LAMINAR BURNING VELOCITY OF PROPANE-AIR
MIXTURES AT HIGH TEMPERATURE AND PRESSURE

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INTRODUCTION

The laminar combustion properties of fossil fuels at high temperatures and pressures are of fundamental importance for analyzing and predicting the performance of internal combustion engines and power plant burners. Of particular interest is the laminar burning velocity which plays an essential role in turbulent combustion processes in determining:

1) the ignition delay which affects the spark advance and the cycle to cycle fluctuation [1],

2) the thickness of the wall quench layers which are the primary source of unburned hydrocarbons and carbon monoxide [2], [3] and

3) the minimum ignition energy to ignite the charge [4] which affects the range of equivalence ratio over which an engine can be operated. Experimental laminar burning velocities are also used to check the theoretical combustion models and calculate apparent activation energies.

There are basically two methods of measuring laminar burning velocities. One employs stationary flames and the other moving flames. Bunsen burner, slot burner, and flat flame burner methods are in the first category while flame tube, soap bubble (constant-pressure bomb), and constant volume bomb methods are in the second.

At the present time there is some information about the laminar burning velocities of propane-air mixtures at low pressures [5 through 11], but none in the range of pressure and temperature encountered in internal combustion engines and burners. The purpose of this paper is to describe a constant volume bomb facility for measuring laminar flame velocities and to present measurements for propane-air mixtures at high temperatures and pressures.

EXPERIMENTAL APPARATUS

A schematic diagram of the combustion bomb used for these measurements is shown in Figure 1. It has an inside diameter of 15,24 cm and was designed to withstand a pressure of 700 atm. Standard 14 mm spark plugs with extended stainless steel electrodes were used to form the spark gap at the center of the bomb. A standard capacitive discharge ignition system in which the energy stored in capacitors can be varied from a few millijoules to 2 Joules, was used for producing the spark.

A "black box" representation of the experimental facility is shown in Figure 2. The bomb is located in an oven and can be heated electrically to a temperature of 500 K. Gaseous fuels and air are introduced through a high pressure line. Pure liquid fuels may be introduced as vapor or injected through a septum. Wide boiling range fuels must be injected. Dynamic pressure was measured with a piezoelectric Kistler pressure transducer and a balanced-pressure indicator was used for absolute calibration. The arrival time of the flame front at the wall was measured using ionization probes located at three positions on the perimeter of the combustion bomb. These probes, which are flush with the spherical inner surface of combustion bomb, were used to check for spherical symmetry of the flame.

For direct measurement of the flame front position a He-Ne laser system shown in Figure 3 was used. The distance from center of the combustion bomb to the laser beam was 6.46 cm. When the flame front passes through the laser beam a diffraction pattern similar to that produced by a knife edge is produced. Using this system the time when the flame front cuts the laser beam can be measured to $\pm$ 0.1 msec and the radius of flame front can be measured

to $\pm$.15 mm. A comparison of this radius with the corresponding value derived from pressure measurements is used to check the assumption of negligible pre-flame reactions made in the analysis of data.

Figure 4 shows the data handling and processing equipment used in the experiment. It consists of a two channel 12 bit analog to digital convertor controlled by a microcomputer. The maximum number of digitized points per channel is 256 and the time increment between two points is 0.25 msec. The instrumentation also includes four counters which are used to read the time when the three ionization probe pulses occur and the balanced-presure switch closes. An oscilloscope is used to monitor all inputs.

To make a measurement the bomb was heated to the desired temperature and filled with the desired fuel/air mixture. A waiting time of 5 minutes was then allowed to permit the fuel and air to mix completely and become quiescent. To check that this was sufficient, tests involving waiting times of 2 to 20 minutes were conducted. No effect on the measurement was observed and 5 minutes was chosen as a reasonable interval.

Figure 5 shows a typical oscillogram for stoichiometric propane-air mixture having initial conditions of 1 atm. and 300 K. The horizontal scale is 10 msec/div. for pressure and ionization probe signals. The vertical scale for a pressure signal is 1.36 atm/div. The laser signal has been delayed 20 msec and the sweep rate is 1 msec/div.

The analog signals from the pressure transducer and the laser were fed directly to the microcomputer and the digitized data were transferred auto-matically from the microcompouter to the host computer. Times from the ioni-zation probe and balanced pressure indicator counters were input manually to

the host computer. The data could be processed immediately or stored in memory for later analysis

THEORETICAL ANALYSIS

In the data reduction process the balanced-pressure indicator was first used to calibrate Kistler pressure transducer data. The dynamic pressure curves were then used to calculate the laminar burning velocity.

In the analysis of the data it is assumed that for a flame radius greater than a centimeter or two it is a good approximation to assume that the thickness of the flame front is negligible and that the gas within the bomb consists of a burned fraction x at thermodynamic equilibrium and an unburned fraction 1.- x frozen at its original composition. It is further assumed that the pressure P is uniform, the flame front is smooth and spherical, the unburned gas is isentropically compressed, heat loss is negligible and there is no stratification of the charge. The conditions in the burned and unburned gases are determined by the equation of state

$$P \bar{v}_b = \bar{R}_b \bar{T}_b \tag{1}$$

$$P \bar{v}_u = \bar{R}_u \bar{T}_u \tag{2}$$

where the subscripts b and u refer to burned and unburned gases. The conservation equations with the stated assumption can be expressed as:

$$V/M = x \bar{v}_b + (1 - x) \bar{v}_u \tag{3}$$

$$E_o/M = x \bar{e}_b + (1 - x) \bar{e}_u \tag{4}$$

where

P = Pressure in the combustion bomb

v = Specific volume

$\bar{R}$ = $\tilde{R}/\bar{M}$

$\tilde{R}$ = universal gas constant

$\bar{M}$ = mean molecular weight of gases in the bomb

V = combustion bomb volume

M = total mass of gases in the combustion bomb

x = mass fraction burned

E_o = initial internal energy

e = specific internal energy

The values of $\bar{v}_b$, $\bar{v}_u$, $\bar{e}_b$, $\bar{e}_a$ are given by

$$\bar{v}_b = \frac{1}{x} \int_0^x v_b \, dx' \qquad (5)$$

$$\bar{v}_u = \frac{1}{(1-x)} \int_x^1 v_u \, dx' \qquad (6)$$

$$\bar{e}_b = \frac{1}{x} \int_0^x e_b \, dx' \qquad (7)$$

and

$$\bar{e}_a = \frac{1}{(1-x)} \int_x^1 e_u \, dx' \qquad (8)$$

The unburned gas properties such as T_u, e_u and $\bar{v}_u$ were calculated using an assumption of isentropic compression and equations (2), (6), and (8). To calculate $\bar{v}_b$ and $\bar{e}_b$, the burned gases are approximated as homogeneous at an equivalence ratio ϕ with uniform temperature throughout so that $T_b = \bar{T}_b$. The Martin and Heywood [12] model of the equilibrium gas is used to calculate $\bar{e}_b$ and $\bar{v}_b$ for any $\bar{T}_b$, P and ϕ.

