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Lean Limit Combustion in an
Expanding Chamber

Owen Irby Smith

September 1977

Lawrence Berkeley Laboratory University of California/Berkeley

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LEAN LIMIT COMBUSTION IN AN EXPANDING CHAMBER

by

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ABSTRACT

Operation of internal combustion engines at very lean fuel-air mixtures is of increasing interest since an increase in operating efficiency estimated at 5 to 10% with simultaneous reduction of most pollutant emissions is expected. Nevertheless, as the lean flammability limit is approached, the typical automotive engine in use today exhibits an increase in unburned hydrocarbon emissions along with an increase in specific fuel consumption which is characteristic of incomplete combustion. The objective of this study is to investigate the propagation of methane-air flames in an enclosure designed to simulate conditions encountered in an internal combustion engine. Emphasis is placed on experimental conditions where incomplete combustion is observed in the bulk gas (as opposed to the thermal boundary layer). This is due to quenching of hydrocarbon oxidation reactions by volume expansion--so called "bulk quenching."

The apparatus used in the experiment provides full optical access to the ignition and combustion processes, so that flame speeds may be extracted from high speed schlieren motion pictures of the propagating deflagration wave. Cases involving flame propagation in a constant volume chamber, an expanding chamber, and a chamber subjected to a

compression-expansion sequence are investigated.

Bulk quenching of mixtures over an equivalence ratio of 0.563 to 0.615 is observed in an expanding chamber initially at 105 kPa pressure and a 300 K temperature. Quenching occurs in all cases before the volume is expanded by a factor of 2.5. The range of conditions under which bulk quenching is observed in compression-expansion cases is greatly restricted (relative to the expansion only) due to the higher initial temperature encountered as a result of compression and effect of turbulence generated by piston motion.

Flame stretch (divergent propagation of the flame front) is found to contribute to the bulk quenching process for values of the Karlovitz number, K , greater than 0.2. Within the limits of the Karlovitz number as a similarity variable, this conclusion should be valid for any fuel, ignitor, chamber geometry, etc.

The occurrence of bulk quenching is found to be related to the amount of volume expansion but independent of the rate of volume expansion. Theoretical analysis indicates that this is due to an imbalance in the rates of chemical processes compared to diffusion processes caused by a decrease in gas density upon expansion. It is further found that the amount of volume expansion necessary to produce bulk quenching in the experimental system used in this study may be approximated by the condition that the adiabatic flame temperature of the unburned gas (under conditions of quenching) be equal to 1600 K.

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CHAPTER 1

Introduction

Increasing requirements for the operation of internal combustion engines under conditions resulting in both high efficiency (low specific fuel consumption) and low emissions of carbon monoxide, oxides of nitrogen and unburned hydrocarbons have resulted in increased interest in the combustion of very lean premixed gasses. As shown in Figure 1.1, the indicated thermal efficiency η increases as the mixture is leaned (decreasing equivalence ratio) for a given compression ratio. The equivalence ratio, ϕ , is defined as the actual fuel/air ratio divided by the stoichiometric fuel/air ratio. Figure 1.2 indicates that the emissions of carbon monoxide and oxides of nitrogen decrease sharply as the mixture is leaned past stoichiometric. Emissions of nitric oxide decrease due to the lower combustion temperatures associated with departure from stoichiometric mixtures, while more CO is oxidized to CO_2 via the reaction

due to higher concentrations of the hydroxyl radical. Leaner mixtures (higher O_2 concentration) lead to higher OH concentrations through the nearly equilibrated H, O, OH shuffle reactions in the post flame zone.

Note that unburned hydrocarbon emissions, along with specific fuel consumption, increase for lean mixtures. This behavior may be attributed to three processes; misfire or failure to ignite (Shiomoto,

Figure 1.1. Theoretical efficiency of a constant-volume fuel-air cycle as a function of equivalence ratio for various compression ratios, r . The fuel is 1-octene and initial conditions are $P=105$ kPa and $T=390$ K. Data taken from Iura, et al. (1975).

Figure 1.2. The relationship of typical engine emissions and performance to mixture ratio. The vertical scale is linear; relative rather than absolute values for each parameter are shown. Data taken from McDonald, et al. (1974).

et al., 1977), wall quenching of the flame inside the thermal boundary layer (Ferguson and Keck, 1972), and quenching in the bulk gas due to chamber expansion--so called "bulk quenching."

Wall quenching takes place under all conditions in which the flame propagates into the boundary layer. Factors affecting the total amount of hydrocarbon left unburned due to this process are the quench layer thickness, the hydrocarbon density in the unburned gas, and to some extent, the exhaust gas temperature. As the mixture approaches the lean flammability limit, the thickness of the quench layer increases dramatically (Andrews and Bradley, 1972) while the density of hydrocarbon species in the unburned gas decreases so that these factors tend to counteract one another to some extent. The lower exhaust gas temperatures observed as the mixture moves from stoichiometric result in less oxidation of unburned hydrocarbons in the exhaust system.

Misfire occurs when the equivalence ratio of the unburned gas in the immediate region of the ignition device falls below the lean flammability limit (at the appropriate temperature and pressure). Usually this is caused by a nonuniform distribution of fuel both among the chambers of a multicylinder engine and within an individual cylinder.

It is also possible that a portion of the fuel may remain unburned due to flame quenching by means of combustion chamber expansion. This process, hereafter referred to as "bulk quenching," is expected to play an increasingly important role in flame quenching as the mixture ratio of the unburned gas approaches its lean flammability limit, as the engine speed (expansion rate) is increased, and as spark timing

is retarded. Since the lean and rich flammability limits for premixed fuel/air mixtures move toward each other as the initial temperature and pressure are lowered due to adiabatic chamber expansion, it seems likely that the bulk quenching process will assume increasing importance relative to wall quenching as the mixture approaches the lean flammability limit (Barnett and Hibbard, 1959).

Among the difficulties involved in the use of very lean ($\phi < 0.8$) mixtures in internal combustion engines are (Iura, Roessler and White, 1975):

- 1) the low flame speed of these mixtures,
- 2) the increased emissions of unburned hydrocarbons, and
- 3) the effect of uneven fuel distribution.

In addition, although thermal efficiency is greater for leaner mixtures, brake efficiency will at some point begin to increase due to frictional losses. In spite of the difficulties in the lean operation of internal combustion engines enumerated above, this technique is currently receiving serious attention due to the possibility of substantial improvement in overall efficiency (estimated at 5 - 10%; Iura, Roessler and White, 1975) with simultaneous reduction in pollutant emissions.

It is easy to see how the effect of uneven fuel distribution and low flame speeds could lead to increased hydrocarbon emissions through the bulk quenching process. In a recent study of limiting processes in the lean combustion of propane-air mixtures performed in a single cylinder CFR engine of 8.3:1 compression ratio, specific indicated hydrocarbon emissions were observed to rise sharply as spark timing was retarded past 40° before top dead center for a $\phi = 0.7$ mixture

(Quader, 1976). Further, at the onset of this dramatic increase in HC emissions, indirect observations of bulk quenching were made using a series of ionization gauges inside the combustion chamber. Similar correlations between unburned hydrocarbon emissions and large cycle to cycle variation in peak cylinder pressures has been observed by others (Shiomoto et al., 1977).

Since increased consideration is being given to the widespread operation of automotive engines under conditions conducive to the bulk quenching process (lean mixtures and retarded spark timing), further investigation of this phenomenon seems worthwhile. This study consists of an experimental investigation of bulk quenching in laminar, premixed methane-air flames and comparison with a corresponding theoretical investigation conducted under roughly the same circumstances (Smith, Westbrook, and Sawyer, 1977). Methane is used as the fuel primarily because the chemical mechanism of combustion, along with values of the kinetic rate constants necessary for theoretical calculations, is relatively well understood. The experimental investigation is intended to provide quantitative knowledge of the circumstances under which the bulk quenching process is important in internal combustion systems. The theoretical study is used to provide insight into the detailed mechanism of bulk quenching and is not intended to model quantitatively the experimental observations.

CHAPTER 2

Experimental Methods and Apparatus

To draw quantitative conclusions regarding the process of flame extinguishment on expansion of a bulk reacting mixture one must, as a minimum, follow the flame front propagation, the reaction chamber pressure, and the reaction chamber volume with time. Experimental methods of following flame front propagation in ducts fall generally into two categories: those involving photography and those employing electrical methods. Electrical methods involving the use of ionization or thin film resistance gauges to measure flame front position are generally unsuitable for use in any system where the shape of the flame front changes with time. Since these devices are usually mounted close to a wall in order to reduce disturbance to the flow field of the unburnt gas, and since they yield information only about the state of the gas in their immediate vicinity, assumptions regarding flame front shape must be made in order to follow its propagation. For the study of laminar flame propagation in horizontal ducts with mixtures near the lean (or rich) flammability limit, the effects of buoyancy result in distinct changes in flame front shape as illustrated by the data of Wheatley (1950), Figure 2.1. Methods based on the photographic (or to some extent photoelectric) detection of flame front position suffer neither of these difficulties. The flow field of unburnt gas ahead of the flame front is unperturbed, while photographic methods allow direct observation

Figure 2.1. A plot of flame speed against volume percentage of ethylene. Full circles denote ignition point 4 cm from open end; others that ignition point was 1 cm from open end. Tailed circles denote flame speeds measured on a slanting flame front; others that flame was upright. Data taken from Wheatley, 1950.

of flame front shape in one or more projections. In view of these considerations, optical methods seem to be more applicable to the present study where emphasis is placed on very lean mixtures, resulting in relatively slowly propagating flames in which bouyancy effects are significant.

The apparatus in which this study was conducted consists of a horizontally mounted duct of square cross-section enclosed on two sides by borosilicate glass windows and on one end by a movable aluminum piston. This apparatus, the single-pulse compression-expansion machine, (hereafter referred to by the acronym SPCEM), is pictured in Figure 2.2. It is designed to simulate, as far as is practical, the environment encountered inside the cylinder of an internal combustion engine while allowing complete optical access to the combustion process.

The SPCEM consists of three mechanical sections, the snubber, driver, and test sections. Piston trajectory is controlled by the snubber section through the use of hydraulic forces on the snubber piston. These forces result from the flow of a light oil (SAE 10) around the snubber piston within the snubber profile segments. By varying the internal diameter of individual snubber profile segments, the piston trajectory can be made to approximate a sine wave for the desired stroke length. Figure 2.3 shows the variation of piston position x_p , normalized with the piston position at top dead center, x_p^{tdc} , with time for a typical expansion stroke. The piston position is taken as zero in the fully expanded state. For comparison, a sine wave trajectory is also shown. It is apparent that the inertia of the test, driver and snubber pistons, along with the rods connecting them, results in retarded

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Figure 2.2. The Single Pulse Compression-Expansion Machine.

Figure 2.3. Comparison of SPCEM piston trajectory with that of an automotive engine.

piston velocity during the initial part of the process. Nevertheless, linear piston speed corresponds well to that of the sine wave trajectory over most of the stroke. Compression strokes show the same behavior.

The piston movement and timing of the compression and expansion strokes is accomplished by the driver section. Force is imparted to the driver piston by means of compressed gas controlled by solenoid valves (not shown in Figure 2.2). Maximum piston speed, equivalent to engine operation at approximately 2200 rpm, is attainable using helium driver gas at a reservoir pressure of 1.1 mPa. Maximum piston speed is constrained by the viscous losses associated with flow through the relatively small (5.07 cm^2 orifice) solenoid valves and the response time of the valves which is dependent on the moving mass of the valve. Maximum piston speed attainable using the laboratory compressed air supply at 756 kPa is equivalent to engine operation at approximately 1250 rpm. Solenoid valve response time may be improved by modification of the valve internal design; however, many such modifications adversely affect the reproducible operation of the valve. In practice, this results in an irreproducible interval between ignition and the start of the expansion stroke so that in the present study no valve modifications (other than general polishing of bearing surfaces) were made.

The test section consists of a square, $3.81 \times 3.81 \text{ cm}$, cross-section duct of 45.7 cm length. Construction is of stainless steel with two vertically mounted windows of borosilicate glass. On compression the aluminum test piston, sealed by means of two teflon gaskets, is moved horizontally from right to left, Figure 2.2. Provision is made for mounting various ignition

devices at the left hand edge of the test section. Instrumentation ports provide access for introduction of reactant gases, removal of product gases for chemical analysis, and pressure measurement.

Overall control of the processes of compression, ignition, and expansion is exercised by an electronic timing circuit through the driver section solenoid valves and the ignition circuit. Initiation of these processes is controlled by type 555 timers which are set by means of potentiometers. Protection against electrical transients introduced by the ignition spark is provided for the compression timing. A schematic of the timing circuit used in this study is presented in Figure 2.4.

Performance and operating limitations of the SPCEM are outlined in Table 2.1. The most severe operating limitation in terms of this study is the restriction of maximum piston speed to the equivalent of 2200 rpm. In practice, this limits the maximum normalized rate of volume expansion ($\frac{1}{v} \frac{dv}{dt}$) to values on the order of 122 sec^{-1} . Although this value could in principle be increased by shortening the stroke at constant compression ratio, practical considerations of minimum flame kernel size and cold wall effects on flame quenching make this impractical. For discussion of additional aspects of SPCEM capabilities, the reader is referred to the paper of Oppenheim, et al., (1976).

Important considerations in the design of the ignition device used in this study include the ability to ignite the reactant mixture reproducibly and uniformly in the horizontal direction with a high degree of precision in ignition timing. Uniformity in the horizontal direction is desirable as it makes the flame front position as nearly two dimensional as possible. This greatly simplifies the extraction of flame speed data from photographic records of the vertical projection of the flame front position.

TABLE 2.1. Operating parameters for the single pulse compression-expansion machine.

Fuel/Oxidizer: gaseous, premixed*

Equivalence Ratio: 0.5 - 1.3*

Ignition Timing: presetable at any point in cycle

Equivalent Piston Speed: ≤ 2200 rpm

Compression Ratio: $\leq 20:1$

Stroke: ≤ 25 cm

Load: uncontrolled

Ignition Energy: 106 - 265 mJ total

Duct Cross-Section: 38 x 38 mm

Initial Temperature: 293 K

Initial Pressure: 105 kPa

* Methane-Air used in current study

The device used in this study is pictured in Figure 2.5. It consists of a row of fifteen 0.0508 cm spark gaps formed by means of sixteen 0.1588 cm diameter brass electrodes mounted in polymethylmethacrylate. The electrodes are filed to a knife edge in the horizontal direction to increase the local field strength across the spark gaps. When this device is mounted in the test section with the row of electrodes running horizontally from window to window, the flame front will initially exhibit the proper two dimensional symmetry. If the effects of the thermal, momentum, and species boundary layers along the borosilicate windows are negligible, this two dimensional structure will be maintained. As will be discussed in Chapter 3 (Data Reduction) this assumption is often valid for the conditions of interest in this study.

