\rho_u}{dt} = S_s - S_g$$

Considering adiabatic compression;

$$P = Cp_u^{\gamma_u}$$

Then we obtain the unburnt gas equation for the burning velocity of Fiock and Marvin

$$\frac{d\rho_u}{dt} = \frac{d\rho_u}{dP}\frac{dP}{dt} = \frac{\rho_u}{\gamma_u P}\frac{dP}{dt}$$

Substituting

$$S_u = \frac{dr_b}{dt} - \frac{(R^3 - R_B^3)}{3R_b^2\gamma_u P}\frac{dP}{dt}$$

Alternative forms of these equations can be obtained by considering the burnt gas behind the flame front. Combustion in a constant volume vessel:

$$m_u = m_o - m_b$$

Thus:

$$\frac{dm_u}{dt} = -\frac{dm_b}{dt}$$

Then we are able to obtain:

$$S_b = \frac{1}{A\rho_u}\frac{dm_b}{d}$$

S_b property of the burnt gas. For a spherical flame font;

$$m_b = \frac{4}{3}\pi r_b^3 \bar{\rho_b}$$

The mean density, $\bar{\rho_b}$, allows us to obtain non-uniform properties of the gas behind the flame front due to recompression:

$$\bar{rho_b} = \frac{3}{r_b^3}\int_0^{r_b} \rho_b r^2 dr$$

when $r_b = R$, $\rho_b = \rho_o$. In this equation total volume and mass are constant. From

$$\frac{dm_b}{dt} = \frac{4}{3}\pi \left[r_b^3\frac{d\bar{\rho_b}}{dt} + 3r_b^2\bar{\rho_b}\frac{d\bar{\rho_b}}{dt} \right]$$

Then we obtain:

$$S_b = \frac{\rho_b}{\rho_u}\frac{dr_b}{dt} + \frac{r_b}{3_{\rho u}}\frac{d\bar{\rho_b}}{dt}$$

Considering adiabatic compression:

$$P = C'\bar{\rho_b}^{\gamma b}$$

Then:

$$\frac{d\bar{\rho_b}}{dt} = \frac{\bar{\rho_b}}{\gamma_b P}\frac{dP}{dt}$$

Finally we obtain the burnt gas equation for the burning velocity

$$S_b = \frac{\bar{\rho_b}}{\rho_u}\left[\frac{dr_b}{dt} + \frac{r_b}{3\gamma_b P}\frac{dP}{dt}\right]$$

It is necessary to find the mean density of the burnt gas(ρ_b). I t is possible to avoid some difficulties.

$$\rho_b = \alpha\rho_o$$

Then:

$$\frac{d\bar{\rho_b}}{dt} = \rho_o\frac{d\alpha}{dt} = \rho_o\frac{d\alpha}{dt}\frac{dP}{dt}$$

The boundary conditions:

$$[\bar{\rho_b}]_{r_o=R} = r\bar{h}o_e = \rho_o$$

$$[\alpha]_{r_b=R} = \alpha_e = 1$$

From these formulas and the perfect gas equation we obtain:

$$\alpha = \frac{\bar{\rho_b}}{\rho_o} = \frac{\bar{m_b}}{m_o}\frac{T_o}{\bar{T_b}\frac{P}{P}}$$

$$\rho_o = \frac{\bar{m_e}P_e}{R\bar{T_e}}$$

$$\alpha = \frac{\bar{m_b}}{m_e}\frac{\bar{T_e}}{T_b}\frac{P}{P_e}$$

From this equations, α is practically proportional to P, $\frac{d\alpha}{dP} = \frac{1}{P}$. Even if the absolute values of $\bar{m_b}$, $\bar{T_b}$ and P are in error. Second equation must yield the contact value of α (unity). The magnitude of any such errors can be estimated by evaluating α at the end of the process from the first equation. The use of the second equation is preferred since errors in the determination of $\bar{m_b}$, $\bar{T_b}$ and P tend to be cancelled out. In fact, it becomes unnecessary to calculate mean values of the burnt gas temperature and molecular weight. For constant pressure combustion $\frac{dP}{dt}$ is zero. Thus:

$$S_b = \frac{\rho_b}{\rho_o}\frac{dr_b}{dt} = \alpha_o S_g = \frac{S_g}{E_o}$$

Being E_o the initial expansion ratio. Lewis and Von Elbe:

$$n = \frac{m_o}{m_b}$$

$$\frac{dn}{dt} = \frac{1}{m_o}\frac{dm_b}{dt} = -\frac{1}{m_o}\frac{dm_u}{dt}$$

Substituting to:

$$\frac{dm_u}{dt} = -A\rho_u S_u$$

$$S_b = \frac{m_o}{A\rho_u}\frac{dn}{dt} = \frac{1}{3}\frac{R^3}{r_b^2}\frac{\rho_o}{\rho_u}\frac{dn}{dt}$$