Equations (3) and (4) were solved for the two unknowns $\bar{T}_b$ and x using the Newton-Raphson, iteration method. The following definitions result from the assumptions of spherical symmetry and mass conservation:

$$V_b = x \, \bar{v}_b \, M = 4/3 \, \pi \, R_f^3 \tag{9}$$

$$R_f = [3V_b/4\pi]^{1/3} \tag{10}$$

$$A_f = 4 \, \pi \, R_f^2 \tag{11}$$

$$S_u = M \, \dot{x}(t)/\rho_u A_f \tag{12}$$

$$S_f = \dot{R}_f(t) \tag{13}$$

$$S_g = S_f - S_u \tag{14}$$

where

R_f = radius of flame

A_f = area of flame

S_u = laminar burning velocity

$\dot{x}$ = rate of mass fraction burned

S_f = flame front velocity

S_g = unburned gas velocity

EXPERIMENTAL RESULT

Before undertaking extensive measurements a statistical study was made to check the reproducibility of data. Four identical runs for stoichiometric propane-air mixtures at an initial temperature of 298 K and 1 atm. pressure were made and the laminar burning velocity was calculated along the isentropes

for each. Figure 6 shown the results plotted as a function of pressure and temperature. It can be seen that data are very reproducible.

Further evidence of the reproducibility is given in Table 1. The parameters shown are peak pressure P_p, time at which peak pressure occurs t_p, the time deviation of the ionization probe pulse from the mean time $t_i - \bar{t}$, the standard deviation of flame radii when ionization probe pulses occur δr_{rms}, the deviation of the calculated flame front radius from that given by the laser beam δr_{laser}, and the unburned mass fraction burned δx_u. As can be seen the maximum pressures and the times at which maximum pressures occurred are very close for all four runs. Although there is some evidence of a systematic variation in the arrival times of the flame front at the ionization probes which might indicate a small assymetry, it should be noted that, since the flame speed is less than 100 cm/sec, the displacements involved are only fractions of a millimeter. This is smaller than the accuracy with which the probes could be positioned and is not considered significant. The other quantities in Table 1 δr_{rms}, δr_{laser} and δx_u are all well within the accuracy of the measurements and the general conclusion is that the data are remarkably reproducible.

Systematic measurements of laminar burning velocities for propane/air mixtures were made at equivalence ratios of 0.8, 1.0 and 1.2. At each equivalence ratio, initial pressures of 0.4, 1.0 and 2.0 atm at room temperature were chosen. Measurements were first made along the isentropes starting at these initial conditions. They were then extended to higher temperatures and pressures by heating the bomb to 400 K and 500 K and chosing initial pressures which lay on the same isentropes. Using this method laminar burning velocities were obtained for the pressure range 0.4 - 40 atm and temperature

range 298 to 750 K.

Figure 7 shows the laminar burning velocity along one of these isentropes for a stoichiometric propane-air mixture having initial conditions of 296 K and 1 atm. Three overlapping runs are shown: the circle points have atmospheric initial conditions; the triangular points have initial conditions of 400 K and 3.13 atm, and the square points have initial conditions of 500 K and 7.6 atm. The scatter in data is about ± 2% which is due to round off error in the analog to digital convertor.

The pressures at which ionization probe pulses occur are shown in the figure, and it can be seen that these probe pulses occur very close to each other.

The laminar burning velocity increases along an isentrope, peaks a little before peak pressure and then falls off. This fall off is due to wall heat transfer from the unburned gas which was neglected in the present analysis. (Correction for this will be included in future work.) The solid and dashed curves are two different fits to the data which will be described in the next section.

Figure 8 shows data for 9 different isentropes. The first column is for propane-air mixtures with an equivalence ratio of 0.8, the second column is for stoichiometric mixtures and the third column is for equivalence ratios of 1.2. These data show that the laminar burning velocity decreases with increasing pressure at constant temperature and increases with increasing temperature at constant pressure.

Figure 9 shows the laminar burning velocity as a function of equivalence

ratio for propane-air mixtures at a temperature of 298 K and pressure of 1 atm. The laminar burning velocity peaks for an equivalence ratio of 1.1 and falls off for the both rich and lean mixtures.

DISCUSSIONS

The measured laminar burning velocities for propane-air mixtures have been fitted to two different functional forms. The first is the simple power law relation

$$S_u = S_{uo} \left(\frac{T_u}{T_{uo}} \right)^\alpha \left(\frac{P}{P_o} \right)^\beta \tag{15}$$

where T_{uo} = 298 K and P_o = 1 atm are the reference temperature and pressure and S_{uo}, α and β are fitted constants. The values of S_{uo}, α and β are given in Table 2 as a function of equivalence ratio along with the percentage of data points falling within ±5% of the fitted curve.

Table 2

ϕ	S_{uo} cm/sec	α	β	% of data within ±5%
0.8	22.5	2.31	-0.24	63
1.0	30.4	2.17	-0.17	64
1.2	32.3	2.03	-0.16	74

The power law fit (15) is also shown graphically by the dashed curves in Figures 7 and 8. For pressures above 2 atm the fit is quite good. Below 2 atm there appear to be some small systematic deviations.