A potential of approximately 46 KV was found to be necessary to achieve a spark across the large total gap of the line ignition source under conditions encountered at the conclusion of an 11:1 compression stroke. The circuit designed to provide ignition energy at this potential is portrayed in Figure 2.6. Uniform pulses of ignition energy are provided by discharge of five 500 pfd, 30 KV capacitors connected in series, yielding a total capacitance of 100 pfd. Capacitance may be increased by removing up to 3 series capacitors, resulting in a maximum capacitance of 250 pfd. Table 2.2 presents the total capacitance and ignition energy at 46 KV for three to five 500 pfd series capacitors.

Series capacitors are discharged through the line ignition source at a precise instant by means of a triggered spark gap which acts as a

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Figure 2.5. End view of the line ignition source.

LINE IGNITER POWER SUPPLY

Figure 2.6. Schematic of the ignition circuit used with the line igniter.

TABLE 2.2. Ignition energy increments available with the line ignition source.

No. Series Capacitors*	Total Capacitance (pfd)	Total Ignition Energy** (mJ)	Ignition Energy/Gap** (mJ)
2	250	265	17.6
3	167	177	11.7
4	125	132	8.8
5	100	106	7.1

* 500 pfd at 30 KV

** 46 KV potential

fast, high voltage switch. It consists of two 3.81 cm diameter aluminum spheres separated by 2.94 cm in air. Triggering is provided by a standard automotive capacitive discharge ignition system (Mallory Model CDN). The 30 k Ω resistor provides a high impedance path through which the series capacitors are charged.

Traces of ignition current and voltage with time are presented in Figure 2.7 for the heavily used condition of 105 kPa pressure, a 300 K temperature, and a $\phi = 0.605$ methane-air mixture. The actual ionization process, which occurs during the first 2 μ sec, is too fast to observe with available equipment. As can be seen from Figure 2.7, ignition energy is deposited over a period of about 16 μ sec. Since this interval is three orders of magnitude less than the characteristic time for combustion (as defined by the ratio of the duct width to the laminar flame speed, for example) we may treat the ignition energy as being instantaneously and uniformly deposited along the line of spark gaps. The oscillations (ringing) observed in the current trace are the result of the L-R-C time constant of the ignition cables.

Since the observation of bulk quenching in the current study is restricted to a narrow range of the equivalence ratio near the lean flamability limit, precise control of reactant mixture composition is essential to its understanding. The equivalence ratio, ϕ , is a dimensionless quantity defined as the ratio of fuel to oxidizer divided by the stoichiometric fuel to oxidizer ratio.

$$\phi = \frac{[\text{fuel}]/[\text{oxidizer}]}{([\text{fuel}]/[\text{oxidizer}])_{\text{stoichiometric}}} \quad (2.1)$$

Thus, the equivalence ratio is equal to one for a stoichiometric mixture, less than one for a lean mixture, and greater than one for a rich mixture.

Gas mixtures may be prepared by static or dynamic methods. Static

Figure 2.7. Current and voltage traces for the line ignitor ignition pulse. Ignition energy is 106 mJ. Current oscillations during the first 2 μ sec. after ignition are too fast to be observed.

methods typically involve manometric preparation by sequential introduction of mixture components into a storage vessel. Dynamic methods involve the mixing of metered streams of individual components. These methods avoid the explosion hazard connected with the storage of large amounts of combustible gas mixtures, as well as assuring homogeneity of the reactant mixture. A dynamic method based on the principle of choked Fanno Line flow (Keenan, et al. 1948) was chosen for use in this study. The apparatus used separately meters the gaseous fuel (methane) and oxidizer (air) through carefully cleaned and deburred hypodermic needles of 2.54 cm length. Although the downstream pressure is essentially constant during introduction of reactant gas into the test section, an effort was made to assure choked flow at the needle exit. For choked Fanno Line flow the molecular flow rate, $\dot{n}$, is a function of the inlet stagnation pressure, stagnation temperature and physical properties of the gas (Kamel and Lundstrom, 1967).

For Reynolds numbers between 1000 and 1750, $\dot{n}$ is a nearly linear function of p_0 so that for a constant air flow rate the methane mole fraction of the mixture should vary linearly with the methane inlet stagnation pressure. At a Reynolds number of ~ 1750 , transition to turbulent flow begins, resulting in decreased molecular flow rate. Reactant gas analysis performed on a Hewlett-Packard 5750 gas chromatograph equipped with thermal conductivity detectors confirms the expected linear relationship between methane mole fraction and methane inlet stagnation pressure over the range $0.05 \leq X_{\text{CH}_4} \leq 0.12$. The same analysis indicates that mixture equivalence ratio is reproducible to within a maximum error of 0.9 percent. Since this figure includes errors introduced in sample handling and injection techniques of two

different analyses, the actual error is expected to be significantly lower. Calibration of the gas metering apparatus in terms of equivalence ratio was done by comparison with manometrically prepared mixtures using the gas chromatograph. Error in the absolute magnitude of the equivalence ratio is estimated at ± 3 percent, due primarily to error in the preparation of calibration standards. Commercially bottled air having a maximum water content of 11 ppm was used as the oxidizer in the current study. Commercial grade methane of ≥ 93 percent purity was used as the fuel. Although commercial grade methane typically contains approximately 3 percent ethane and 1 percent propane by volume, neither of these species was observed in the gas chromatographic analysis of reactant mixtures.

Table 2.3 lists pertinent operating conditions for the gas mixing system used in this study. For an extensive theoretical treatment of the process, the reader is referred to the literature (Kamel and Lundstrom, 1967; Kamel, Lundstrom and Oppenheim, 1968).

As stated at the beginning of this chapter, knowledge of the flame front position and area, along with the combustion chamber pressure, as functions of time are necessary to determine the flame speed with respect to the unburned gas. Since quenching may be conveniently defined to have occurred when the flame speed with respect to the unburnt gas has been reduced to zero, the technique used to follow the flame front position (and area) with time is of primary interest. For reasons discussed earlier in this chapter, optical methods seem to be best suited for this task.

In this study the method used is based on high speed schlieren cinematography. The image produced by the schlieren process portrays

TABLE 2.3. Operating parameters for the gas mixing system.

	<u>Methane</u>	<u>Air</u>
Needle Gauge	30	23
Needle Inside Diameter (cm)	0.00152	0.00356
Needle Length (cm)	2.54	2.54
Upstream Pressure Range (kPa)	225	420 - 725
Downstream Pressure (kPa)	105	105

areas of suitably high refractive index gradient. This is done by marking light rays which, on passing through the test section, are refracted to a given degree as a result of traversing a gradient in the refractive index, η . The apparatus which performs this function is diagramed schematically in Figure 2.8. Light provided by a high intensity xenon arc lamp (Oriel model C-60-50) is passed through a 1.5 mm diameter pinhole at point S. It is then formed into parallel rays by means of the spherical mirror M_1 (focal length f_c) and passed horizontally through the test section. The test section image thus produced is focused by means of another spherical mirror M_2 onto the schlieren stop S' , and thence onto the image plane of a high speed motion picture camera by means of a lens.

In the idealized schlieren schematic presented in Figure 2.9, the light provided by the point source S is deflected at point A by an angle θ as a result of traversing the refractive index gradient $(\frac{\partial \eta}{\partial y})$. The relationship between θ and $(\frac{\partial \eta}{\partial y})$ is given by

$$\theta = - \int_0^Z \frac{1}{\eta} \left(\frac{\partial \eta}{\partial y} \right) dz \quad (2.2)$$

where the minus sign indicates that the deflection is in the direction of higher refractive index. Following the formalism of Weinburg (1963), we introduce the quantity δ , the deviation of refractive index from that of a vacuum ($\eta_{\text{vacuum}} \equiv 1$), defined by equation 2.3.

$$\eta = 1 + \delta \quad (2.3)$$

Numerical values for δ are on the order of 10^{-4} for gases at standard temperature and pressure. Further, for an ideal gas, this value decreases with increasing temperature (see Eq. 2.7). Since $\delta \ll 1$, Eq. 2.2 may be written

$$\theta = - \int_0^Z \left(\frac{\partial \delta}{\partial y} \right) dz \quad (2.4)$$

Figure 2.8. Schematic of the schlieren cinematographic system. $f_s = f_c = 394$ cm.

Figure 2.9. Ray deflection diagram illustrating the effect of a refractive index gradient at point A on the path of a transmitted ray. The deflected ray is indicated by the broken line.

For the case where the refractive index gradient is normal to the incident radiation, a situation which is often true to a good approximation in the current study due to the use of the line ignitor, $(\frac{\partial \delta}{\partial y})$ will not be a function of z so that Equation 2.4 may be integrated yielding

$$\theta = z \left(\frac{\partial \delta}{\partial y} \right) \quad (2.5)$$

For the two dimensional case (uniform in the z -direction) considered in the current study, Equation 2.5 may be generalized

$$\theta_y = z \left(\frac{\partial \delta}{\partial y} \right) \text{ and } \theta_x = z \left(\frac{\partial \delta}{\partial x} \right) \quad (2.5a)$$

where

$$\theta = (\theta_x^2 + \theta_y^2)^{1/2}$$

The empirical expression of Gladstone and Dale as well as the equivalent theoretical expression derived by Lorenz for the relationship between η and ρ may be expressed as

$$\frac{\eta - 1}{\rho} = \text{constant} \quad (2.6)$$

As a result, for an ideal gas at constant pressure and molecular weight

$$\eta - 1 \propto \frac{1}{T} \text{ or } \delta \propto \frac{1}{T} \quad (2.7)$$

Also, for the case of an ideal gas of constant molecular weight and specific heat ratio undergoing an adiabatic change in pressure

$$\frac{P}{P_o} = \left(\frac{\rho}{\rho_o} \right)^\gamma = \left(\frac{\delta}{\delta_o} \right)^\gamma \quad (2.8)$$

where γ represents the ratio of specific heats. Combining Equations 2.7 and 2.8 and taking the derivative of δ with respect to y yields

$$\frac{\partial \delta}{\partial y} = \delta_o T_o P_o^{-1/\gamma} \left\{ -\frac{1}{T^2} \left(\frac{\partial T}{\partial y} \right) P^{1/\gamma} + \frac{1}{T^\gamma} P^{(1/\gamma - 1)} \left(\frac{\partial P}{\partial y} \right) \right\} \quad (2.9)$$

For the current study, where both the piston speed and the flame speed are slow with respect to the speed of sound, the pressure inside the combustion chamber may be approximated as being spatially uniform so that the last term of Equation 2.9 may be neglected. Combining Equations 2.9 and 2.5 yields

$$\theta = \frac{\delta_o T_o Z}{T^2} \left(\frac{\partial T}{\partial y} \right) \left(\frac{P}{P_o} \right)^{1/\gamma} \quad (2.10)$$

With reference to Figure 2.9, the distance Δ from the center of the schlieren stop at which the deflected ray intersects the stop can be expressed

$$\Delta = f_s \tan \theta \quad (2.11)$$

or for small θ

$$\Delta \sim f_s \theta \quad (2.11a)$$

Combining Equations 2.10 and 2.11a and rearranging yields

$$\frac{\partial}{\partial y} \left(\frac{1}{T} \right) = \frac{\Delta}{f_s \delta_o T_o Z} \left(\frac{P_o}{P} \right)^{1/\gamma} \quad (2.12)$$

Equation 2.12 provides a relationship between the temperature gradient (or really $\frac{\partial(1/T)}{\partial y}$) and the deflection distance Δ on the schlieren stop. The function of the schlieren stop is to label the deflected ray so that it may be identified as having passed through a specified temperature gradient when returned to the image plane at A'. This is usually done by means of a neutral density filter for black and white film or by a frequency selective (color) filter in the case of color film. In the current study, a 2.11 mm diameter solid aperture was normally used with Eastman Kodak Tri-X reversal film. A few cases were examined using a stop consisting of concentric rings of different color along with

High Speed Ektachrome-EF film. A Wollensac Fastax Model WF-17 16 mm camera capable of framing rates up to 7000 frames/sec was used to record the event.

Equation 2.12 may be used to obtain an estimate of schlieren sensitivity for the parameters used in this study. For a methane-air mixture of equivalence ratio $\phi = 0.65$, initially at 293 K, and at a constant pressure of 105 kPa, δ_o is calculated from Equation 2.13

$$\delta_o = \sum_j \chi_j \delta_j \quad (2.13)$$

where χ_j represents the mole fraction of species j .

Using published values of δ for methane and air (Weinburg, 1963)

$$\left. \begin{array}{l} \delta_{CH_4} = 4.44 \times 10^{-4} \\ \delta_{AIR} = 2.93 \times 10^{-4} \end{array} \right\} \begin{array}{l} 293 \text{ K} \\ 105 \text{ kPa} \end{array}$$

Equation 2.13 yields a value of 3.03×10^{-4} for δ_o . Equation 2.12 then yields a minimum sensitivity

$$\left(\frac{\partial T}{\partial y}\right)_{\min} \sim 260 \text{ K/cm}$$

for observation of a schlieren image.

In theory, a point source of light should yield a schlieren image of infinite contrast. In practice, the finite size of the source at S results in an image of graduated contrast with sensitivity distributed about the minimum theoretical value. For an analysis of the resolution of the schlieren system used in this study the reader is referred to the work of Ishikawa and Daily (1977). For a more general discussion of schlieren photography the reader may refer to the extensive literature available (Landenberg, et al. 1954, Weinberg, et al.

1963; Holman, et al. 1975; Eckert, et al. 1976).

The test section pressure was measured using a Kistler Model 610 A (3 μ sec rise time) piezoelectric pressure transducer mounted 0.7 cm from the ignition source in the bottom plane of the test section. The diaphragm was covered with a thin coat of RTV-102 silicone rubber in order to insulate the transducer from the heat of the combusted gases. This has been reported to make transducer temperature coefficient errors negligible in experiments similar to the present study (Steiner, 1977). Pressure records along with an event marker for the ignition pulse were recorded on an oscilloscope.