During the early stages of combustion:

$$n = \frac{P - P_o}{P'_e - P_o}$$

Hence:

$$\frac{dn}{dt} = \frac{1}{P'e - P_o}\frac{dP}{dt}$$

Eliminating r_b:

$$\frac{m_u}{m_o} = 1 - n = \frac{(R^3 - r_b^3)}{R^3\rho_o}\rho_u$$

$$r_b = R\left[1-(1-n)\frac{\rho_o}{\rho_u}\right]^{\frac{1}{3}}$$

Then we obtain n's exact value:

$$n = \frac{r_b^3 \bar{P_b}}{R^3 \rho_o} = \alpha \frac{r_b^3}{R^3}$$

$$\alpha = \frac{\bar{m_b}}{m_e}\frac{\bar{T_e}}{\bar{T_b}}\frac{P}{P_e};$$

$$n = \frac{r_b^3}{R^3}\frac{P}{P_e} = \frac{P\left(\frac{\rho_o}{\rho_u}\right)P}{P_e - \left(\frac{\rho_o}{\rho_u}\right)P}$$

Substituting.

$$r_b = R\left[\frac{\frac{\rho_u}{\rho_o}-1}{\frac{\rho_u}{\rho_o}-\alpha}\right]\frac{1}{3}$$

Introduction

Several equations have been used to calculate the burning velocities of a stoichiometric acetylene-air mixture, fired in a spherical vessel.Due to the low rate of pressure rise during the early stages of combustion two pressure traces were recorded.

- The Fiock and Marvin equation is the only one which doesn't require a knowledge of the properties of the burn gas. It has the disadvantage of magnifying small errors in the observations
- The Lewis and Von Elbe equation claimed claimed to be accurate only over the initial stages

The calculated values of r_b are nearly always less than the observed radius. This difference suggests the existence of a reaction zone of significant thickness, particularly during the early stages when the spatial velocity is high. Values based on the low range pressure record one constantly nearer the observed radius than values from the high range record.

Justification for Use of Proposed Burning Velocity Equation

The discrepancy between the calculated and observed flame radius suggests a lock of equilibrium in the burnt gas, probably confined to a reaction zone adjacent to the flame front. With the equations derive, on estimate of the degree of lack of equilibrium is possible. Consider the parameter α which is defined as the ratio of the mean density of the burnt gas to the density of the unburnt mixture before ignition:

$$\alpha = \frac{\bar{\rho_b}}{\rho_o} = \frac{\bar{b}}{m_u}\frac{T_o}{\bar{T_b}}PP_o$$

Using the observed maximum pressure, P_e, m_e and T_e, corresponding to final conditions in the burnt gas at the flame front, may be calculated assuming equilibrium conditions. An approximate value of α may be calculated:

$$\alpha_e = \frac{m_e}{m_o}\frac{T_o}{T_e}\frac{P_e}{P_o}$$

In all cases α_e is less than unity. Since the total mass of gas in the vessel remains constant, the mean density of the products when the flame has reached the bomb wall must equal the initial density of the unburnt mixture, $\rho_b = \rho_o$; hence α_e should have a value of value of unity at the end of the process. The discrepancy must therefore be attributed to P_e and $\frac{m_e}{T_e}$ being too low.

· Consider P_e: an error could arise from

(a) Incorrect calibration of the pressure measuring system
(b) Inadequate transient response of the pressure transducer
Use of the correct value would lower α_e still further.

Consider $\frac{m_e}{T_e}$ instead of $\frac{m\bar{e}_e}{T_e}$

(a) The temperature at the flame front is less than that at the centre of the vessel. Thus T_e is less than $\bar{T}_e$.
(b) The difference between m_e and $m\bar{e}_b$ is small compared with the difference between T_e than $\bar{T}_e$.
Hence the use of mean temperatures to calculate α_e would yield even lower values than those obtained by using flame front temperatures.