The second relation used to fit the data is that used by Lavoie [13] to correlate data from previous experiments. It is given by

$$V_{STP} \equiv \frac{\rho_u S_u}{\rho_{STP}} = A \left(\frac{P}{P_o} \right)^\beta e^{-E/2RT_b^o} \tag{16}$$

where V_{STP} is the mass average burning velocity, T_b^o is the adiabatic flame temperature and A, β and E are fitted constants. The values of A, β and E are given in Table 3 along with the percentage of data points within $\pm 5\%$ of the fitted curve.

Table 3

ϕ	A cm/sec	β	E Cal/(gm.mole)	% of data within $\pm\%5$
0.8	17.1×10^4	0.752	72,900	62
1.0	152.3×10^4	0.705	96,800	70
1.2	5.03×10^4	0.805	64,100	81

The exponential fits (16) are shown graphically by the solid curves in Figures 7 and 8. It can be seen from these figures and the last columns in Tables 2 and 3 that the overall fit of the power law and exponential relations are about equally good. The exponential relation appears to be slightly better at pressures below 2 atm but it is very sensitive to the calculation of the adiabatic flame temperature and is much less convenient to use than the power law relation. There might be some tendency to prefer the exponential relation on fundamental grounds, however, in view of the strong variation of both the preexponential coefficient A and the apparent activation energy E with equivalence ratio, the physical significance of these quantities is extremely doubtful.

Comparison of the data in Table 3 with the corresponding values obtained by Lavoie from previous data show reasonable agreement for the pressure exponent but significant disagreement in the values of A and E. The most probable reason for this is the limited amount of high pressure and temperature data

with which Lavoie had to work.

The variation of the reference laminar flame speed S_{uo} with equivalence ratio shown in Figure 9 is in good agreement with the low pressure data obtained by Kuehl [5] using a slot burner.

One general conclusion we would like to draw from the present work is that the constant volume bomb method of measuring adiabatic flame speed is both an accurate and efficient technique. Further refinements such as the use of interferrometry [14] to measure unburned gas density, laser scattering to measure flame thickness and the inclusion of wall heat transfer corrections have the potential to make it even more accurate.

Future work with the bomb facility will include measurements of flame speeds for wide boiling range liquid fuels and studies of the effect of "residual gases" in the mixture.

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Table 1

Run No.	P_p (atm)	t_p (msec)	$t_1 - \bar{t}$ (msec)	$t_2 - \bar{t}$ (msec)	$t_3 - \bar{t}$ (msec)	δr_{rms} (mm)	* δr_{Laser} (mm)	δx_u
1	9.327	38.95	-0.32	0.68	-0.36	0.24	+0.004	0.001
2	9.135	39.21	-0.58	0.32	0.25	0.23	-0.069	0.025
3	9.210	39.21	-0.26	0.38	-0.11	0.15	-0.021	0.008
4	9.221	38.95	-0.49	0.45	0.04	0.21	+0.019	0.015

P_p : Max. Pressure

t_p : Time of P_p

$$\bar{t} = \frac{t_1 + t_2 + t_3}{3}$$

δ_r : STD Diviation of I.P.