CHAPTER 3

Data Reduction

In studies involving internal combustion engines, values for the flame-front propagation rate are commonly inferred from knowledge of the cylinder pressure and cylinder volume (crank-angle) with respect to time (Krieger and Borman, 1966). In extracting the flame speed from such limited data, one must make numerous assumptions as to the shape of the flame-front, temperature of the burned gas and heat transfer rates. In the present study, use is made of experimental observations of flame-front position to effect a considerable reduction in the scope of such assumptions.

The model on which flame speed measurements made in this study are based is portrayed in Figure 3.1. The following assumptions are made in order to extract flame speeds from experimental observations:

- 1) $\int_{V_u} \vec{q} \cdot \vec{n} \, dV = 0$, No net heat flux is allowed across the boundaries of the unburned volume.
- 2) The flame front itself is considered to be a negligibly thin zone which is uniform in the z direction. It need not, however, be symmetric about the horizontal plane defined by the ignition source.
- 3) The unburned gas is assumed to behave as an inviscid ideal gas of constant specific heat ratio. The composition is

Figure 3.1. Idealized representation of flame front geometry using the line ignition source. Flame front is uniform in the z - direction.

taken as that of the initial mixture.

- 4) The pressure is assumed to be spatially uniform inside the combustion chamber.

The net heat transfer across the boundaries of the unburned volume may be broken down into that component across the flame front and that across the chamber walls. The magnitude of first component may be estimated from the adiabatic flame temperature obtained from thermodynamic calculations and the flame front thickness obtained from schlieren photographs. For typical initial conditions of ambient temperature and pressure, an equivalence ratio of approximately 0.6 and an initial (compressed) volume of 26 cm^3 , the adiabatic flame temperature is approximately 1900 K. A few milliseconds after ignition, the average thickness of the schlieren image remains approximately constant at $\sim 2 \text{ mm}$. Thus, the heat flux conducted through the flame front is

$$q = k \frac{dT}{dn} \sim 2.00 \text{ J sec}^{-1} \text{ cm}^{-2}$$

Approximating the flame front area as the duct cross-sectional area, about $3 \times 10^{-1} \text{ J}$ will be conducted in the 10 msec interval during which the process of interest occurs. The average temperature increase of the unburned gas due to adsorption of this energy may then be calculated from

$$H_f - H_i = \int_{T_i}^{T_f} C_p dT \sim C_p (T_f - T_i) \sim 3 \times 10^{-1} \text{ J}$$

Since there is typically $\sim 10^{-3}$ mole of unburned gas remaining at flame extinguishment, Equation 3.2 leads to an average temperature increase of $\sim 10^\circ \text{K}$ in the unburned gas. Thus, neglecting heat transfer across

the flame front leads to errors in unburned gas temperature on the order of 3 percent. Error due to conduction of the chamber walls may be treated in the same manner and is of similar magnitude.

The second assumption of our analysis, horizontal isotropy, is probably the poorest of any made and can lead to considerable error. Evidence of retarded flame propagation in the boundary layer along the glass windows can often be seen in the schlieren photographs. This makes the measured values of both the flame front area and unburned volume based on the assumption of horizontal isotropy low. The effect of these errors on the calculated flame speed is discussed in detail elsewhere in this chapter. It should be noted, however, that in this study flames are typically quenched before significant three-dimensional flame front geometry is observed in the schlieren images and that uncertainty in the flame front area does not affect the calculated point of flame extinguishment (see Equation 3.6).

For the experimental conditions used in this study, the assumption of perfect gas behavior for the unburned gas introduces negligible error. The assumption of isotropic pressure is also good since the speed of sound in both the burned and unburned regions exceeds the maximum piston or flame front velocities by a factor of ~ 10 .

The flame speed with respect to the unburned gas is defined by

$$S = - \frac{\dot{m}_u}{\rho_u A_f} \quad (3.1)$$

where $\dot{m}_u$ is the time rate of change of the mass of unburned gas, ρ_u is the unburned gas density and A_f represents the area of the flame front. The first quantity may be expressed as follows:

$$\dot{m}_u = \frac{\partial}{\partial t} m_u = \frac{\partial}{\partial t} (\rho_u V_u) \quad (3.2)$$

where V_u is the volume of unburned gas remaining at a given time.

Accordingly, we may write

$$S = - \frac{V_u}{A_f} \frac{\partial}{\partial t} \{ \ln(\rho_u V_u) \} \quad (3.3)$$

Under the assumptions outlined earlier, the unburned gas temperature is given by the equation for adiabatic compression

$$T V^{\gamma-1} = \text{constant} \quad (3.4)$$

where γ represents the ratio of specific heats. Applying Equation 3.4 along with the ideal gas equation of state to Equation 3.3, one may easily derive an expression for S in terms of P , V_u , γ_u and A_f

$$S = - \frac{V_u}{A_f} \frac{\partial}{\partial t} \{ \ln(P^{\frac{1}{\gamma_u}} V_u) \} \quad (3.5)$$

Defining the quenching condition as $S = 0$, the criterion for flame extinguishment becomes

$$\frac{\partial}{\partial t} \{ \ln(P^{\frac{1}{\gamma_u}} V_u) \} = 0 \quad (3.6)$$

The unburned volume and flame front area can be estimated from schlieren photographs while the test section pressure is measured, so that under the assumptions of our model the flame speed may be calculated from available data.

Analysis of the effect of an uncertainty, δ_x , in one of the parameters of Equation 3.5 on the flame speed may be conveniently broken into two parts; the analysis of so called steady error ($\frac{\partial}{\partial t} \delta_x = 0$), and that of unsteady error ($\frac{\partial}{\partial t} \delta_x \neq 0$). All of the

former are of a systematic nature and, in theory, none should impact the detection of the quenching condition according to Equation 3.6.

As an example of the effect of a steady error on S , consider an uncertainty in the test section pressure, δP . The test section pressure is calculated by means of a calibration curve from the voltage output of a Kistler charge amplifier. The calibration curve is of linear form

$$P = C + kv \quad (3.7)$$

where v represents the output voltage, k the transducer sensitivity (atm/volt) and C is a constant indicating the zero point of the amplifier and is always equal to 1 atm in the current study. Thus

$$\delta P = \delta C + (\delta k)v. \quad (3.7a)$$

Taking first the effect of δC and defining

$$C' = C + \delta C \quad \text{and} \quad P' = C + \delta C + kv$$

we may write from Equation 3.5, after some algebraic manipulation

$$S' = \frac{V_u}{A_f} \left[[\gamma(P + \delta C)]^{-1} \frac{\partial P}{\partial t} + \frac{1}{V_u} \frac{\partial V_u}{\partial t} \right]. \quad (3.8a)$$

In the same manner, for $k' = k + \delta k$ and $P' = C + (k + \delta k)v$ we may write

$$S' = \frac{V_u}{A_f} \left[\left(1 + \frac{\delta k}{k}\right) [\gamma(P + \delta kv)]^{-1} \frac{\partial P}{\partial t} + \frac{1}{V_u} \frac{\partial V_u}{\partial t} \right]. \quad (3.8b)$$

The percentage error in the flame speed, ΔS , is then given by

$$\Delta S = \left(\frac{S - S'}{S} \right) \times 10^2. \quad (3.9)$$

Equations 3.8 and 3.9 may be applied to a typical set of experimental conditions of interest in this study. A case involving flame propagation during an expansion stroke approximately 6 msec before

quenching has been chosen for this purpose. Details of the experimental conditions are included in Table 3.1.

The maximum value of δC is estimated to be 0.106 atm, corresponding to a maximum charge amplifier zero point error of 10 mv. Charge amplifier offset due to radiated noise from the ignition pulse is responsible for this relatively large uncertainty. In the absence of an ignition pulse $\delta C_{\max} \leq 1$ mv since the charge amplifier is always shorted to ground immediately before measurements are taken. Calibration with a high quality digital voltmeter indicates that the pressure-voltage calibration curve is linear to within one percent. Thus for $k = 10.627 \frac{\text{atm}}{\text{volt}}$, $\delta k_{\max} = 0.106 \frac{\text{atm}}{\text{volt}}$. Application of these values, along with those of Table 3.1, to Equations 3.8 and 3.9 yields

$$\Delta S \text{ for } \delta C = 0.106 \text{ atm} \sim 17\%$$

$$\Delta S \text{ for } \delta k = 0.106 \text{ atm/volt} \sim 2\%$$

Thus, one could expect as a worst case, a maximum error of approximately 19% due to a steady uncertainty in the test section pressure.

A similar analysis has been performed for steady uncertainty in the unburned volume and flame front area. The results are summarized in Table 3.2. Due to the presence of oscillator supplied timing marks on the schlieren film, uncertainty in time is expected to be negligible.

As stated earlier, only unsteady uncertainties can affect the time at which quenching is observed to occur. Since this is the event of primary interest in this study, we now direct our attention toward these random errors.

We need consider only those parameters found in Equation 3.6. Of these, we again neglect δt for reasons already stated. The unsteady

TABLE 3.1. Results of film analysis for three sequential points in a $\phi = 0.577$ laminar expansion.

	$t(\text{msec})$	$V_u(\text{cm}^3)$	$V_{\text{total}}(\text{cm}^3)$	$A_f(\text{cm}^2)$	$P(\text{kPa})$	$v(\text{volt})$	$\frac{\partial V_u^*}{\partial t}(\frac{\text{cm}^3}{\text{sec}})$	$\frac{\partial P^*}{\partial t}(\frac{\text{atm}}{\text{sec}})$	$S(\frac{\text{cm}}{\text{sec}})$
j-1	6.67	23.685	27.736	10.192	104.7	-.0003			
j	8.33	23.781	29.353	11.538	98.6	-.0057	294.6	-38.44	-35.16
j+1	10.00	24.666	31.675	13.354	91.2	-.0123			

$\phi = 0.577$, $T_o = 303 \text{ K}$, $P_o = 105 \text{ kPa}$, $\gamma_u = 1.39$, ignition energy = 106 mJ

$$* \left(\frac{\partial \ell}{\partial t} \right)_j = \frac{1}{2} \left(\frac{\ell_j - \ell_{j-1}}{t_j - t_{j-1}} + \frac{\ell_{j+1} - \ell_j}{t_{j+1} - t_j} \right)$$

TABLE 3.2. Effect on the flame speed of the maximum estimated variation in a parameter X for the data of Table 3.1.

<u>X</u>	<u>X₀</u>	<u>ΔX_{max}</u>	<u>ΔS_{max}</u>
P	105 kPa	11.1 kPa	17%
k	1.115 $\frac{\text{MPa}}{\text{volt}}$	11.1 $\frac{\text{kPa}}{\text{volt}}$	2%
V _u	23.7 cm ³	1.50 cm ³	10%
A _f	11.5 cm ²	.5 A _f	100%

uncertainty in pressure is controlled by the precision with which the output voltage from the charge amplifier can be read from an oscilloscope trace. The corresponding uncertainty in the unburned volume is much harder to ascertain, since it involves not only the precision with which the flame front position can be measured from schlieren images, but also the degree of validity of our assumption of flame front horizontal isotropy. Since the schlieren photographs show only the vertical (x-y) projection of the flame front, the latter effect is very difficult to assess.

An attempt was made to verify the assumed flame front symmetry experimentally by orienting the line ignition source vertically with respect to the schlieren optical path. Although care was taken to isolate the ignition system ground from that of the remainder of the apparatus, the extremely fast ignition current pulse took the lower impedance path between the high potential end of the line ignitor electrodes and the adjoining stainless steel test section wall. As a result of this, we can only estimate the magnitude of uncertainty in the unburned volume due to deviation from horizontal isotropy.

This estimate was made for experimental conditions under which we are barely able to quench the flame. Since deviation from horizontal isotropy typically increases during the initial stage of combustion, a relatively long interval between ignition and extinguishment increases the effect, making deviations in the case examined among the largest of any observed. Exposures at 15.00, 16.67 and 18.33 msec after ignition are presented in Figure 3.2. The rightmost image in each each frame represents the cross section of the flame front in

Figure 3.2. Sequential schlieren images showing horizontal anisotropy.

Frame 90; $t = 15.0$ msec.

Frame 100; $t = 16.7$ msec.

Frame 110; $t = 18.3$ msec.

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the central vertical plane. The trailing images represent its position along the glass windows. Corresponding experimental conditions are reported in Table 3.3. In the estimation of the error in unburned volume introduced by the assumption of horizontal isotropy, the scheme outlined in Figure 3.3 is used. The image of the flame front in the x-y plane at $z = \frac{L}{2}$ is assumed to accurately portray the flame front position to within a distance $2\delta_q$ of each window. The flame front is then assumed to slope to the image in the x-y plane at $x=0=L$. If the actual flame front is assumed to behave as described above, and if the quenching distance for a $\phi = 0.654$ mixture at one atmosphere, $\delta_q = 2.4$ mm (Andrews and Bradley, 1972), is used, our model underestimates V_u by 2.2% at 15 msec, 3.0% at 16.67 msec and 3.3% at 18.33 msec.

The unburned volume, V_u is calculated by a computer program from coordinates of the flame front and piston positions obtained from an optical film reader. The program used, FILM, is reproduced in Appendix 1. Numerical integration is performed on monotonically increasing or decreasing segments of the flame front in the subroutine CRUNCH. A set of points defining a curve segment is first approximated by cubic splines (with arbitrary second derivative and end conditions) via the IMSL routine ICSICU (International Mathematical and Statistical Libraries, 1975). Another IMSL routine, DCSQDU, then computes the integral of the segment. Finally, the integrals are summed appropriately in FILM.

Accuracy of the integration depends on the quality of the spline approximation to the flame front position. This, in turn, depends on the complexity of the flame front shape and the positions at which

Figure 3.3. Method of error estimation due to deviation from horizontal isotropy. δ_q represents the quenching distance.

TABLE 3.3. Result of film analysis for the sequential frames of Figure 3.2.

	<u>frame</u>	<u>$V_{\text{total}}(\text{cm}^3)$</u>	<u>$V_u(\text{cm}^3)$</u>	<u>time (msec)</u>	<u>$A_f(\text{cm}^2)$</u>	<u>P (kPa)</u>	<u>S (cm/sec)</u>
j - 1	90	54.9	32.4	15.00	31.0	46.2	---
j	100	66.9	38.4	16.67	39.4	35.9	9.12
j + 1	110	81.0	47.1	18.33	47.5	26.9	---

$\phi = 0.605$, $T_0 = 298 \text{ K}$, $P_0 = 105 \text{ kPa}$, $\gamma_u = 1.39$, ignition energy = 106 mJ

co-ordinates are recorded. Typically, between 10 and 20 points are taken, spaced at uneven intervals appropriate to defining the curve. When in a test case, it was attempted to extract the known volume ahead of ten equally spaced points defining an idealized parabolic arc the program overestimated the actual volume by 0.12%. This procedure, then, contributes a negligible amount to the total unburned volume uncertainty.

