

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188		
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1. REPORT DATE (DD-MM-YYYY) 20-10-2008		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 1-Mar-2005 - 31-Aug-2008	
4. TITLE AND SUBTITLE Experimental and Theoretical Studies of Autoignition and Burning Speed of JP8 and DF-2			5a. CONTRACT NUMBER W911NF-05-1-0051		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 611102		
6. AUTHORS Mohamad Metghalchi			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES Northeastern University Office of Sponsored Programs Northeastern University Boston, MA 02115 -5000			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 46835-EG.1		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT Experimental facilities have been built to measure burning speed, determine flame structure and observe auto-ignition of fuel/oxidizer/diluent for a wide range of pressure, temperature and fuel-air equivalence ratio. Experimental facilities include a spherical vessel and a cylindrical chamber. The spherical vessel is housed in an oven to increase initial temperature of the mixture to 500 K. The cylindrical chamber has two large windows at the end for flame observation. Dynamic pressure has been measured during the combustion process in both vessels. A thermodynamic model has been developed to calculate burning speed from pressure data. The model is a very complicated one and is described in detail in the text. Laminar burning					
15. SUBJECT TERMS combustion, burning speed, autoignition					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Mohamad Metghalchi
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U			19b. TELEPHONE NUMBER 617-373-2973

Report Title

Experimental and Theoretical Studies of Autoignition and Burning Speed of JP8 and DF-2

ABSTRACT

Experimental facilities have been built to measure burning speed, determine flame structure and observe auto-ignition of fuel/oxidizer/diluent for a wide range of pressure, temperature and fuel-air equivalence ratio. Experimental facilities include a spherical vessel and a cylindrical chamber. The spherical vessel is housed in an oven to increase initial temperature of the mixture to 500 K. The cylindrical chamber has two large windows at the end for flame observation. Dynamic pressure has been measured during the combustion process in both vessels. A thermodynamic model has been developed to calculate burning speed from pressure data. The model is a very complicated one and is described in detail in the text. Laminar burning speeds of JP8-air, JP8-He-Oxygen and JP8-Ar-Oxygen mixtures at high temperatures and pressures have been measured and reported. A power law fit has been developed to correlate burning speed to temperature, pressure and fuel air equivalence ratio. In all cases the structures of the flames were studied qualitatively by a high speed CMOS camera set up in a shadowgraph optical system.

Burning speeds of diesel-air mixtures were calculated at high temperatures and pressures and the structure of the flame was studied with shadowgraph system.

The instability and cell formation analyses were performed for JP8-O₂-diluent mixtures at high temperatures and pressures and different diluents.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. Parsinejad, F., Keck, J.C. and Metghalchi, H., "On the Location of Flame Edge in Shadowgraph Pictures of Spherical Flames; Experimental and Theoretical Study", Experiments in Fluids, Volume 43, Number 6: 887-894, December 2007.
2. Rahim, F., Eisazadeh Far, K., Parsinejad, F., Adrews, R. J. and Metghalchi, H., "A Thermodynamic Model to Calculate Burning Speed of Methane-Air- Diluent Mixtures", Accepted for publication in International Journal of Thermodynamics.

Number of Papers published in peer-reviewed journals: 2.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

1. Parsinejad, F., Shirk, E., Eisazadeh Far, K., and Metghalchi, H., "Laminar Burning Speed Measurements of Premixed JP-8, Oxygen and Helium Flames", Proceedings of 2006 IMECE ASME International Mechanical Engineering Congress & Exposition, November 2006, Chicago, IL.
2. Janbozorgi, M., Gao, Y., Metghalchi, H., and Keck, J.C., "Rate-Controlled Constrained-Equilibrium Calculations of Ethanol-Oxygen Mixture", Proceeding of 2006 IMECE ASME International Mechanical Engineering Congress & Exposition, November 2006, Chicago, IL.
3. Eisazadeh Far, K., Andrews, R., Parsinejad, F., and Metghalchi, H., "Structure of Fuel/Oxygen/Diluent (Argon, Helium, Nitrogen) Premixed Flames at High Pressures and Temperatures" Proceedings of Eastern States Section of the Combustion Institute, October 2007, University of Virginia.
4. Janbozorgi, M., Goldthwaite, D., Metghalchi, H., and Keck, J. C., "RCCE calculations of the Combustion Products in the Expansion Stroke of an Internal Combustion Engine" Proceedings of Eastern States Section of Combustion Institute, October 2007, University of Virginia.

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

4

(d) Manuscripts

1. Janbozorgi, M., Ugarte, S., Metghalchi, M., Keck, J. C., "Combustion Modelling of Mono-Carbon Fuels Using the Rate-Controlled Constrained-Equilibrium Method", submitted to Combustion and Flame.
2. Janbozorgi, M., Metghalchi, M "Maximum Entropy Principle Applied to Chemical Relaxation Phenomena", submitted to International Journal of Thermodynamics.