* $\delta r_{Laser} = R_{Calc} - 6.464$

- 14 -
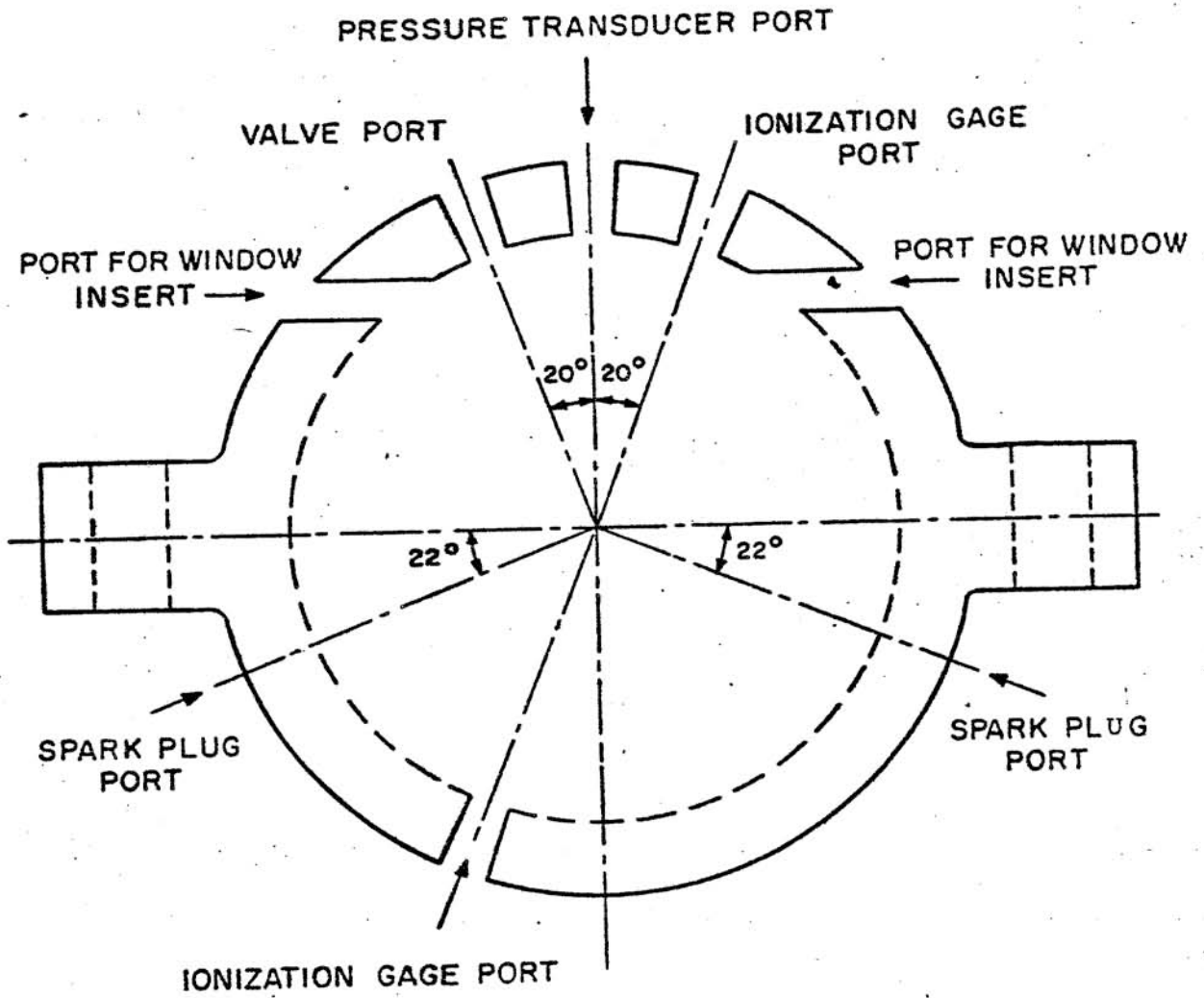
Figure 1 : Schematic Diagram of the Combustion Bomb
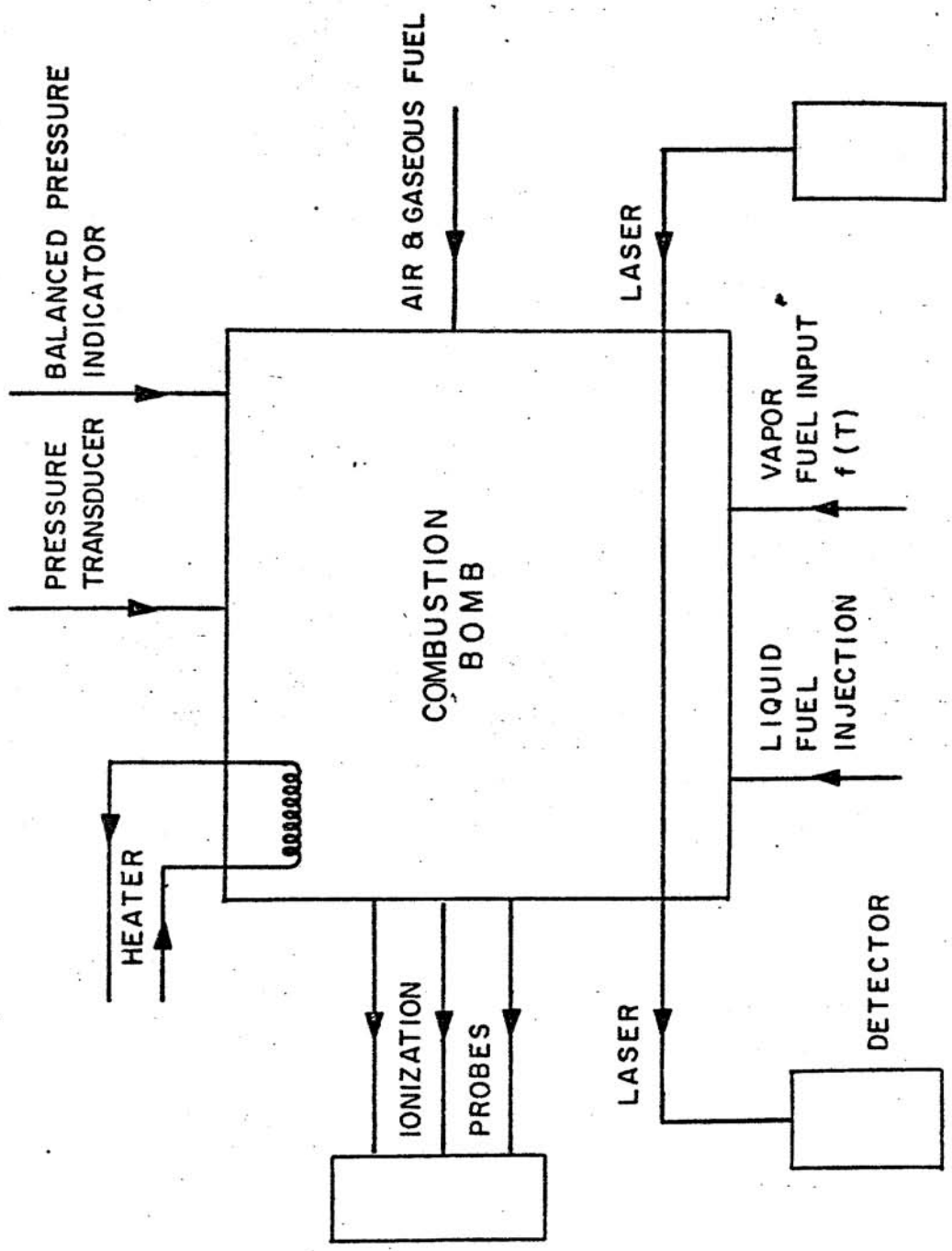