Maximum error in flame front position measurement estimated to be ± 1 mm, or approximately half the schlieren image thickness, while the piston measurement should be within 0.5 mm of the true value. Equation 3.10 expresses the uncertainty in V_u due to measurement error...

$$(\delta V_u)_{\text{meas.}} = N^{-1/2}(A_{f1} \cdot 0.1) + (A_{xs} \cdot 0.05)\text{cm}^3 \quad (3.10)$$

The factor $N^{-1/2}$ represents the improvement in signal to noise resulting from taking N samples. Since a given curve is sampled 10 to 20 times, we will assume $N = 15$. A_f represents the flame front area and A_{xs} represents the duct cross-sectional area. For the example of Figure 3.2 and Table 3.3...

frame	$V_u(\text{cm}^3)$	$(\delta V_u)_{\text{symm.}}(\text{cm}^3)$	$(\delta V_u)_{\text{meas}}(\text{cm}^3)$	$\delta V_u(\text{cm}^3)$
90	32.4	-0.7/+0	± 1.5	+1.5/-2.2
100	38.4	-1.2/+0	± 1.7	+1.7/-2.9
110	47.1	-1.5/+0	± 1.9	+1.9/-3.4

Applying these data to Equation 3.5, using the centered difference scheme of Table 3.1 to evaluate the appropriate derivations with $(\delta V_u)_{j-1}$ and $(\delta V_u)_{j+1}$ taken in the opposite directions, we obtain for frame 100 $S' = 79.7$ cm/sec, or over eight times the unperturbed value. A similar analysis for a maximum uncertainty in test section pressure of 0.01 atm

corresponding to an uncertainty of ± 1 mv in reading the oscilloscope trace yields $S' = 16.2$ cm/sec, or ~ 1.8 times the unperturbed value.

The large errors produced in the preceding analysis result from combining the largest possible errors in the various parameters in such a manner as to cause the greatest effect. No deviations on the same order as these maximum values have been observed. Nevertheless, it is obvious that considerable smoothing will be necessary in the extraction of the time derivative of Equations 3.5 and 3.6 if meaningful results are to be obtained. In practice, this was found to be most easily accomplished by hand.

CHAPTER 4

Experimental Results

Experimental investigations conducted as part of this study utilize the methods described in previous chapters to follow flame front propagation in three different situations; a constant volume duct (no piston motion), and expanding volume (piston withdrawal only), and a volume undergoing a compression-expansion sequence (piston extension and withdrawal). Laminar flame speeds are frequently deduced from combustion in constant volume systems (i.e. bombs) so that comparison of our results obtained in the constant volume duct with literature values should serve to check the applicability of approximations made in the data reduction.

Flame propagation in an expanding volume initially at ambient pressure and temperature, hereafter referred to as laminar expansion, was the subject of most of the experimental work performed in this study. The laminar expansion is the simplest case in which flame quenching due to expansion may be observed since the complicating effect of flow field turbulence induced by compression is absent. In addition, the lower initial flame speeds associated with a gas mixture at ambient temperature (as opposed to the significantly higher temperatures resulting from adiabatic compression) and the lower leak rate around the piston seals as a result of the lower pressure gradient across them are advantageous from a practical standpoint. These effects will be discussed later in this chapter.

Flame propagation in a volume undergoing a compression-expansion sequence most closely approximates the actual conditions inside an internal combustion engine of any situation investigated in this study. Missing are the turbulence and fluid motion which result from intake processes. As explained later in this chapter, experimental difficulties limit the amount and scope of useful information that can be extracted from compression-expansions.

Flame speed measurements in a constant volume duct were made for two values of the equivalence ratio, ϕ . Initial conditions are presented in Table 4.1. Sequential schlieren photographs of flame front propagation for the $\phi = 0.563$ and $\phi = 0.923$ cases are presented in Figures 4.1a and 4.1b respectively. The mixture of Figure 4.1a ($\phi = 0.563$) represents the lean flammability limit in our apparatus under the conditions specified in Table 4.1. The time interval between frames is approximately 15 msec. The retarding effect of the thermal and momentum boundary layers along the glass windows on the flame propagation rate is easily noticeable in frames three through seven. This results in the illusion of a second flame front following the first down the duct. After frame nine the process appears to be nearly two dimensional (uniform in the horizontal direction) and the effect of bouyancy becomes quite noticeable. Flame speeds extracted from the schlieren photographs of Figure 4.1a by means of Equation 3.5 are plotted against time in Figure 4.2, $t = 0$ being taken as one frame prior to the occurrence of the spark. For purposes of comparison, laminar flame speeds calculated from expressions cited in a recent review (Andrews and Bradley, 1972) are included. Flame speeds calculated from experimental records are seen to exhibit only fair agreement with accepted literature values.

Figure 4.1a. Flame propagation in a constant volume duct. $\phi = 0.563$. Frames at 15 msec. intervals. Initial conditions as specified in Table 4.1.

Figure 4.1b. Flame propagation in a constant volume duct. $\phi = 0.923$. Frames at 4.5 msec. intervals. Initial conditions as specified in Table 4.1.

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TABLE 4.1

Experimental Conditions, Constant Volume Duct

Fuel: Methane-Air

Duct Dimensions: 3.81 x 3.81 x 14.92 cm

Film: Kodak Tri-X reversal

Schlieren Stop: 2.11 mm solid aperture

Camera Speed: 6000 frames/sec

Ignition Energy: 106 mJ

Initial Pressure: 105 kPa

Initial Temperature: 303 K

Equivalence Ratio: 0.563 and 0.923

Figure 4.2. Plot of flame speed versus time for flame propagation in a constant volume duct at the lean flammability limit. Initial conditions are $P = 105$ kPa and $T = 303$ K. Ignition energy is 106 mJ. Broken line shows the laminar flame speed, calculated from the correlation of Andrews & Bradley, (1972), under the same conditions.

The very high flame speeds observed initially may be attributed to the rather large ignition energy (106 mJ) used in this case. This is over two orders of magnitude higher than the minimum ignition energy for stoichiometric methane air mixtures. The flame speed stabilizes briefly at approximately twice the literature value between 20 and 50 msec, then decreases until good agreement is obtained with literature values for times greater than 100 msec. With reference to Figure 4.1a, 100 msec after ignition corresponds approximately to frame seven. Since the time at which measured flame speeds reach agreement literature values and the time at which horizontal anisotropy effects begin to disappear coincide closely, it seems likely that they are connected.

According to the analysis of steady error summarized in Table 3.2, the only measurement error capable of producing a uniform error of a factor of two in the calculated flame speed is error in the estimation of the flame front area, A_f . For the case where the flame front is not uniform in the horizontal direction, the analysis will underestimate this value, leading to a corresponding overestimate of the flame speed from Equation 3.5. To summarize, it seems probable that deviations in flame speed from literature values evidenced in Figure 4.2 for times greater than 15 msec are due to underestimation of the flame front area, A_f , due to deviations from horizontal isotropy. This difficulty encountered in measuring A_f is perhaps not surprising in view of conclusions in the literature that even when the flame is photographed in three projections, accurate determination of flame front area is often impossible (Andrews & Bradley, 1972). Fortunately, as explained in Chapter 3, errors in flame speed calculation brought about by inaccurate estimates of flame front area have no effect on the calculated quenching times in the expanding volume experiments.

Figure 4.1b illustrates the combustion of a near stoichiometric ($\phi = 0.923$) mixture in a constant volume duct. The time interval between frames is approximately 4.5 msec. Notice that the flame front propagates much faster in this case than in the lean limit case, covering half the duct length in about 22.5 msec as compared to ~ 100 msec for the leaner mixture. Wall effects on flame propagation are initially present (frames 1 and 2) but disappear quickly as the flame flattens. This classical behavior, called Taylor instability, is observed for flames in closed ducts due to the interaction of an adverse pressure gradient created by compression of the unburnt gas ahead of the flame front with the momentum boundary layer along the walls. This results in eventual separation of the laminar boundary layer and the creation of turbulent eddies in the region of the walls. Since turbulence greatly increases the flame speed, the flame accelerates near the wall resulting in an apparent collapse of the flame front in the center of the duct exhibited beginning with frame 5. Taylor instability is most readily observed in fast burning mixtures which create relatively large adverse pressure gradients. In the lean limit mixture (Figure 4.1a) the effect of Taylor instability may be observed beginning with frame 12 near the bottom of the picture.

A rather extensive experimental investigation of bulk quenching in the laminar expansion process has been performed in the course of this study. Parameters examined include the effect of spark timing and ignition energy, rate and amount of volume expansion, and mixture equivalence ratio on bulk quenching. Flame extinguishment by means of the bulk quenching process has been observed over an equivalence ratio range between the lean flammability limit ($\phi = 0.563$)

and $\phi = 0.615$. Experimental constraints (maximum piston speed) prohibit the extension of this range to higher equivalence ratios.

The concept of ignition timing is made somewhat hazy by the elimination of the compression stroke in the laminar expansions. In this study the ignition timing is represented by the parameter τ_i , which is defined as the time interval between the ignition pulse and volume expansion to 1.1 times the compressed (top dead center) volume. Since laminar expansions are always started with the fully compressed volume and since the time of ignition is always taken as $t = 0$, τ_i is given by Equation 4.1

$$\tau_i = t \Big|_{V = 1.1V_0} \quad (4.1)$$

τ_i is plotted against the volume expansion ratio at which quenching is observed, $\theta_{s=0}$, in Figure 4.3 for a number of $\phi = 0.557$ mixtures. The volume expansion ratio, θ , is defined as the amount of volume expansion that the combustion chamber has undergone at a given time, non-dimensionalized by the initial volume V_0 .

$$\theta \equiv \frac{V - V_0}{V_0} \quad (4.2)$$

Experimental conditions for the points plotted in Figures 4.3 - 4.13 may be found in Table 4.2. Figure 4.3 indicates that a relatively larger degree of volume expansion is necessary to quench the $\phi = 0.577$ mixtures as τ_i increases over the range $0 < \tau_i < 7$ msec. For $\tau_i > 7$ msec a volume expansion ratio of 0.126 (a 12.6% increase in the initial volume) seems sufficient to quench the flame.

No such relationship seems to exist between τ_i and the rate of volume expansion, $\frac{\partial}{\partial t}(\ln V)$, as shown in Figure 4.4. As indicated by

Figure 4.3. Variation of volume expansion ratio at quenching with the ignition timing parameter τ_i , defined by equation 4.1. $\phi = 0.577$ laminar expansions with ignition energy of 106 mJ except as otherwise noted.

□ - 1105 kPa driver pressure	◇ - 533 kPa driver pressure
○ - 750 kPa driver pressure	▽ - 320 kPa driver pressure

TABLE 4.2 Experimental Conditions - Laminar Expansions

Experiment #	512-1	706-3	706-7	711-2	711-3	711-4	712-1a	712-1b	803-1a	803-1b	512-2
Equivalence Ratio	0.577	0.577	0.577	0.577	0.577	0.577	0.577	0.577	0.586	0.586	0.591
τ_i (msec)	11.0	6.3	3.0	2.3	3.3	7.4	4.4	4.0	7.7	6.8	11.7
Driver Pressure (kPa)	750	750	1105	750	533	320	750	750	320	320	750
Approx. Expansion Speed (rpm)	1250	940	1000	882	750	460	860	860	1070	1150	1250
Compression Ratio	8.57:1	8.15:1	8.15:1	7.51:1	7.51:1	7.51:1	7.51:1	7.51:1	6.98:1	6.98:1	8.57:1
Stroke (cm)	13.18	13.22	13.22	12.84	12.84	12.84	12.84	12.84	11.94	11.94	13.18
Compressed Volume (cm ³)	25.26	26.84	26.84	28.63	28.63	28.63	28.63	28.63	28.98	28.98	25.26
Expanded Volume (cm ³)	216.52	218.79	218.79	215.01	215.01	215.01	215.01	215.01	202.24	202.24	216.52
Ignition Energy (mJ)	106	106	106	106	106	106	265	177	106	106	106
Experiment #	803-3a	803-2b	803-3b	814-1a	814-1b	814-2a	814-2b	414-6	315*	420-9	
Equivalence Ratio	0.586	0.586	0.605	0.611	0.605	0.602	0.615	0.577	0.795	0.923	
τ_i (msec)	6.7	10.5	4.1	7.7	7.2	6.7	6.4	8.5	2.4	<1.0	
Driver Pressure (kPa)	1105	1105	1105	1105	1105	1105	1105	622	750	750	
Approx. Expansion Speed (rpm)	1580	1580	1875	2300	2300	2300	2300	750	1460	830	
Compression Ratio	6.98:1	6.98:1	6.98:1	6.98:1	6.98:1	6.98:1	6.98:1	8.2:1	8.2:1	8.2:1	
Stroke (cm)	11.94	11.94	11.94	11.94	11.94	11.94	11.94	13.18	13.18	13.18	
Compressed Volume (cm ³)	28.98	28.98	28.98	28.98	28.98	28.98	28.98	26.50	26.50	26.50	
Expanded Volume (cm ³)	202.24	202.24	202.24	202.24	202.24	202.24	202.24	217.77	217.77	217.77	
Ignition Energy (mJ)	106	106	106	106	106	106	106	106	106	106	

Fuel: Methane-Air
 Camera Speed: 6000 frames/sec
 Film: Kodak Tri-X reversal
 *Kodak Ektachrome EF 7241

Schlieren Stop: 2.11 mm dia. solid aperture
 *color stop #101
 Initial Pressure: 105 kPa
 Initial Temperature: 300 K

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Figure 4.4. Variation of volume expansion rate at quenching with ignition timing parameter τ , defined by Equation 4.1. $\phi = 0.557$ laminar expansions with ignition energy of 106 mJ except as noted.