The only term left to account for the discrepancy between the deserved and expected values of α_e is the temperature of the burnt gas. It appears that the calculated equilibrium value of flame front temperature is too high. There are two factors which may account for the calculated value of T_b being too high:

(a) Combustion may not occur adiabatically due to heat loss. But, the quantity of heat loss by radiation up to the time the flame reaches the bomb wall is negligible. Conductive heat loss, due to buoyancy, is likely to be longer for slow burning mixtures, and should lead to lower values of α_e for the rich and lean mixtures tested. Therefore, heat loss can not explain discrepancy.

(b) The assumption that equilibrium is attained immediately behind the flame front may not be justified: insufficient time may be available for the reactions to go to completion. If this is so then at any air/fuel ratio the thickness of such a reaction zone should increase with flame speed.

The lowest value of α_e coincides with the greatest observed spatial velocity. Thus if a non-equilibrium condition exists at the end of the precess ($\alpha_e < 1$), on even greater departure from equilibrium probably exits over the initial stages since the spatial velocity is then higher. Using the alternative approximate expression for α:

$$\alpha = \frac{m_b}{m_e}\frac{T_e}{T_b}\frac{P}{P_e}$$

which must yield the correct value of α_e (unity). All previous burning velocity equations have been based on the assumption that chemical equilibrium exists in the burnt gas. In the burning velocity equation any such lack of equilibrium is partly allowed for by using the dimensionless density ratio α calculated from the above equation.

D. Burning Velocity Measurement of Fluorinated Compounds By The Spherical-Vessel Method

Abstract

Burning velocity has been measured using the spherical vessel (SV) method for four hydrofluorocarbons (HDCs). Experiments were conducted for initial pressures in the range 78-108 kPa and initial temperatures in the range 280-330 K, over wide ranges of HCF-air. The burning velocities were determined from the rate of pressure increase by applying a spherical-flame propagation model. It is found that the SV method is adequate for determining the burning velocity for weakly flammable HCFs as well as for moderately flammable compounds. The magnitude of the burning velocity is strongly dependent on the ratio of H atoms to F atoms in the HFC molecules.

Introduction

There are a number of flammable compounds among the alternatives. In order to ensure safe use of these substances, assessment of their flammability is important. For the burning velocity measurement, numerous techniques have been developed. The method of measurement is in general chosen according to the properties of compounds and experimental requirements. Fluorinated compounds usually have low burning velocities. in addition, some refrigerants and cleaning solvents have a higher boiling point than room temperature. The SV method is more appropriated than the Bunsen method. It has been widely used for flammable gases such as hydrogen and hydrocarbons because it provides experimental accuracy as well as operational simplicity: the burning velocity of a compound together with its temperature and pressure dependence is obtained simultaneously by measuring the pressure time history in the vessel. There is a concern about using the SV method for weakly flammable compounds. It is necessary to assume that the flame front is spherical and smooth. But for a compound with low burning velocity such as NH_3, the buoyancy force may distort the flame front which can not be regarded as spherical.

Result and Discussion

Method of Analysis The Data Obtained With The SV Method

The burning velocity S_u:

$$S_u = \frac{R}{3}\left[1-(1-x)\left(\frac{P_o}{P}\right)^{\frac{1}{\gamma_u}}\right]^{-\frac{2}{3}}\left(\frac{P_o}{P}\right)^{\frac{1}{\gamma_u}}\frac{dx}{dt}$$

In order to use this equation, we have to obtain the relationship of P with x, γ_u, r_f, and burned and unburned gas temperatures T_u and T_b. The obtained S_u has been fitted to the following:

$$S_u = S_{uo}\left(\frac{T}{T_s}\right)^{\alpha}\left(\frac{P}{P_s}\right)^{\beta}$$

Taking into account that: $T_s = 298K$
$P_s = 1atm$
S_{uo}= burning velocity at T_s, P_s
α and β: coefficients of temperature and pressure dependence.
S_{uo}, α and β are dependent on ϕ;$S_{uo} = S_{uo,max} + S_1(\phi-\phi_{max})^2 + S_2(\phi-\phi^3_{max})\alpha = a_1 + a_2(\phi-1)\beta = b_1 + b_2(\phi-1)$