Figure 2 Black Box Representation of the Experimental Facility
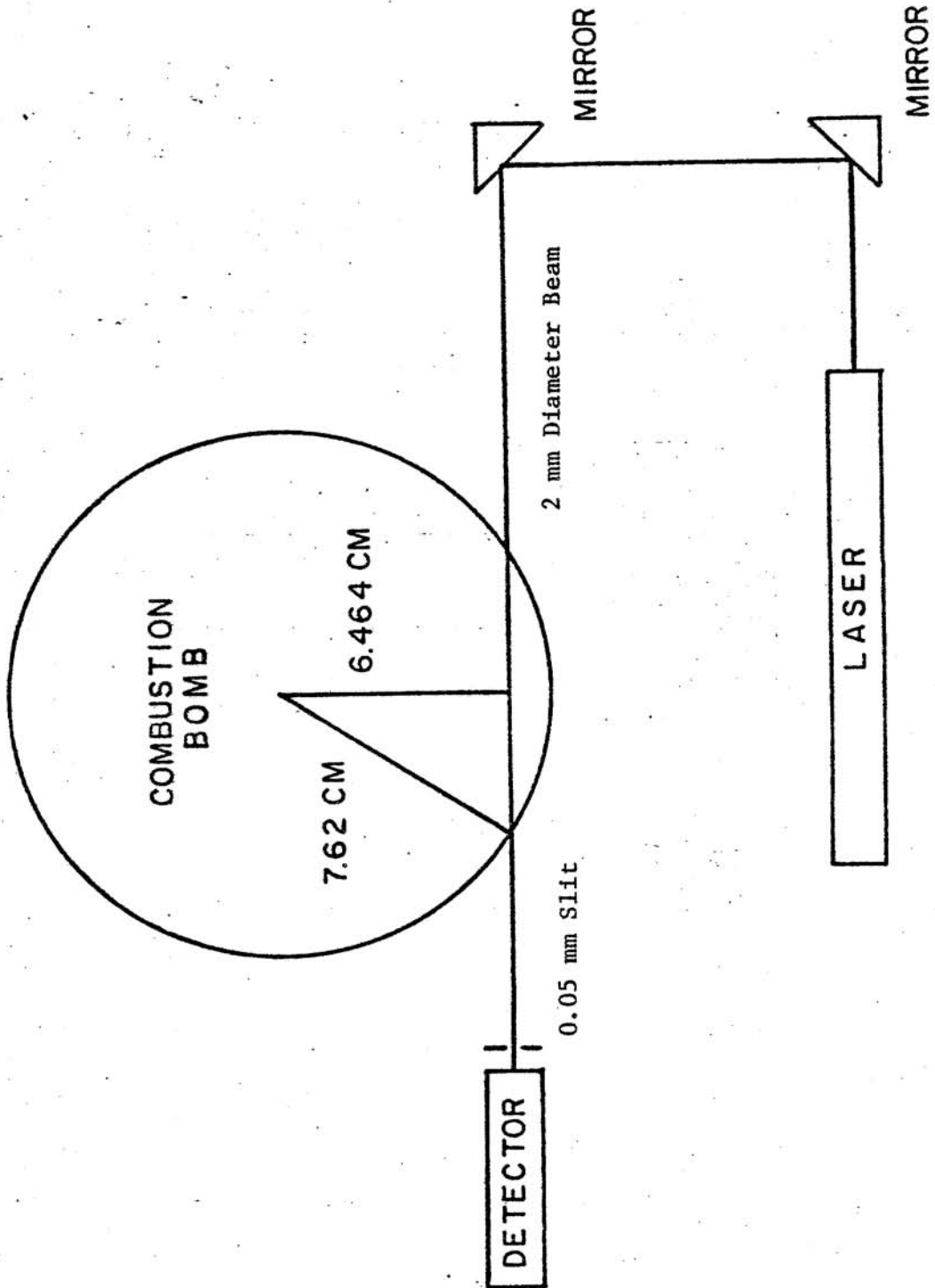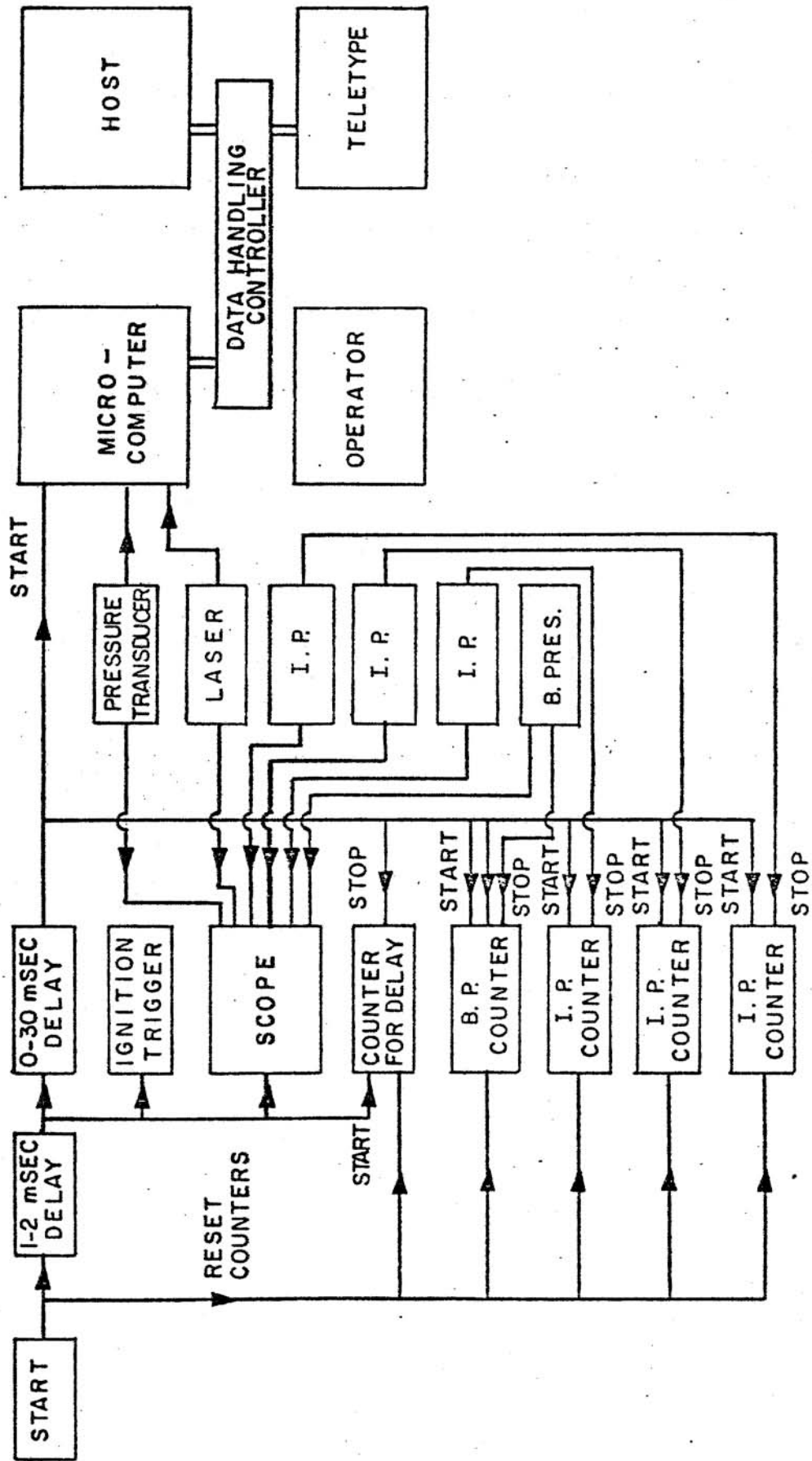
Figure 3   Schematic Diagram of Laser System