□ - 1105 kPa driver pressure
○ - 750 kPa driver pressure

◇ - 533 kPa driver pressure
▽ - 320 kPa driver pressure

Figure 4.5, for different expansion driver pressures, the volume expansion rate will differ at constant θ . During the initial part of the expansion, where the piston speed increases as the piston is withdrawn, higher driver pressures result in a higher rate volume expansion at a given value of θ . Therefore, when the quenching of mixtures of identical initial composition are compared over a range of driver pressures one would not expect a correlation with both the volume expansion rate and ratio.

Figures 4.6 and 4.7 ($\phi = 0.586$) and Figures 4.8 and 4.9 ($\phi = 0.605$ except as noted) illustrate the same general trend. The lack of correlation between the occurrence of quenching and the volume expansion rate is less apparent in Figures 4.7 and 4.9 due to the fact that most experiments on these richer mixtures were conducted at the highest driver pressure available, 1105 kPa. It is necessary to use this driver pressure to insure that, while maintaining τ_i above the value for which $\theta_{s=0}$ is not affected, the expansion is rapid enough so that quenching occurs before the flame front is substantially influenced by chamber walls. Even at the highest driver pressure available, the influence of the chamber walls on the quenching process may be observed in the points for $\tau_i > 6$ msec in Figures 4.8 and 4.9. This will become apparent in the later discussion of the effect of equivalence ratio on the quenching process.

In addition to the experimental limitations on the observation of bulk quenching for relatively rich ($\phi > 0.6$) mixtures described previously, the reader should note that for relatively lean mixtures ($\phi < 0.577$) the determination of the quenching point where $s=0$ is difficult due to scatter in the measurement of unburned volume. In

Figure 4.5. Piston trajectory for typical laminar expansions at:

- - 1105 kPa driver pressure
- ▽ - 320 kPa driver pressure.

Figure 4.6. Variation of volume expansion ratio at quenching with the ignition timing parameter τ_i , defined by Equation 4.1. $\phi = 0.586$ laminar expansions. Driver pressure is 1105 kPa.

Figure 4.7. Variation of volume expansion rate at quenching with ignition timing parameter τ_i , defined by Equation 4.1. $\phi = 0.586$ laminar expansions; driver pressure = 1105 kPa.

Figure 4.8. Variation of volume expansion ratio at quenching with the ignition timing parameter θ_s , defined by Equation 4.1. $\phi = 0.605$ laminar expansions except as noted. Driver pressure is 1105 kPa.

Figure 4.9. Variation of volume expansion rate at quenching with ignition timing parameter τ_i , defined by Equation 4.1. $\phi = 0.605$ laminar expansions except as otherwise noted. Driver pressure is 1105 kPa.

order to obtain several sequential values of the function $\ln(P^{1/\gamma} V_u)$ necessary to evaluate the derivative of Equation 3.6, the time interval between volume measurements is often limited to ~ 1 msec. Since the laminar flame speed of these lean mixtures is very low, this effect results in taking a small difference between two sequential large values of V_u . The impact of this practice on data quality is most obvious in the comparison of Figures 4.3 and 4.8.

Finally, it should be noted that the value of τ_i for which $\theta_{s=0}$ becomes independent of τ_i , denoted τ_i^* in Figures 4.3-4.9, is dependent on the mixture equivalence ratio; richer mixtures resulting in lower values of τ_i^* . For a $\phi = 0.577$ mixture, $6 \leq \tau_i^* \leq 8$ msec, while for mixtures of $\phi = 0.686$ and 0.605 $4.3 < \tau_i^* < 6.8$ msec and $4.1 < \tau_i^* < 6.4$ msec respectively.

Two experiments were conducted in which ignition energies greater than the normal 106 mJ were used. Results are displayed in Figure 4.3. The points of interest are annotated with their ignition energies. Both points fall within the scatter of data for this relatively lean mixture. Since the effect of increased ignition energy would be expected to be most apparent at the small values of τ_i and lean mixtures used, and since there is no correlation whatever between $\theta_{s=0}$ and the ignition energy, it is concluded that this is not an important parameter in the quenching process.

In the course of this study, attempts were made to quench mixtures considerably richer than those discussed so far by means of laminar expansion. For mixtures of $\phi = 0.795$ and 0.923 , we were unable to quench the reacting mixture. Schlieren images of the flame front position for the $\phi = 0.923$ case are presented in Figure 4.10a,

with an interval between frames of 2.5 msec. This flame displays much the same behavior as the equivalent constant volume duct case, Figure 4.1b. Effects of Taylor instability on flame front shape are noticeable beginning with frame 8. In a $\phi = 0.795$ case (#315, Table 4.2), the piston was fully withdrawn yielding an 8.2 fold volume increase ($\theta = 7.2$) before the reactant mixture was completely consumed. No Taylor instability was noticed, probably due to the faster expansion rate and slower laminar flame speed. This would tend to reduce the magnitude of the unfavorable pressure gradient, or perhaps eliminate it altogether.

Schlieren photographs of flame propagation for a quenched flame (#512-2, Table 4.2) are displayed in Figure 4.10b. The time interval between frames is 1.67 msec. Based on the criterion of Eq. 3.6, quenching occurs approximately at frame 9, following which the schlieren image grows due to expansion of the chamber volume along with dissipation of the thermal gradients due to conduction. The variation of the volume expansion ratio at quenching with equivalence ratio is displayed in Figure 4.11. Only points for which $\tau_i \geq \tau_i^*$ are included. The fall-off in the curve for $\phi > 0.60$ is probably due to the fact that a considerable portion of the flame front is in close proximity to the chamber walls at the time of quenching. Thus, flame extinguishment may be only partly due to mechanisms acting in the bulk gas. This apparently results in quenching at lower values of volume expansion ratio than would otherwise be observed. Flame proximity to chamber walls at quenching is displayed in Figure 4.12 for $\phi = 0.601, 0.605, 0.611$, and 0.615 mixtures. Notice that for mixtures of $\phi \geq 0.605$, the flame front at the instant of quenching lies well within the laminar flame quenching distance of the piston face (Andrew and Bradley, 1972).

Figure 4.10a. Flame propagation in a laminar expansion. $\phi = 0.923$. Case 420-9, Table 4.2. Frames at 2.5 msec. intervals.

Figure 4.10b. Flame propagation in a laminar expansion. $\phi = 0.591$. Case 512-2, Table 4.2. Frames at 1.67 msec. intervals.

Figure 4.11. Variation of volume expansion ratio at quenching with the equivalence ratio for laminar expansions with $\tau_i \geq \tau_i^*$.

- - 1105 kPa driver pressure
- - 750 kPa driver pressure
- ▽ - 320 kPa driver pressure

$$\phi = 0.601$$

CASE : 814-2a

$$\phi = 0.605$$

CASE : 814-1b

$$\phi = 0.611$$

CASE : 814-1a

$$\phi = 0.615$$

CASE : 814-2b

Figure 4.12. Pictorial representation of flame front and piston position at quenching for several laminar expansions. The distance from the broken line to the piston face is the quenching distance (Andrews and Bradley, 1972).

Figure 4.13 shows the variation of the volume expansion rate at quenching with equivalence ratio. As in Figure 4.11, only points for which $\tau_i > \tau_i^*$ are included. Note the divergence of the points at $\phi = 0.577$ as compared to Figure 4.11. As explained earlier, this is due to the fact that at a given θ , higher driver pressures result in a greater volume expansion rate.

To summarize the results of investigation into the bulk quenching process during a laminar expansion, the following points may be made:

- 1) For $\tau_i < \tau_i^*$, a longer interval between ignition and the onset of expansion results in higher degree of volume expansion necessary for quenching. For $\tau_i > \tau_i^*$, the degree of volume expansion at which quenching is observed is independent of τ_i . τ_i^* is a function of the equivalence ratio, and probably the initial pressure and temperature as well.
- 2) The volume expansion ratio for quenching is independent of ignition energy for energies between 106 mJ and 265 mJ for the line ignitor used in this study.
- 3) The amount of volume expansion seems to be a parameter of more fundamental importance to the bulk quenching process than does the rate of volume expansion.

Considerable difficulty was encountered in quenching a reacting mixture undergoing a compression-expansion sequence. The principal reason for this is the existence of a turbulent zone near the piston face, resulting from the scraping-up of the momentum boundary layer along the chamber walls by the piston during compression. This is illustrated by Figure 4.14, extracted from Oppenheim, et al. (1976). Notice that for a compression ratio of 8.5:1 the turbulent regime

Figure 4.13. Variation of the volume expansion rate at quenching with the equivalence ratio for laminar expansions with $\tau_i \geq \tau_i^*$.

- - 1105 kPa driver pressure
- - 750 kPa driver pressure
- ▽ - 320 kPa driver pressure

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Figure 4.14. Cinematographic sequence of schlieren photographs of rolling vortex. Compression ratio: 8.5:1; Stroke: 13.3 cm.

occupies a significant part of the total chamber volume so that the flame front has only to travel a short distance to penetrate this zone. In addition, the leak rate by the piston is increased substantially relative to the laminar expansion because the maximum pressure gradient across the seals increases by an order of magnitude. This leads to difficulties in the data reduction. As a result, conclusions regarding bulk quenching in a compression-expansion case are largely qualitative.

Experimental conditions for compression-expansions conducted as part of this study are presented in Table 4.3. As can be seen from Figure 4.15, quenching was not observed in a $\phi = 0.712$ mixture. Sequential flame front traces for this case are presented in Figure 4.16. Notice that the flame speed initially decreases as the piston is withdrawn; however, at frame 60 the flame speed begins to increase in spite of the expansion. This coincides with penetration of the roll-up vortex turbulence zone by the flame front, as is indicated by the wrinkling of the flame front trace subsequent to frame 60 in Figure 4.16.

Quenching was observed for a $\phi = 0.496$ mixture (case 805-1a, Table 4.3). Although the high leak rate from the chamber prevents quantitative determination of the time of quenching, the volume expansion ratio at quenching is estimated to be approximately one from the schlieren photographs.

Quenching is complete before the flame front is able to propagate into the turbulent zone near the piston face. For an identical mixture (case 805-1b, Table 4.3) no quenching was observed when the spark was advanced from $\tau_i = 0.6$ to ~ 8 msec. In this case, the flame front

TABLE 4.3

Experimental Conditions - Compression-Expansions

Experiment #	011*	805-1a	805-1b
Equivalence Ratio	0.712	0.496	0.496
τ_i (msec)	~ 1	0.6	~ 8
Driver Pressure (kPa)	960	1105	1105
Equivalent Speed (rpm)	1250	1580	1030
Compression Ratio	8.52:1	6.98:1	6.98:1
Stroke (cm)	13.20	11.94	11.94
Compressed Volume (cm ³)	25.48	28.98	28.98
Expanded Volume (cm ³)	217.10	202.24	202.24
Ignition Energy (mJ)	3	106	106

Fuel: Methane-Air

Camera Speed: 6000 frames/sec

Film: Kodak Tri-X Reversal

*Kodak Ektachrome EF 7241

Schlieren Stop: 2.11 mm dia. solid aperture

*Color stop #71

Ignitor: Line ignitor

*NGK C-GH spark plug

Initial Pressure: 105 kPa

Initial Temperature 300 K

Figure 4.15. Flame speed versus time for compression-expansion Case 011, Table 4.3. $\phi = 0.712$.

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FLAME FRONT POSITION (frame number $\times 10^{-1}$)

METHANE / AIR CASE 011

Figure 4.16. A plot of flame front and piston position versus film frame number for a $\phi = 0.712$ compression-expansion; Case 011, Table 4.3. Appearance of the ignition spark identifies frame zero.

was able to penetrate the turbulent zone before extinguishment.

In summary, quenching was never observed in compression-expansion experiments once the flame front propagated into the turbulent zone caused by the roll-up vortex. Bulk quenching was observed for a $\phi = 0.496$ mixture and compression ratio of 6.98:1 at a volume expansion ratio of order 1, provided that ignition is retarded or expansion is sufficiently rapid so that the chamber volume may be doubled before the flame front reaches the turbulent regime.

CHAPTER 5

Discussion

To understand the effect of ignition timing on the bulk quenching process it is helpful to invoke arguments of minimum flame kernel size. These arguments are based on consideration of the conservation equations for mass and energy across a flame front of diverging geometry.

In the steady, adiabatic propagation of a plane wave flame front, a mass element crossing the front receives a given amount of energy by means of conduction as it traverses the pre-heat zone. After burning, it then gives up the same amount of energy to the unburned gas via conduction. Thus, there is no net enthalpy change over and above that brought about due to chemical reaction and the final temperature of this mass element is the adiabatic flame temperature. In a divergent geometry (such that the radius of curvature of the flame front is small compared to the characteristic length of the system) the mass element gives up more energy to the unburned gases. As a result, its final temperature is lower than the adiabatic flame temperature calculated from purely thermodynamic considerations. This phenomenon is illustrated in Figure 5.1 for a spherical volume element. The total heat flux conducted into the volume across the surface $r = r_0$ as the flame front approaches r_0 will be less than that lost across the surface $r = r_1$ as the flame front passes r_1 . Whereas the heat flux per unit area as given by the conduction equation

$$q = k \nabla T \quad (5.1)$$

Figure 5.1. Pictorial representation of a spherically propagating flame front. The volume element is bounded by the surfaces A_0 and A_1 .

is approximately constant, the areas across which the conduction occurs is proportional to r^2 so that the total heat flux at $r = r_1$ exceeds that at $r = r_0$. Clearly, for a given radius of curvature, this effect will be more significant for a spherical geometry ($A \propto r^2$) than for a cylindrical geometry ($A \propto r$). As the radius of curvature of the flame front is decreased, there will exist a point where a balance between loss by conduction and heat production by chemical reaction can just be maintained. This is referred to as the minimum flame kernel size. A flame kernel smaller than this will be quenched by the unburned gas itself.

The Karlovitz number K is a dimensionless quantity that is frequently used as a measure of flame stretch (Karlovitz, et al., 1953). In order to serve as a similarity variable for the process described in the preceding paragraph, the Karlovitz number must serve to measure the net heat deficit as a result of the diverging flame front. With reference to Figure 5.1 and Equation 5.1, the heat conducted across the flame front at $r = r_0$ is given by $q A_0 \Delta t$ where Δt represents the time interval over which the heat flux occurs. Thus Δt will be proportional to the thickness of the preheat zone. Thus,

$$K = \frac{A_1 - A_0}{A_0} = \frac{A_1}{A_0} - 1 \quad (5.2)$$

where A_0 and A_1 are defined as areas subtended by a unit solid angle and separated by the width of the preheat zone η_0 .