Conclusion

The present study focus on determination of burning velocities of HFCs. The burning velocities of HFC-32, HFC-143, HFC-143a and HFC-152a together with CH_4 and C_3H_8 were investigated.
Burning velocities were determined by analyzing the pressure time profiles in the spherical vessel and were checked by direct observation of flame propagation using the schlieren photograph in a wide range of concentrations.
Direct measurement of flame propagation showed that a flame with a longer burning velocity is less affected by buoyancy than those with smaller burning velocity.
For HFC-32 and HFC-143a concentrations that are far from stoichiometric, the flame shapes were distorted by buoyancy. For the concentrations that were used for the measurement, the burning velocity was obtained with good accuracy and buoyancy affects were negligible. Thus the SV method is appropriate for determining the burning velocity even for weakly flammable HFCs.

E. Impact of Dissociation and End Pressure on Determination of Laminar Burning Velocities In Constant Volume Combustion

Abstract

Determining laminar burning velocities S_u from the pressure trace in constant volume combustion requires knowledge of the burnt fraction as a function of pressure x(p). x(p) is either determined via numerical modeling or via the oversimplified assumption that x(p) is equal to the fractional pressure rise.
In this paper we systematically compare our analytical models with a numerical two-zone model and with a 1D unsteady simulation (1DUS) of a spherical stoichiometric methane-air flame in a constant volume.
Results indicate that our analytical models reasonable describe the burnt fraction as a function of fractional pressure rise. However the x(p) relation also involves the end pressurep_e. Its value significantly affects S_L and influenced by dissociation.
Evaluating p_e from an equilibrium code, in combination with the analytical x(p) model, provides S_L is achieved using numerical x(p) models that account for dissociation also for intermediate stages.

Introduction

Laminar burning velocities of a combustible mixture can be obtained by recording the pressure p as a function of time in a constant volume vessel.
The burning velocity values (S_u) are obtained for a range of pressures and temperatures in one single experiment. Only the pressure is needed to determine S_L
In the analysis of pressure data, a set of assumptions commonly made, including uniformity of pressure, negligible external heat loss or gain (ignition), no buoyancy effects, isentropic compression of the burnt gas, and an infinitely thin and spherical flame front with no heat transfer between the burnt and unburnt zones. Using these assumptions, S_u can be related to the pressure trace through a differential equation:

$$\frac{dp}{dt} = \frac{3}{R}\left(\frac{dx}{dp}\right)^{-1}\left[1-\left(\frac{P_i}{P}\right)^{\frac{1}{\gamma_u}}(1-x)\right]^{\frac{2}{3}}\left(\frac{P}{P_i}\right)^{\frac{1}{\gamma_u}} S_L$$

Being:
P_i: initial pressure
γ_u: isentropic exponent of the unburnt gas
R: vessel radius
x: burnt mass fraction
Relation between x and p must be known
Lewis and von Elbe argue that relation between x and p is very close to linear, and they introduce the relation:

$$x = \frac{p - p_i}{p_e - p_i}$$

In the derivation of analytical relations, we have to assume perfect gas behaviour of both unburnt and burnt gas. This implies (besides having constant specific heats) that the average molar mass before and after combustion remains constant. Hence, shifting chemical equilibrium due to the changing temperature of successively burnt shells is not taken into account.
A second point of concern is that analytical x(p) relations require the end pressure p_e as input. The P_e value required in the evaluation is necessarily the theoretical end pressure (which would be achieved when a perfectly spherical and adiabatic flame would develop in a spherical vessel in the absence of gravity).
Finally, we will show how the combined effect of x(p) model and end pressure affects the differences between S_u values.
Stoichiometric methane-air will be used.

Theory

Analytical models for both two and multiple zones are briefly described. The most restrictive simplification is the assumption of perfect gas behaviour.
The two-zone analytical model neglects the burnt temperature gradient. This simplification was slow not to affect the x(p) results within a perfect gas. However, when both a burnt temperature gradient and dissociation are allowed, this may no longer hold true: enchanced dissociation near the core of the vessel may affect the mass-averaged burnt temperature leading to different results for x(p) as wall.