MIRROR

MIRROR

2 mm Diameter Beam

LASER

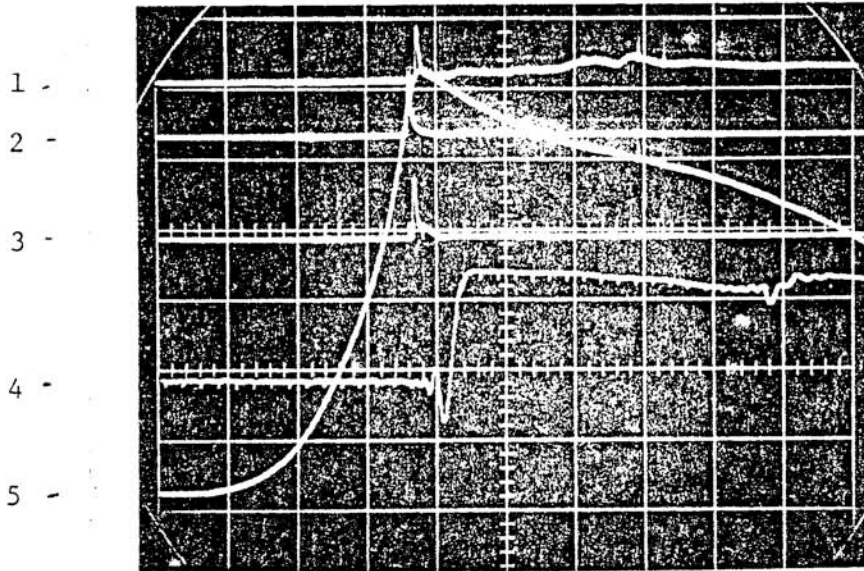COMBUSTION BOMB

6.464 CM

7.62 CM

0.05 mm Slit

DETECTOR

Figure 4   Schematic Diagram of Data Acquisition System

Propane - Air Mixture

$$P_i = 1 \text{ ATM} \quad T_i = 300 \text{ °K}$$

10 msec/div. Laser trace delayed 20 msec, sweep rate 1 msec/div.