The width of the preheat zone may be approximated as

$$\eta_0 = T_1 - T_u \left(\frac{dT}{dx} \right)_1 \quad (5.3)$$

where T_u represents the temperature of the unburned gas, T_1 represents the temperature of the inflection point in Figure 5.2, and $\left(\frac{dT}{dx} \right)_1$ is the temperature gradient normal to the flame front surface evaluated at

Figure 5.2. Schematic representation of the temperature profile across a flame front.

the inflection point. The point of inflection on the T versus X curve, denoted T_i in Figure 5.2 represents the boundary between regions of net heat liberation $\left(\frac{d^2T}{dx^2} < 0\right)$ and net heat adsorption $\left(\frac{d^2T}{dx^2} > 0\right)$, and as such is used to define the pre-heat zone.

η_0 has been related to measurable data by Lewis and Von Elbe (1961) by means of the conservation equations for a plane, adiabatic wave.

Their expression is

$$\eta_0 = \frac{k}{C_p \rho_u S_u} \quad (5.4)$$

where k represents the thermal conductivity, C_p the heat capacity at constant pressure, ρ_u the density of the unburned gas and S_u the flame speed with respect to unburned gas.

An expression for the Karlovitz number may be calculated for the desired geometry from Equation 5.2. For a spherical geometry

$$K_{\text{sphere}} = \frac{\pi(d^2 + 2\eta_0 \frac{\rho_u}{\rho_b})^2}{\pi d^2} - 1 \sim 4 \frac{\eta_0(\rho_u)}{d} \left(\frac{\rho_u}{\rho_b}\right) \quad (5.5)$$

The ratio of densities accounts for expansion between surfaces due to combustion and terms of order $\left(\frac{\eta_0}{d}\right)^2$ have been dropped since η_0 is typically much smaller than the kernel diameter, d . For a cylindrical geometry

$$K_{\text{cyl}} = \frac{\pi(d + 2\eta_0 \frac{\rho_u}{\rho_b})\ell}{\pi d \ell} = 2 \frac{\eta_0}{d} \left(\frac{\rho_u}{\rho_b}\right) \quad (5.6)$$

Note that $K_{\text{cyl}} = \frac{1}{2} K_{\text{sphere}}$. For a planar geometry $A_0 = A_1$ so that $K_{\text{planar}} \equiv 0$.

Since K increases as the flame stretch effect increases, there should be some critical value of K above which the flame will not propagate. This corresponds to the minimum flame kernel diameter, d_{cr} ,

through Equation 5.5 or 5.6.

The critical Karlovitz number for a spherical geometry is plotted against equivalence ratio in Figure 5.3. Data utilized in the calculation were taken from Lewis and Von Elbe (1961) except for values of the critical flame kernel diameter and the flame speed which were taken from a more recent review (Andrews and Bradley, 1971), and is summarized in Table 5.1. It is seen that the data fall in the range $0.5 \leq K_{cr} \leq 1.0$. Further, this data shows fair agreement with K_{cr} values calculated from geometrically different experiments such as blowout at the entrance to a diverging nozzle.

The initial size of the flame kernel produced by the line ignition source used in this study may be estimated from the schlieren image on the first frame after ignition. This portrays the flame kernel of some time in the interval $0 \leq t \leq 133 \mu\text{sec}$, where $t = 0$ is taken at the moment of ignition. This measurement has been performed for a large number of cases, yielding image sizes over the range $3.0 \leq d \leq 3.5 \text{ mm}$. Of these, the smallest should be closest to the true image size at $t = 0$.

The high sensitivity ($\sim 260 \text{ K/cm}$) of the schlieren system results in the pre-heat zone adjacent to the flame front being included in the schlieren image. To correct for this effect, the schlieren image size d' was corrected by subtracting $2\eta_0$, yielding within a close approximation the true initial flame kernel size d

$$d = d' - 2\eta_0 = (.30 - 2\eta_0)\text{cm} \quad (5.7)$$

For the experimental conditions of interest in this study, η_0 varies over the range $.012 \leq \eta_0 \leq .015 \text{ cm}$, resulting in initial flame kernel sizes of $d \sim 0.27 \text{ cm}$. Since the gap spacing of the line ignition

TABLE 5.1. Data used in the calculation of the critical Karlovitz number.

x_{CH_4}	ϕ	S_u (cm/sec)	T_b (K)	$k \times 10^5$ (cal/sec·cm·K)	C_p (cal/g·K)	$\rho_u \times 10^3$ (g/cm ³)	ρ_u/ρ_b	$\eta_o \times 10^3$ (cm)	d_{cr} (cm)	K_{cr}
.0543	0.547	11.6*	1568 [†]	6.5	.30	1.14	5.2	16.4	.65*	.52
.0593	0.6	15.6*	1665 [†]	6.5	.30	1.14	5.6	12.2	.34*	.80
.0684	0.7	22.1*	1900	6.5	.30	1.14	6.3	8.6	.22*	.98
.0776	0.8	28.7*	2000	6.5	.31	1.14	6.7	6.4	.18*	.95
.0862	0.9	35.3*	2150	6.5	.32	1.13	7.2	5.1	.17*	.86
.0950	1.0	43.3*	2250	6.5	.32	1.12	7.5	4.2	.18*	.70

$$\theta = 0$$

$$p_o = 105 \text{ kPa}$$

$$T_o = 300 \text{ K}$$

*Values taken from Andrews and Bradley, 1972.

[†]Values taken from Gordon and McBride, 1971.

Values for η_o and K_{cr} calculated from Equations 5.4 and 5.5.

All other values taken from Lewis and Von Elbe, 1961.

Figure 5.3. A plot of Karlovitz number versus equivalence ratio for conditions of Tables 5.1, 5.2 and 5.3.
 I - K for expanding Kernel, $\theta = 0.1$, evaluated over $\tau_{\text{min}}^* < t < \tau_{\text{max}}^*$ (see Table 5.3)
 ○ - K_{critical} (see Table 5.1)
 □ - K for minimum kernel diameter, $\theta = 0$ (see Table 5.2)
 ◇ - K for minimum kernel diameter, $\theta = 0.1$ (see Table 5.2)

source is 0.224 cm, it is apparent that the flame kernel evolving from the line ignitor is better represented in a cylindrical geometry as the individual kernels (if they exist separately at all) conduct no heat across their adjacent sides. Accordingly, Equation 5.6 is used to calculate the Karlovitz number in cases using the line ignitor.

Results of Karlovitz number calculations for the experimental conditions of Figures 4.3, 4.6, and 4.8 and the initial flame kernel size as given by Equation 5.7, are summarized in Table 5.2. Calculations were performed using the laminar expansion initial conditions ($\theta = 0$) of $T = 300$ K and $P = 105$ kPa and the laminar expansion conditions at $\theta = 0.1$ as calculated from Equation 3.4 and the perfect gas law. For the $\theta = 0$ cases, the calculated Karlovitz number should be below the critical Karlovitz number, since these mixtures were all observed to burn to completion in the absence of piston withdrawal. As can be seen from Figure 5.3, this is indeed the case. For the $\theta = 0.1$ cases, K increases due primarily to the decrease in ρ_u . Notice from Table 5.2 that the flame speed and adiabatic flame temperature (T_b) are practically unaffected by expansion. In the case of the flame speed, calculated from the correlation of Andrews and Bradley, 1971

$$S_u = (10 + 3.71 \times 10^{-4} T_u^2) P^{-1/2} \left(\frac{S_u^0}{43.3} \right) \quad (5.8)$$

the effects of decreasing temperature and pressure during the expansion nearly cancel. In Equation 5.8, S_u^0 represents the flame speed at standard conditions of $P = 105$ kPa and $T = 300$ K for a given equivalence ratio. The small change observed in T_b reflects the fact that since for the methane-air system there is practically no change in the number of moles during combustion, the adiabatic flame temperature is essentially

TABLE 5.2. Data used in the calculation of the Karlovitz number for the initial flame kernel size produced by the line ignition source at 106 mJ ignition energy.

x_{CH_4}	ϕ	S_u^* (cm/sec)	$T_b^\dagger$ (K)	$k \times 10^5$ (cal/sec·cm·K)	C_p (cal/g·K)	$\rho_u \times 10^3$ (g/cm ³)	ρ_u/ρ_b	$\eta_o \times 10^3$ (cm)	d (cm)	K_{cr}
.0571	0.577	14.1	1624	6.5	.30	1.14	5.4	13.5	.266	.55
.0580	0.586	14.6	1641	6.5	.30	1.14	5.5	13.1	.268	.54
.0598	0.605	16.1	1676	6.5	.30	1.14	5.6	11.9	.272	.49
(θ = 0, P = 105 kPa, T _u = 300 K)										
.0571	0.577	14.2	1613	6.4	.30	1.04	5.6	14.5	.266	.61
.0580	0.586	14.6	1630	6.4	.30	1.04	5.7	14.0	.268	.60
.0598	0.605	16.1	1665	6.4	.30	1.04	5.8	12.7	.272	.54
(θ = 0, P = 91 kPa, T _u = 298 K)										

*Values taken from Andrews and Bradley, 1972.

†Values taken from Gordon and McBride, 1971.

Values for η_o , d and K calculated from Equations 5.4, 5.7 and 5.6.

All other values taken from Lewis and Von Elbe, 1961.

independent of pressure. The K values calculated for these cases appear to be somewhat low. As can be seen from Figure 5.3, the $\phi = 0.577$ case is approaching the critical value of K. This is satisfying since according to Figure 4.3, a $\phi = 0.577$ mixture is observed to quench $\theta = 0.125$.

To determine a value of the Karlovitz number for less than which the bulk quenching process is independent of flame kernel size (i.e. K evaluated with $d(t) = d(\tau_i^*)$) it is necessary to allow for growth of the kernel from its initial size. From Equations 3.1 and 3.2 one may write

$$S = \frac{1}{\rho_u A_f} \left(\frac{d\rho_b}{dt} V_b + \rho_b \frac{dV_b}{dt} \right) \quad (5.9)$$

Assuming a cylindrical flame kernel as explained earlier, Equation 5.9 may be written

$$\frac{dr}{dt} + r \frac{1}{2} \frac{d \ln \rho_b}{dt} = \frac{\rho_u}{\rho_b} S \quad (5.10)$$

This linear differential equation may be solved using the integrating factor $\beta = \rho_b^{1/2}$ yielding

$$r = \rho_b^{-1/2} \int_t \rho_u \rho_b^{-1/2} S dt \quad (5.11)$$

Assuming that piston withdrawal begins at $t = 0$ and continues at a constant rate until $t = \tau_i^*$ (at which time $\theta = 0.1$ by the definition of τ_i^* , Equation 4.1), ρ_u may be expressed as

$$\rho_u(t) = \frac{\bar{M}_u P_0 (1.1) \tau_i^*}{RT_0 t} \quad (5.12)$$

by means of the adiabatic expansion relationship 3.4 and the perfect gas law. Since the adiabatic flame temperature changes less than 2 percent

for a $\theta = 0.1$ expansion we may assume $T_b \sim T_{ad}^0 = \text{constant}$ where T_{ad}^0 represents the adiabatic flame temperature with initial conditions T_0 and P_0 . Thus

$$\rho_b(t) = \frac{\bar{M}_b P_0}{RT_{ad}^0} (1.1 \frac{t}{\tau_i^*})^{-\gamma} \quad (5.13)$$

We may also assume that $S \sim S^0 = \text{constant}$ since, as explained earlier, for an adiabatic expansion the effects of pressure and temperature change nearly cancel. Equation 5.11 is now easily integrated with initial condition $r(t = 0) = r_0$.

$$r(t) \sim \left(\frac{\bar{M}_u T_{ad}^0}{\bar{M}_b T_0 \gamma} \right) \left(\frac{1.1}{\tau_i^*} \right)^{\gamma-1} S t^\gamma + r_0 \quad (5.14)$$

$r(\tau_i^*)$ is given by

$$r(\tau_i^*) \sim \left(\frac{T_{ad}^0}{T_0 \gamma} \right) (1.1)^{\gamma-1} S \tau_i^* + r_0 \quad (5.15)$$

where the ratio of molecular weights has been dropped since it is very close to unity.

Equation 5.15 has been applied to the experimental cases of Figures 4.3, 4.6 and 4.8. As stated in Chapter 4, τ_i^* (the value of τ_i such that for $\tau_i \geq \tau_i^*$ the bulk quenching process is independent of τ_i) is known to within the following limits:

$\phi = 0.577$	$6 \leq \tau_i^* \leq 8 \text{ msec}$
$\phi = 0.586$	$4.3 \leq \tau_i^* \leq 6.8 \text{ msec}$
$\phi = 0.605$	$4.1 \leq \tau_i^* \leq 6.4 \text{ msec.}$

Values of the flame kernel size d and the Karlovitz number K evaluated at $t = \tau_{i_{\max}}^*$ and $\tau_{i_{\min}}^*$ are presented in Table 5.3. As shown by Figure

TABLE 5.3. Data used in the calculation of the minimum Karlovitz number $K(\tau_i^*)$ for which flame stretch effects the bulk quenching process.

x_{CH_4}	ϕ	S_u (cm/sec)	T_b (K)	ρ_u/ρ_b	$\eta_o \times 10^3$ (cm)	$\tau_i^* \times 10^3$ (sec)	$d(t = \tau_i^*)$ (cm)	$K(t = \tau_i^*)$
.0571	0.577	14.2	1613	5.6	14.5	> 6.0, < 8.0	> .97, < 1.21	< .17, > .13
.0580	0.586	14.6	1630	5.7	14.0	> 4.3, < 6.8	> .80, < 1.10	< .20, > .15
.0598	0.605	16.1	1665	5.8	12.7	> 4.1, < 6.4	> .84, < 1.16	< .18, > .13

$$\theta = 0.1 \quad k = 6.4 \times 10^{-5} \text{ cal/sec}\cdot\text{cm}\cdot\text{K}$$

$$P = 91 \text{ kPa} \quad C_p = 0.30 \text{ cal/g}\cdot\text{K}$$

$$T_u = 289 \text{ K} \quad \rho_u = 1.04 \times 10^{-3} \text{ g/cm}^3$$

Values for τ_i^* extracted from Chapter 4.

Values for d and K calculated from Equations 5.15 and 5.7.

All other values extracted from Table 5.2.

5.3, $K \left|_{t = \tau_{ij}^*} \right.$ is far below the critical value for all cases.