Analytical Two-Zone Model

In a two zone model, both the burnt and unburnt zones have uniform temperatures and compositions:
Conservation of specific volume:

$$v_t = xv_b + (1+x)v_u$$

Conservation of specific internal energy:

$$e_t = xe_b + (1+x)e_u$$

The specific internal energy is evaluated: Unburnt mixture

$$e_u = C_{vu}(T_u - T_o) + D_e$$

Burnt mixture

$$e_b = C_{vb}(T_b - T_o) + D_e$$

Being T_o: the reference temperature. The above equations can be manipulated to:

$$x = \frac{p - p_i f(p)}{p_e - p_i f(p)}$$

Where:

$$f(p)0\frac{\gamma_b - 1}{\gamma_u - 1} + \left(\frac{\gamma_u - \gamma_b}{\gamma_u - 1}\right)\left(\frac{P}{P_i}\right)^{\frac{\gamma_u - 1}{\gamma_u}}$$

The resulting equation obeys energy conservation.
This equation does not hold true for linear relation between x and p. This observation can be attributed to an underestimation of entropy production by the linear model.
The end pressure p_e in the two-zone model is obtained from conservtion of internal energy for $x = 1$:

$$cv_u(T_i - T_o) + D_e = cv_b(T_e - T_o)$$

The unburnt specific heat is evaluated at $T_i = 298{,}15K$
Specific heat of the burnt gas evaluated at $\frac{(T_I + T_e)}{2}$
In this way we have;

$$Cp_u = 1078Jkg^{-}1K^{-}1$$

$$Cp_u = 777Jkg^{-}1K^{-}1$$

$$Cp_b = 1425Jkg^{-}1K^{-}1$$

$$Cv_b = 1124Jkg^{-}1K^{-}1$$

and

$$\gamma_u = 1{,}39$$

$$\gamma_b = 1{,}27$$

$$\Delta e = 276 MJkg^{-}1$$
$$T_e = 2744K$$
$$P_e = 9{,}2bar$$

Analytical Multi-Zone Model

The approach sketched above for two zones can be extended to multiple negleting heat loss to the vessel wall.

$$v_t = \sum_{j=1}^{n=1} x_j v_{bj} + x_n v_{bn} + \left[1 - \sum_{j=1}^{1} x_j\right] v_u$$

$$e_t = \sum_{j=1}^{n=1} x_j e_{bj} + x_n e_{bn} + \left[1 - \sum_{j=1}^{1} x_j\right] e_u$$

Shells with lower indices have burnt previously, and are compressed in a isentropic way during burning of the nth shell. For this reason, the nth terms are treated differently. Specific heats are taken identical as in the two-zone model. Heat exchange between zones are neglected. The total burnt fraction x after burning of N zones:

$$x = \sum_{n=1}^{N} x_n$$

Numerical Two-Zone Model

The numerical two-zone model starts from the conservation equations. Heat losses are neglected. The perfect gas assumption is dropped. Temperature dependent caloric properties are evaluated from polynomial fits. The numerical model was run in two modes: -**"No dissociation"**, complete combustion is assumed into CO_2 and H_2O.
-.**Equilibrium"**, the burnt gas is assumed to be in chemical equilibrium. Depending on pressure and temperature, the composition of the burnt mixture is computed using an equilibrium solver.
The conservation equations are solved for x and T_b for every incremental pressure step. The pressure profile is input by the user.
The model is run until the burnt mass fraction reaches unity, the corresponding pressure at that point is the end pressure p_e.

Conclusions

Evaluation of laminar burning velocities S_u from the pressure trace in constant volume combustion necessarily requires the burnt mass fraction as a function of pressure.
Manipulation of volume and energy conservation laws for perfect gases leads to an analytical x(p) relation that is as easy to implement as the linear one. The derivation requires the assumption of perfect gas behaviour, thus neglecting dissociation and other potentially important effects.

The numerical models used for comparison allowed for temperature dependent specific heats and dissociation. Both effects were shown to affect x(p), with about equal magnitudes.
The one-dimensional unsteady simulation was also used to confirm that flame stretch does not affect x(p) for stoichiometric combustion of methane with air.
We have demonstrated new relations for x and p that well capture deviation from the linear relation found from the numerical models. This proves that neglect of the difference between burnt and unburnt specific heat ratios is the major pitfall of the linear approximation.
Any analytical x(p) relation requires the end pressure as input. Its value affects S_L values is achieved using a numerical model that correctly accounts for dissociation throughout the experiment.