Traces No. 1,2 and 3: Ionization Probe Signals

Trace No. 4: Laser Signal

Trace No. 5: Pressure Transducer Signal

Figure 5. A Typical Oscillograom for Stoichiometric Propane-Air Mixture

- 19 -
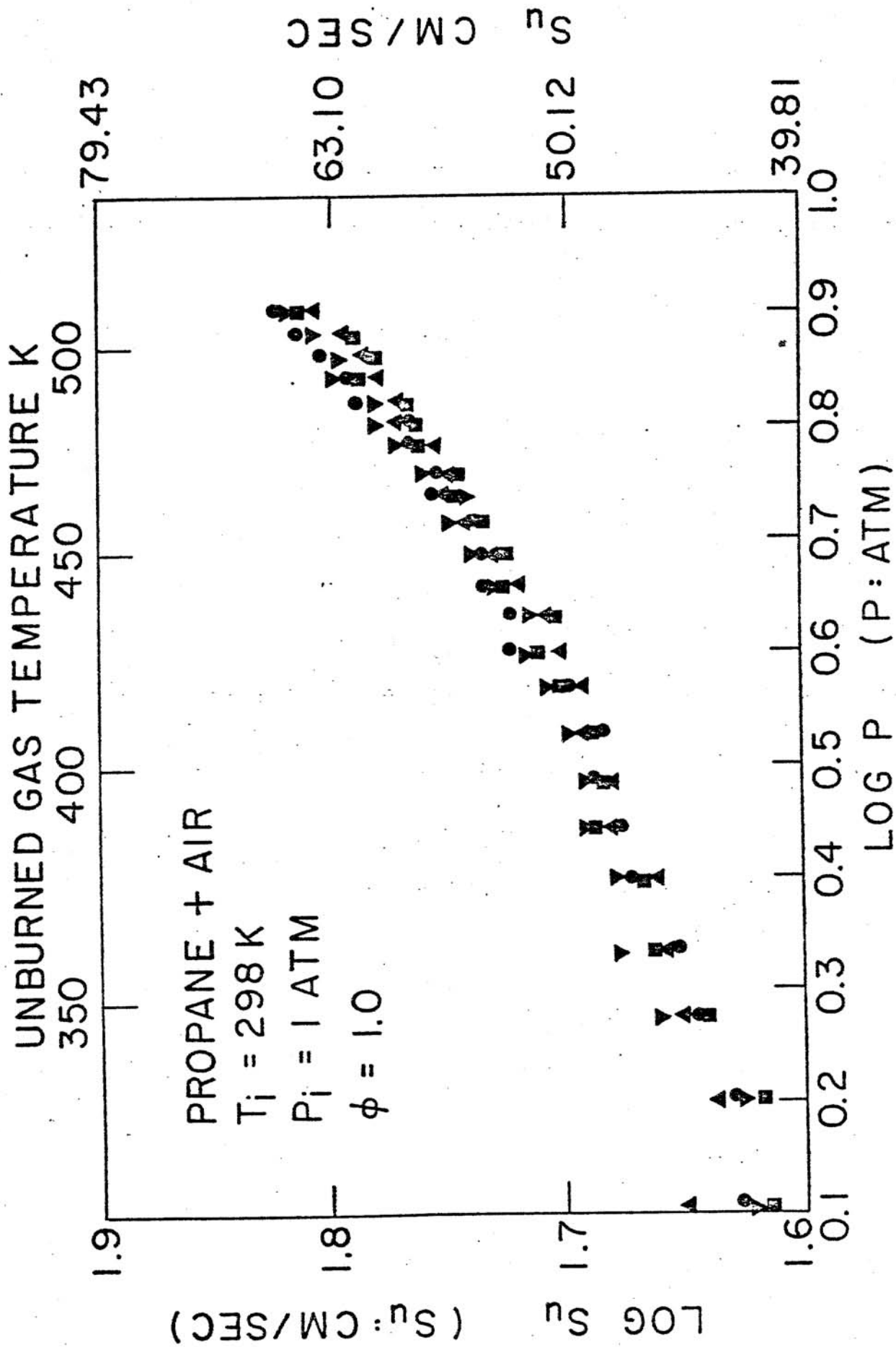
Figure 6   Laminar Burning Velocity of Stoichiometric Propane-Air Mixture having Atmospheric Initial
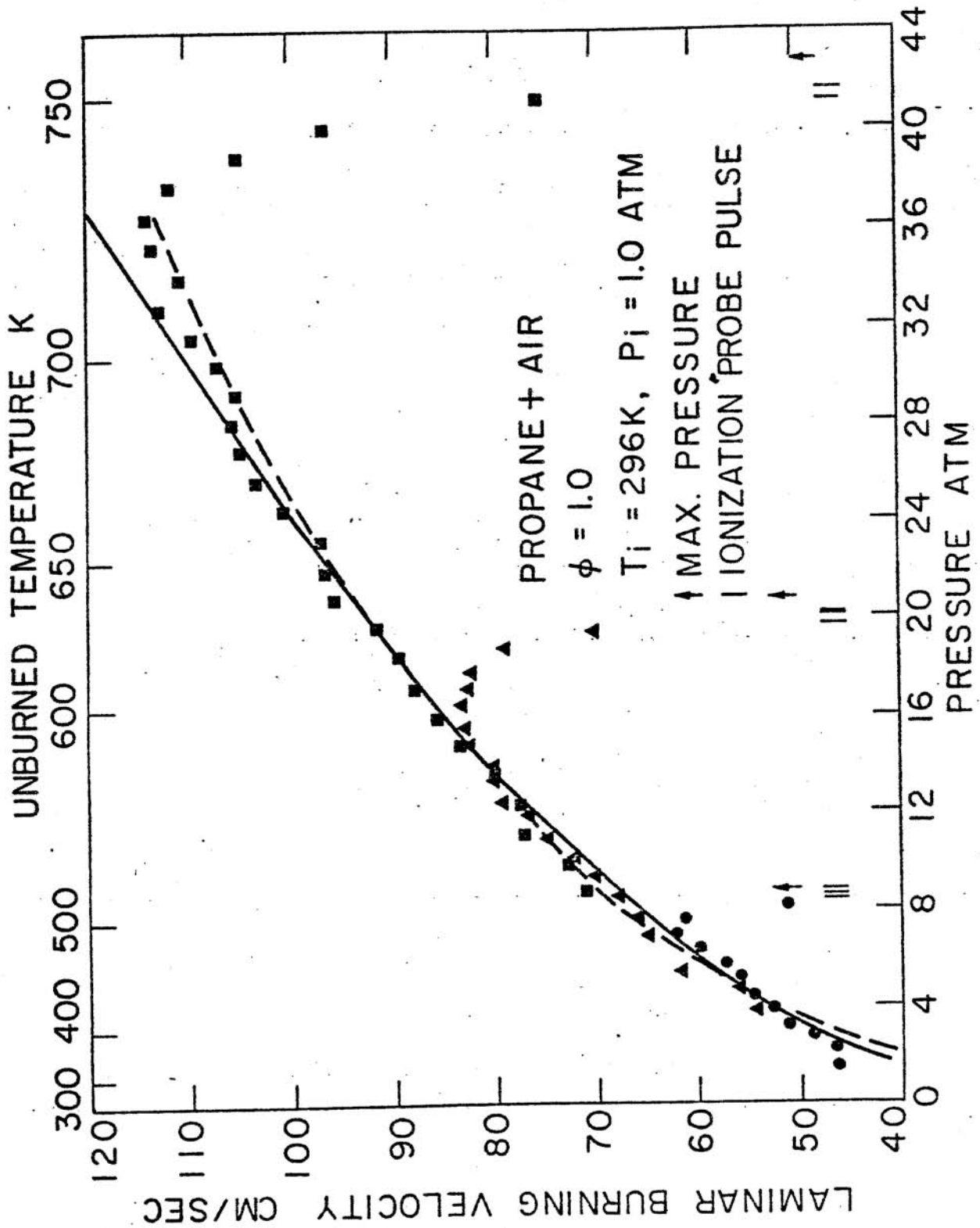Condition for Four Identical Runs.

Figure 7   Laminar Burning Velocity for Stoichiometric Propane-Air Mixture Having
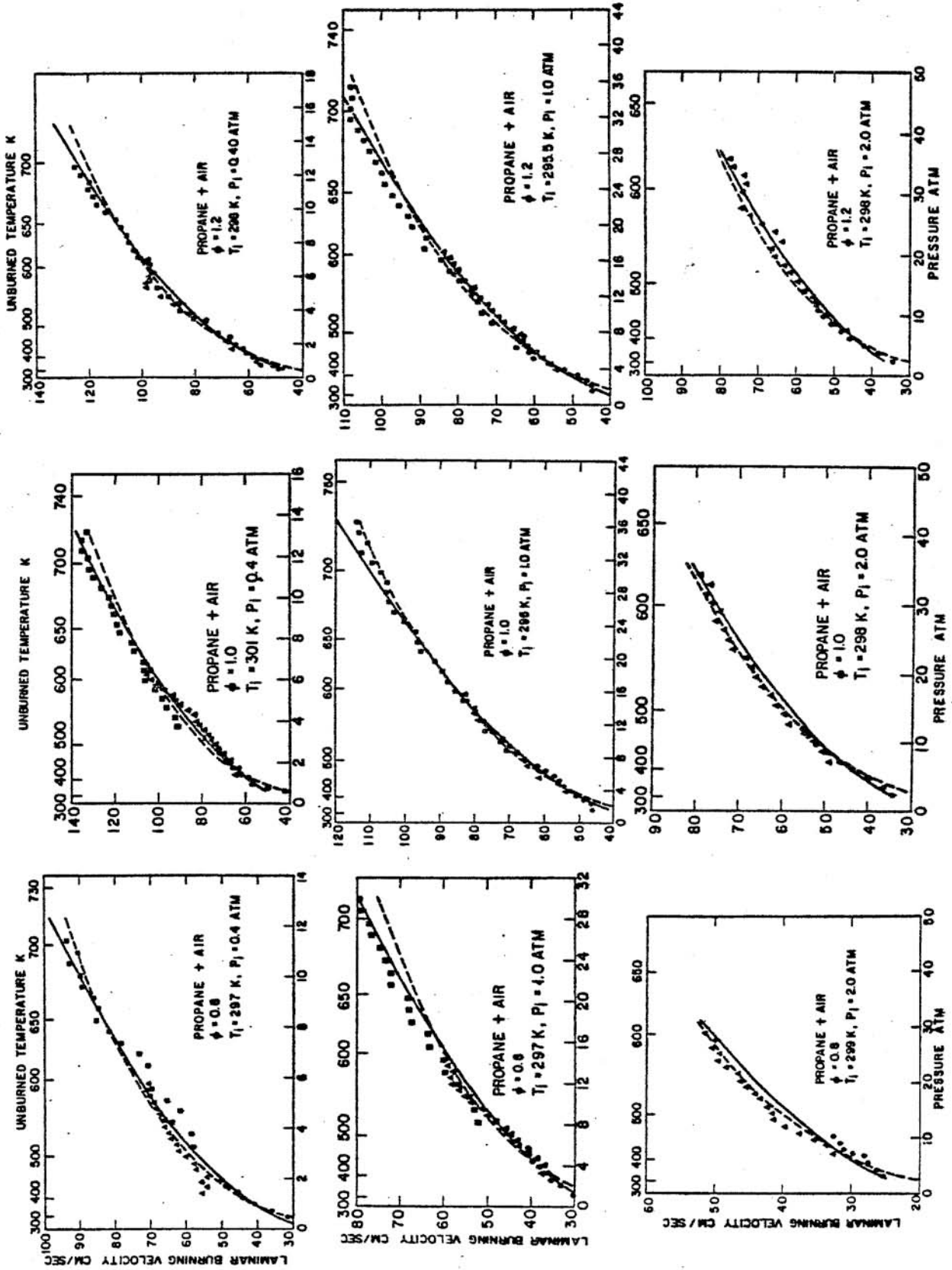Initial Conditions of 296 K and 1 a).