Apparently, flame stretch has a very significant impact on the bulk quenching process. Figure 5.3 indicates that noticeable contributions to flame quenching are made by flame stretch for $K > 0.2$ while for $K < 0.15$ such contributions are negligible, so that all the observations presented in Chapter 4 regarding ignition timing may be summarized in one sentence. If the Karlovitz number $K \leq 0.15$, the bulk quenching process will not be influenced by ignition timing.

The independence of the bulk quenching process and initial flame kernel growth from the magnitude of ignition energy observed in this study for ignition energies between 106 mJ and 265 mJ has also been observed by others (Laderman, Urtiew and Oppenheim, 1962). One would expect these processes to be independent of ignition energy until the energy deposited in the gas is either strong enough to generate a pressure wave affecting the state of the unburned mixture or so weak that the mixture cannot be ignited. Hydrocarbon-air mixtures at atmospheric pressure have minimum ignition energies of 0.2 to 0.3 mJ (Gaydon and Wolfhard, 1970). Thus, the ignition energy deposited in each gap of the line source exceeds the minimum ignition energy by a factor of at least 20. Apparently even this large ignition energy is not sufficient to disturb significantly the state of the unburned gas.

Figure 5.4 illustrates an interesting feature of the bulk quenching process under study. It consists of a plot of mixture equivalence ratio against the adiabatic flame temperature of the unburned gas under the conditions at which quenching has been observed in this study. Circular points represent laminar expansion cases (taken from Figure 4.11), the diamond shaped point represents the quenched

Figure 5.4. Variation of adiabatic flame temperature of unburned gas at quenching with equivalence ratio.

- - Laminar expansions; see Figure 4.11 for conditions.
- - No expansion; lean flammability limit at $P=105$ kPa and $T=300$ K.
- ◇ - Compression-Expansion; consult text of Chapter 4 for conditions.

compression-expansion case referred to in Chapter 4, and the square point represents the lean flammability limit at 105 kPa and 300 K.

The flame temperature for adiabatic, constant pressure combustion has been calculated by means of a computer code developed by Gordon and McBride (1971) using as initial conditions the temperature and pressure of the unburned gas at the moment of quenching, or in the case of the lean flammability limit, 300 K and 105 kPa. These conditions were calculated from the experimentally observed expansion ratio at quenching, $\theta_{s=0}$, by means of the adiabatic compression-expansion relationship, Equation 3.4, and the perfect gas law. The assumptions involved in this procedure are those already stated in Chapter 3. Note that the adiabatic flame temperature is approximately 1600 K in all cases except those for which wall effects have been observed ($\phi \geq 0.605$). As expected, the latter points exhibit a deviation in the direction of higher adiabatic flame temperature.

The correlation observed between the adiabatic flame temperature of the unburned mixture and the bulk quenching process is not unexpected, since many flames exhibit flammability limits (both rich and lean) that correspond to a certain minimum value of the adiabatic flame temperature. For methane-air mixtures, this is reported to correspond to a temperature of approximately 1400 K (Gaydon and Wolfhard, 1970). The 200 K discrepancy between this value and our result is probably related to the fact that the lean flammability limit ($P = 105$ kPa and $T = 300$ K) in our apparatus, $\phi = 0.563$, is somewhat higher than the literature value, $\phi = 0.53$. This may well be due to the duct size used in the current study, since it has been reported that for a lean

limit methane-air flame ($P = 105$ kPa and $T = 300$ K) a duct diameter of about 5 cm is needed to eliminate wall effects on the flammability limit (Barnett and Hibbard, 1959). Further, when the chamber pressure is reduced (as in the laminar expansions) one would expect these effects to become more significant.

Figure 5.5 is a prediction of volume expansion ratio at quenching as a function of equivalence ratio for types of cases examined in this study. Predicted values of $\theta_{s=0}$ are based on the assumption that quenching occurs when the unburned gas has been cooled by expansion to such an extent that its adiabatic flame temperature is equal to 1606 K.

For the compression-expansion cases, initial conditions consist of a fully expanded chamber filled to a pressure of 105 kPa at 300 K. The value of ϕ at $\theta_{s=0} = 0$ represents the flammability limit mixture at conditions encountered after compression to top dead center. As in the experiment, initial conditions for the laminar expansion case consist of a fully compressed chamber filled to a pressure of 105 kPa at 300 K. $\phi = 0.563$ is the experimentally determined lean flammability limit under these conditions.

The triangular point represents the estimated value of $\theta_{s=0}$ for the compression-expansion case 805-1a (Table 4.3, 6.98:1 compression ratio). Circular points represent the laminar expansions of Figure 4.11. Deviation observed for laminar expansion cases of $\phi \geq 0.605$ is due to wall effects.

Figure 5.5. Prediction of volume expansion ratio at quenching as a function of equivalence ratio. Initial conditions are $P = 105$ kPa and $T = 300$ K. θ is defined by equation 4.2 with V_0 taken as the chamber volume at top dead center.

As explained in Chapter 4, these predictions are expected to be valid only for cases where spark timing and expansion rate combine to quench the flame before it comes in close proximity to a wall and, in the case of compression-expansions, before the turbulent region is penetrated.

In order to better understand the details of the bulk quenching process, it is helpful to review the results of a recent calculation of chemical and hydrodynamic properties in an expanding combustion chamber (Smith, Westbrook and Sawyer, 1977). The numerical model used is a one-dimensional, unsteady code for the solution of the governing conservation equations of mass, momentum, species and energy by means of implicit finite difference techniques. At a given time step, hydrodynamic variables such as temperature, density and velocity are determined by an implicit finite difference technique while the chemical species concentrations are determined by a different implicit technique more suited to the solution of stiff systems of differential equations. The two solutions are then combined by the method of operator splitting to give the overall solution. The chemical integrator made use of an extensive chemical mechanism, for which the rate constants are given in Table 5.4. The hydrodynamic code neglects wall heat loss and all boundary layer effects. This numerical technique and chemical mechanism have been used previously in a number of investigations of methane-air combustion (Westbrook and Chang, 1977; Westbrook, 1977; Westbrook, et al., 1977).

In the model, the flame front is considered to be a one-dimensional (planar) deflagration propagating normal to the axis of a combustion chamber of 0.2 cm length. The restriction to one-dimensional geometry

TABLE 5.4. Rate constants used in the study of Smith, Westbrook & Sawyer, 1977.

Rate constants ($k=AT^n\exp(-E_a/RT)$) in cm^3 , mole, K units

	Reaction	log A	n	E_a
1	$\text{CH}_4 + \text{M} = \text{CH}_3 + \text{H} + \text{M}$	17.30	0.	88.4
2	$\text{CH}_4 + \text{H} = \text{CH}_3 + \text{H}_2$	14.10	0.	11.9
3	$\text{CH}_4 + \text{OH} = \text{CH}_3 + \text{H}_2\text{O}$	12.50	0.	3.8
4	$\text{CH}_4 + \text{O} = \text{CH}_3 + \text{OH}$	13.30	0.	9.2
5	$\text{CO} + \text{HO}_2 = \text{CO}_2 + \text{OH}$	14.00	0.	23.0
6	$\text{HCO} + \text{OH} = \text{CO} + \text{H}_2\text{O}$	14.00	0.	0.0
7	$\text{CO} + \text{OH} = \text{H} + \text{CO}_2$	11.40	0.	1.1
8	$\text{H} + \text{O}_2 = \text{O} + \text{OH}$	14.34	0.	16.9
9	$\text{H}_2 + \text{O} = \text{H} + \text{OH}$	10.20	1.	8.9
10	$\text{O} + \text{H}_2\text{O} = \text{OH} + \text{OH}$	13.80	0.	18.4
11	$\text{H} + \text{H}_2\text{O} = \text{OH} + \text{H}_2$	13.98	0.	20.3
12	$\text{HCO} + \text{M} = \text{H} + \text{CO} + \text{M}$	14.10	0.	19.0
13	$\text{O} + \text{H} + \text{M} = \text{OH} + \text{M}$	16.00	0.	0.0
14	$\text{O} + \text{O} + \text{M} = \text{O}_2 + \text{M}$	15.70	-0.25	0.0
15	$\text{H}_2 + \text{M} = \text{H} + \text{H} + \text{M}$	14.34	0.	96.0
16	$\text{O}_2 + \text{H}_2 = \text{OH} + \text{OH}$	14.90	0.	45.0
17	$\text{NO} + \text{O} = \text{N} + \text{O}_2$	9.40	1.	38.6
18	$\text{N}_2 + \text{O} = \text{N} + \text{NO}$	14.15	0.	75.2
19	$\text{NO} + \text{M} = \text{N} + \text{O} + \text{M}$	20.60	-1.5	151.0
20	$\text{N}_2\text{O} + \text{M} = \text{N}_2 + \text{O} + \text{M}$	14.70	0.	58.0
21	$\text{NO} + \text{NO} = \text{N}_2\text{O} + \text{O}$	14.00	0.	76.0
22	$\text{NO}_2 + \text{M} = \text{NO} + \text{O} + \text{M}$	16.00	0.	65.0
23	$\text{NO} + \text{O}_2 = \text{NO}_2 + \text{O}$	12.00	0.5	45.5
24	$\text{N} + \text{OH} = \text{NO} + \text{H}$	13.60	0.	0.0

*See Westbrook and Chang, 1977, for references

	Reaction	log A	n	E _a
25	$\text{H}_2\text{O} + \text{M} = \text{H} + \text{OH} + \text{M}$	16.34	0.	105.1
26	$\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$	15.18	0.	-1.0
27	$\text{CO} + \text{O} + \text{M} = \text{CO}_2 + \text{M}$	15.77	0.	4.1
28	$\text{CO}_2 + \text{O} = \text{CO} + \text{O}_2$	13.28	0.	54.2
29	$\text{HCO} + \text{H} = \text{CO} + \text{H}_2$	14.30	0.	0.0
30	$\text{HCO} + \text{O} = \text{CO} + \text{OH}$	14.00	0.	0.0
31	$\text{CH}_2\text{O} + \text{M} = \text{HCO} + \text{H} + \text{M}$	16.70	0.	72.0
32	$\text{CH}_2\text{O} + \text{OH} = \text{HCO} + \text{H}_2\text{O}$	14.70	0.	6.3
33	$\text{CH}_2\text{O} + \text{H} = \text{HCO} + \text{H}_2$	13.10	0.	3.8
34	$\text{CH}_2\text{O} + \text{O} = \text{HCO} + \text{OH}$	13.70	0.	4.6
35	$\text{CH}_3 + \text{OH} = \text{CH}_2\text{O} + \text{H}_2$	12.60	0.	0.0
36	$\text{CH}_3 + \text{O} = \text{CH}_2\text{O} + \text{H}$	14.10	0.	2.0
37	$\text{CH}_3 + \text{O}_2 = \text{CH}_3\text{O} + \text{O}$	13.40	0.	29.0
38	$\text{CH}_3 + \text{CH}_2\text{O} = \text{HCO} + \text{CH}_4$	10.00	0.5	6.0
39	$\text{HCO} + \text{CH}_3 = \text{CH}_4 + \text{CO}$	11.50	0.5	0.0
40	$\text{CH}_3\text{O} + \text{M} = \text{CH}_2\text{O} + \text{H} + \text{M}$	13.70	0.	21.0
41	$\text{O} + \text{OH} + \text{M} = \text{HO}_2 + \text{M}$	17.00	0.	0.0
42	$\text{HO}_2 + \text{O} = \text{O}_2 + \text{OH}$	13.70	0.	1.0
43	$\text{HCO} + \text{HO}_2 = \text{CH}_2\text{O} + \text{O}_2$	14.00	0.	3.0
44	$\text{CH}_3\text{O} + \text{O}_2 = \text{CH}_2\text{O} + \text{HO}_2$	12.00	0.	0.6
45	$\text{CH}_3 + \text{HO}_2 = \text{CH}_4 + \text{O}_2$	12.00	0.	0.4
46	$\text{HCO} + \text{O}_2 = \text{CO} + \text{HO}_2$	12.48	0.	7.0
47	$\text{H} + \text{HO}_2 = \text{OH} + \text{OH}$	14.40	0.	1.9
48	$\text{H} + \text{HO}_2 = \text{H}_2 + \text{O}_2$	13.40	0.	0.7

	Reaction	log A	n	E _a
49	$\text{OH} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}_2$	13.70	0.	1.0
50	$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	12.30	0.	0.0
51	$\text{H}_2\text{O}_2 + \text{M} = \text{OH} + \text{OH} + \text{M}$	17.08	0.	45.5
52	$\text{H} + \text{H}_2\text{O}_2 = \text{HO}_2 + \text{H}_2$	12.23	0.	3.8
53	$\text{CH}_4 + \text{HO}_2 = \text{CH}_3 + \text{H}_2\text{O}_2$	12.70	0.	12.5
54	$\text{CH}_2\text{O} + \text{HO}_2 = \text{HCO} + \text{H}_2\text{O}_2$	12.00	0.	8.0
55	$\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$	13.00	0.	1.8

and very small chamber length is made to restrict the cost of the analysis to reasonable proportions, while allowing the inclusion of a full chemical kinetic mechanism and a sufficient number of spatial nodes to resolve gradients across the flame front. Twenty-five equally spaced nodes are utilized, resulting in about four spatial nodes within the flame front. Laminar values for the species diffusion coefficients and thermal conductivities were used.

The flammable mixture is ignited by introduction of energy into the spatial zone nearest the endwall at a constant rate of 1.46×10^8 J/gm-sec over a period of 35 μ sec. The ignition energy per unit of duct cross-section is more than 100 times greater than that of the line ignitor and is added over roughly twice the time interval.

Unlike the experiment, the model combustion chamber was expanded in a direction normal to the direction of flame propagation for reasons of practical consideration. As noted in Chapter 3, both piston motion and flame speed are so much slower than the sound speed in both experiment and model that the primary result of piston motion is to lower the gas density.

The nature of the simplifications made in this analysis regarding flame front geometry, chamber size, and ignition method make it unlikely that quantitative agreement with experimental results will be produced. Accordingly, the model is used to gain a qualitative insight into the details of the flame quenching process which the gross nature of the experimental information obtained in this study cannot provide.