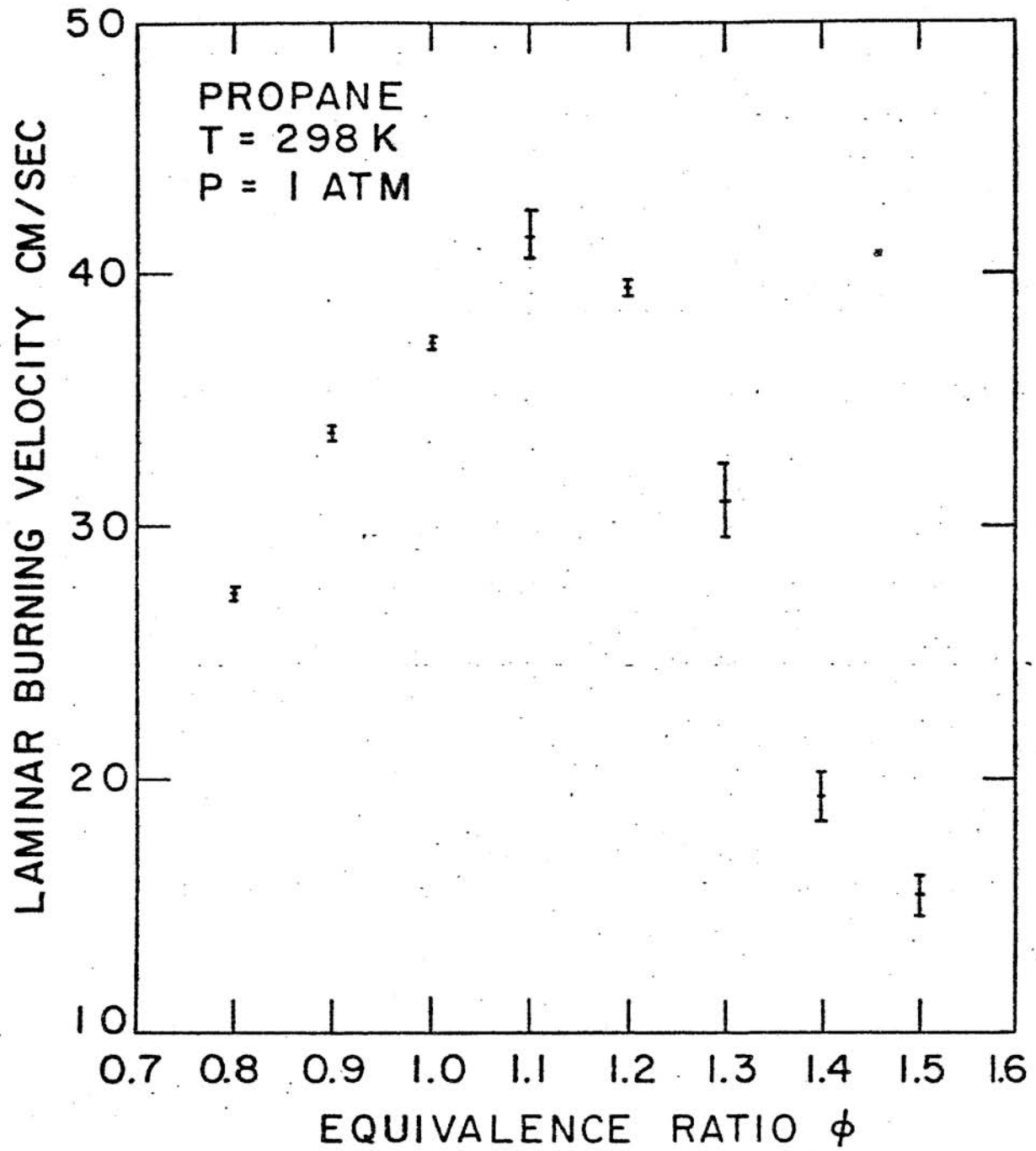Figure 8. Laminar Burning Velocity of Propane-Air Mixtures at Equivalence Ratios of 0.8, 1.0 and 1.2

Figure 9 Laminar Burning Velocity of Propane-Air Mixture at Atmospheric
Condition as a Function of Equivalence Ratio