A number of calculations have been performed on a $\phi = 0.86$ methane-air mixture initially at 298 K and 105 kPa. They consist of ignition at $t = 0$, followed by flame propagation without volume expansion

over the interval $0 \leq t \leq 685 \mu\text{sec}$, at which time the flame front (defined arbitrarily as the point where $T = 1500 \text{ K}$) has propagated 0.04 cm through the chamber. The flame front velocity is 46 cm/sec at this point. Various rates of volume increase were then introduced, ranging from no expansion (constant volume duct) to expansion at a constant rate by a factor of 9 over an interval of 685 μsec . An intermediate expansion resulting in a 9 fold volume increase over a 6.85 msec interval was also studied.

Some results from these calculations are displayed in Figures 5.6 through 5.21. In these figures, the solid line represents the unexpanded case, the closely spaced dotted line represents the intermediate rate expansion and the widely spaced dotted line represents the highest rate expansion. Flame front position and speed are plotted against time in Figures 5.6 and 5.7. The decrease in flame speed in the unexpanded case follows closely the $P^{-1/2}$ dependence given by Andrews and Bradley (1972).

The flame speed decreases dramatically once expansion is begun. Further, the slower rate expansion seems to retard the flame more, per unit of volume expansion, as seen by comparison of the points at $\theta = 1$ where the initial volume has been doubled. Whether this effect will disappear by the time quenching occurs as observed in the experimental study, is a matter of conjecture since the pertinent data for intermediate rate expansion are not available past 2 msec. The flame speed for this case does seem to exhibit a decreasing slope as expansion occurs, indicating that this could be the case. Although the concept of flame quenching cannot be strictly applied to a one-dimensional, adiabatic model, note that the flame speed in the rapidly expanded case is reduced

Figure 5.6. Theoretical flame front trajectory for a $\phi = 0.86$ mixture

— No expansion
 Moderate rate expansion
 Rapid expansion

Figure 5.7. Theoretical calculation of flame speed versus time for a $\phi = 0.86$ mixture.

— No expansion
 Moderate rate expansion
 Rapid expansion

Figure 5.8. Theoretical calculation of temperature versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate rate expansion
 - - - - - Rapid expansion

Figure 5.9. Theoretical calculation of density versus axial position for a $\phi = 0.86$ mixture.

- No expansion
- - - Moderate expansion rate
- Rapid expansion

Figure 5.10. Theoretical calculation of hydrogen atom mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate expansion rate
 Rapid expansion

Figure 5.11. Theoretical calculation of hydrogen molecule mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
..... Moderate expansion rate
- Rapid expansion

Figure 5.12. Theoretical calculation of hydroxyl radical mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate rate expansion
 Rapid expansion

Figure 5.13. Theoretical calculation of oxygen atom mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
..... Moderate expansion rate
- Rapid expansion

Figure 5.14. Theoretical calculation of peroxy radical mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
..... Moderate expansion rate
- Rapid expansion

Figure 5.15. Theoretical calculation of H₂O mole fraction versus axial position for a $\phi = 0.86$ mixture.

- No expansion
- Moderate expansion rate
- Rapid expansion

Figure 5.16. Theoretical calculation of H_2O_2 mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate expansion rate
 Rapid expansion

Figure 5.17. Theoretical calculation of HCO mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
..... Moderate rate expansion
..... Rapid expansion

Figure 5.18. Theoretical calculation of formaldehyde mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate rate expansion
 - Rapid expansion

Figure 5.19. Theoretical calculation of CH_3O mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
 Moderate rate expansion
 Rapid expansion

Figure 5.20. Theoretical calculation of carbon monoxide mole fraction versus axial position for a $\phi = 0.86$ mixture.

- No expansion
- Moderate rate expansion
- Rapid expansion

Figure 5.21. Theoretical calculation of carbon dioxide mole fraction versus axial position for a $\phi = 0.86$ mixture.

— No expansion
..... Moderate rate expansion
- Rapid expansion

to a few centimeters per second although according to Figure 5.3 such a result would not be expected for mixtures of $\phi > 0.64$ at $\theta = 8$ on the basis of experimental evidence.

Figures 5.6 through 5.19 portray variations in hydrodynamic and chemical properties over the chamber length. These figures are plotted for times such that, in each case, the flame front has propagated approximately 0.077 cm down the duct. For the unexpanded case this time is 1.57 msec after ignition, while for the intermediate and rapid rate expansions the appropriate times are 1.94 and 4.04 msec respectively. At these times, the rapid rate case is fully expanded (by a factor of 9) while the intermediate rate case is expanded by a factor of ~ 2.4 .

Figure 5.8 shows that the expansion process has little effect on the temperature distribution. This is a consequence of the very weak dependence of the adiabatic flame temperature on pressure. The abnormally high temperatures exhibited at the ignition end of the chamber result from the large ignition energy used. As indicated by Figure 5.9, expansion has a much greater effect on the mixture density.

Mole fraction distributions for a number of species are plotted in Figures 5.10 through 5.21. Note that in the region of the flame front most stable intermediate and radical species, including H_2 , HCO , CH_3 , CH_2O , HO_2 and CH_3O , reach their peak mole fraction. Mole fractions of O , OH and H are greatest in the post flame gas, where dissociation of H_2O at the very high temperatures observed there (~ 3000 K) contributes to their numbers. The relative mole fractions of these species are controlled by the nearly equilibrated H , O , OH shuffle reactions.

The large radical populations to the left of the flame front result

in diffusion of these species into the unburned gas, greatly decreasing the induction time of the unburned mixture. This is particularly true of the species O and OH, which are formed rapidly at the flame front via the reaction $H + O_2 \rightarrow O + OH$. These species diffuse from the high temperature post flame gasses as well. These species are usually short-lived, being destroyed in the induction zone by the fast reactions:

When the chamber is expanded, resulting in a lower mixture density, the rates of these bimolecular reactions decrease quadratically with the density. The rates of diffusion processes, however, decrease at a rate proportional to the density making the diffusion processes relatively faster in the expanded cases. This is responsible for the enhanced population of the hydrogen and oxygen atom, along with the hydroxyl radical, in the induction zone as indicated by Figures 5.10, 5.12, and 5.13. Indeed, these species show not only higher mole fractions, but higher concentrations as well in the induction zone for expanded cases.

The modeled flame seems to quench when, due to density decrease upon expansion, the induction reactions become so slow that they can

no longer soak up the diffusing radical species. Diffusional processes then stretch the flame structure, and the flame ceases propagation. This concept is consistent with the experimental observation that, in the bulk quenching process, the amount of volume expansion (density decrease) is a more fundamental parameter than the rate of volume expansion.

It is more difficult to find a fundamental connection between the role apparently played by density in the bulk quenching mechanism and the experimental observation that quenching occurs when the unburned gas is expanded to a state such that its adiabatic flame temperature is ~ 1600 K. These phenomena are not incompatible, however.

As explained earlier, the lowering of adiabatic flame temperature during expansion is almost entirely a consequence of initial temperature decrease in the unburned gas. This is expressed by Equation 3.4

$$TV^{\gamma-1} = \text{const.}$$

The sensitivity of initial temperature to volume expansion, and therefore to a close approximation of the sensitivity of the adiabatic flame temperature, is given by

$$dT = c(1 - \gamma) V^{-\gamma} dV \quad (5.16)$$

where $\gamma \sim 1.4$. Equation 5.16 indicates that the initial part of the expansion, where V is small, will produce a relatively large part of the total change in T during the expansion. This is responsible for the shape of the curves in Figure 5.5.

Note that the density is affected in a similar manner during expansion. At constant mole number, the density is inversely proportional to the volume so that

$$d\rho = -C V^{-2} dV \quad (5.17)$$

where C is a constant. The sensitivity of the density change on volume is just slightly greater than that of the temperature. For mixtures which are quenched early in the expansion ($\theta_{s=0} < 2$) this difference would probably not be detectable. Apparently this is the case in the current study, where the observation of quenching is limited to $0.1 \leq \theta_{s=0} \leq 1.4$.

To summarize the conclusions of this study, we may say that bulk quenching does indeed occur, having been directly observed for methane-air mixtures over the range $0.563 \leq \phi \leq 0.615$ in laminar expansions carried out as part of the current study. The range of conditions under which bulk quenching is observed in compression-expansion cases is greatly restricted due to the higher initial temperatures as a result of compression and the effect of turbulence.

Flame stretch was found to contribute to the bulk quenching process for Karlovitz numbers greater than 0.2. Within the limits of the Karlovitz number as a similarity variable, this conclusion should be valid for any fuel, ignitor, chamber geometry, etc.

The amount of volume expansion was found to be directly related to the bulk quenching process whereas the rate of volume expansion was not. Theoretical considerations indicate that this is because chemical processes become too slow in relation to diffusional processes (species diffusion and heat conduction) as the density is decreased. Finally, it was found that the amount of volume expansion necessary to produce quenching in the experimental system used may be approximated by the condition that the adiabatic flame temperature of the unburned gas (under the conditions of quenching) be equal to 1600 K.

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APPENDIX I

Input for program FILM:

<u>CARD</u>	<u>VARIABLE</u>	<u>FORMAT</u>	
1	D	E15.5	Image size of duct diameter (used to obtain the conversion factor between image size and actual duct size).
2	NFRAME	I10	Frame number
2	NPTS ¹	I10	Number of data points on NFRAME
2	YP	E10.3	Piston displacement from end wall
3	RX _j , RY _j ²	5(F6.4, 1x, F6.4, 2x)	Flame front coordinate pairs, $j = j_0 \rightarrow j_0 + 5$
$2 + \frac{\text{NPTS}}{5}$	"	"	" " " " " " $j \rightarrow j_{\text{NPTS}}$

Repeat cards 2 and 3 through $2 + \frac{\text{NPTS}}{5}$ for each frame analyzed.

Last card NPTS I10 Use any negative integer

¹If NPTS = 0, omit cards 3 through $2 + \frac{\text{NPTS}}{5}$

²Coordinate pairs RX_j and RY_j must proceed sequentially around the flame front, $j \leq 30$, RX_j ≠ RX_{j+1}.

Output from program FILM:

NFRAME = Frame number

YP = Piston displacement from endwall (cm)

VT = Total chamber volume (cm³)

VU = Volume of unburned gas (cm^3)

AF = Area of flame front (cm^2)

Subroutines ICSICU and DCSQDU are IMSL Library 3, Edition 5 routines (International Mathematical and Statistical Libraries, Inc., 1975) which approximate the curve defined by a set of points by the method of cubic splines, then compute the area under the curve.


```

PROGRAM FILM(INPUT,OUTPUT)

DIMENSION RX(30),RY(30)
CGMMCN/BLOCK1/X(30),Y(30),XSTART,XSTOP,MFLAG,VB,AF,D,MAX
DIA = 3.81

READ 10, D
C = DIA / D
PRINT 14

100 READ 11, NFRAME,NPTS,YP
    IF (NPTS.LT.0) GO TO 900
    IF (NPTS.EQ.0) GO TO 226

    DO 110 J=1,NPTS,5
110  READ 12, RX(J),RY(J),RX(J+1),RY(J+1),RX(J+2),RY(J+2),RX(J+3),RY(J+
    *3),RX(J+4),RY(J+4)

    N = NPTS - 1 $      K = 1 $      VB1 = AF1 = 0.

115  DO 120 J=K,N
    IF (RX(J).GE.RX(J+1)) GO TO 125
120  CONTINUE

    MFLAG = 1 $      GO TO 200
125  IF (J.EQ.K) GO TO 140

    XSTART = RX(K) $      XSTOP = RX(J)
    MFLAG = 1 $      MAX = J - K + 1

    DO 130 M=1,MAX
    X(M) = RX(K+M-1)
130  Y(M) = RY(K+M-1)

    IF (MAX.LT.3) MFLAG = 2
    CALL CRUNCH

    VB1 = VB1 + VB $      AF1 = AF1 + AF $      K = J

140  DO 150 J=K,N
    IF (RX(J).LE.RX(J+1)) GO TO 155
150  CONTINUE

    MFLAG = -1 $      GO TO 200
155  XSTART = RX(K) $      XSTOP = RX(J)
    MFLAG = -1 $      MAX = J - K + 1

    DO 160 M=1,MAX
    X(MAX+1-M) = RX(K+M-1)
160  Y(MAX+1-M) = RY(K+M-1)

    IF (MAX.LT.3) MFLAG = -2
    CALL CRUNCH

    VB1 = VB1 - VB $      AF1 = AF1 + AF $      K = J
    GO TO 115

```

```

200 XSTART = RX(K) $      XSTOP = RX(NPTS)
    MAX = NPTS - K + 1
    IF(MFLAG.LT.0) GO TO 215

    DO 210 M=1,MAX
        X(M) = RX(K+M-1)
210  Y(M) = RY(K+M-1)

    GO TO 225

215 DO 220 M=1,MAX
    X(MAX+1-M) = RX(K+M-1)
220  Y(MAX+1-M) = RY(K+M-1)

225 CALL CRUNCH

    VB1 = MFLAG * VB + VB1 $      AF1 = AF1 + AF
    VT = YP * D ** 2 $      VU = VT - VB1
    VU = VU * C **3
    VT = VT * C **3
    IF (RX(1).GT.0.) AF1 = AF1 + RY(1) * D
    IF (RX(NPTS).LT.D) AF1 = AF1 + RY(NPTS) * D
    AF = AF1 * C **2
    YP = YP * C
    GO TO 227

226 AF = 0. $      YP = YP * C $      VU = VT = YP * (D*C)**2
227 CONTINUE

    PRINT 13, NFRAME,YP,VT,VU,AF
    GO TO 100

10  FORMAT(E15.5)
11  FORMAT(2I10,E10.3)
12  FORMAT(5(F6.4,1X,F6.4,2X))
13  FORMAT(1I10,4F8.3)
14  FORMAT(6X,6HNFRAME,3X,2HYP,6X,2HVT,6X,2HVU,6X,2HAF,/)

900 CONTINUE
    END

```

SUBROUTINE CRUNCH

COMMON/BLOK1/X(30),Y(30),XSTART,XSTOP,MFLAG,VB,AF,D,MAX
DIMENSION C(29,3),BPAR(4)

IC = 29

BPAR(1) = BPAR(2) = BPAR(3) = EPAR(4) = 0.

CALL ICSICU(X,Y,MAX,BPAR,C,IC,IER)

CALL DCSQDU(X,Y,MAX,C,IC,XSTART,XSTOP,VB,IER)

VB = ABS(VB)

VB = VB * D

AF = 0.

N = MAX - 1

DO 200 K=1,N

AL = ((Y(K) - Y(K+1))**2 + (X(K) - X(K+1))**2) ** 0.5

200 AF = AL + AF

AF = AF * D

RETURN

END

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