Number of Manuscripts: 2.00

Number of Inventions:

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Kian Eisazadeh	0.90
Colin Fredette	0.05
Raymond Andrews	0.05
FTE Equivalent:	1.00
Total Number:	3

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Farzan Parsinejad	0.15
FTE Equivalent:	0.15
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Mohamad Metghalchi	0.08	No
FTE Equivalent:	0.08	
Total Number:	1	

Names of Under Graduate students supported

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Reynolds Andrews

Total Number:

1

Names of personnel receiving PhDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Final Report

Experimental and Theoretical Studies of Autoignition and Burning Speed of JP8 and DF-2

Submitted to:

U. S. Army Research Office

ATT: AMSRL-RO-S (IPR)

P. O. Box 12211

Research Triangle Park, NC 27709-2211

Grant No. W911NF0510051

October 20, 2008

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

1. One Ph.D. student, two Master's student.
2. No inventions.
3. Experimental facilities have been modified. More modification has been added to the burning model.
4. No patents.
5. Kian Eisazadeh Far earning a Ph.D. and Raymond J. Andrews (received his MS in Spring 2008) and Collin Fredette earning a Master's degree (Spring 2009).

Introduction

The United States Army and Air Force use MIL-T-83133C grade JP8 as the main source of energy for military land vehicles and aircraft. JP-8 is very similar to Jet A-1 with three military specified additives, fuel system inhibitor, corrosion inhibitor/lubricity improver and static dissipater. The conversion to JP-8 occurred primarily to improve the safety of aircraft, although the "single fuel for the battlefield" concept is centered on the use of aviation kerosene in all Air Force and Army aircraft and ground vehicle.

Detailed chemical kinetic mechanisms that describe combustion of many of the components in JP-8 are not available and are unlikely to be developed in the near future. Hence there is a need to study the characteristics of JP-8 experimentally. One of the important thermo-physical properties of JP-8/air mixtures is its laminar flame speed. There are many more difficulties in the accurate measurement of the laminar burning speeds of liquid fuels such as JP-8 than that of gaseous fuels. The process of creating a precise initial mixture of the fuel/oxidizer/diluents can present many challenges. In this research the unique experimental facility in Northeastern University allows to prepare correct mixture at high temperatures and pressures to perform the experiments.

The following is the final report on our developments and accomplishments for the three years period. In this report, a brief description of the experimental facilities which includes two combustion chambers, spherical and cylindrical, optical set up, a high

temperature oven will be presented. The structure of JP8-O₂-diluent flames have been studied, laminar burning speeds of JP8-O₂-He, JP8-O₂-Ar and JP8-air mixtures have been calculated and a power law fit has been developed for the calculation of laminar burning speed of these fuels at different conditions. Also, the cell formation and instability of these mixtures have been investigated.

Autoignition and explosion limits of JP-8/air mixtures have been measured by performing some experiments in the spherical vessel. The experiments were performed at high initial pressures and temperatures to observe autoignition. The explosion limits temperatures and pressures were measured at different equivalence ratios.

Experimental Set up

Burning speed measurements were made in the existing spherical combustion chamber. The spherical chamber consists of two hemispheric heads bolted together to make a 15.4 cm inner diameter sphere. The chamber was designed to withstand pressures up to 425 atm and is fitted with ports for spark electrodes, diagnostic probes, and ports for filling and evacuating it. A thermocouple inserted through in one of the chamber ports was used to check the initial temperature of the gas inside the chamber. A Kistler 603B1 piezo-electric pressure transducer with a Kistler 5010B charge amplifier was used to obtain dynamic pressure vs. time records from which the burning speed was determined. Ionization probes mounted flush with the wall located at the top and bottom of the chambers were used to measure the arrival time of the flame at the wall and to check for spherical symmetry and buoyant rise.

Spherical vessel is housed in an oven which can be heated up to 500 K. Liquid fuel is stored in a 115 cc heated vessel and is transferred through a heated line inside the oven to the spherical chamber. Several thermocouples are located on the line from the fuel reservoir to the vessel to monitor temperature of the fuel passageway. A heated strain gauge (Kulite XTE-190) in the oven is used to measure partial pressure of fuel in the vessel.

The companion cylindrical chamber is made of SAE4140 steel with an inner diameter and length of 133.35 mm. The two end windows are 34.93 mm thick Pyrex with a high durability against pressure and temperature shocks as well as having very good optical

properties. A Z-type Schlieren/Shadowgraph ensemble has been set up to visualize the flame propagation. A high speed CMOS camera (MotionXtra HG-LE, Redlake Inc.) with a capture rate of up to 40,000 frames per second is placed very close to the focal point of the second mirror. Two band heaters and a rope heater wrapped around the cylindrical vessel are used to heat up the inside temperature of the vessel up to 500 K. This chamber is equipped with a heated liquid fuel line system, a pressure strain gauge and thermocouples similar to the spherical vessel. The oven was omitted to permit flame observation for this application.

Gas handling system used with these facilities consists of a vacuum pump for evacuating the system and a valve manifold connected to gas cylinders for preparation of the fuel/oxidizer/diluent mixtures. Partial pressures of the fuel mixtures were measured using Kulite strain gauge pressure transducers in the 0-15 psi range. Two spark plugs with extended electrodes were used to ignite the mixture at the desired location in the chambers. An electronic ignition system controlled by the data acquisition program provides a spark with the necessary energy. The data acquisition program synchronizes the ignition with the dynamic pressure recording and Schlieren/Shadowgraph photography.

The data acquisition system consists of a Data Translations 16 bit data acquisition card, which records the pressure change of the combustion event at a rate of 250 kHz. The analog to digital converter card receives the pressure signal from the charge amplifier and the signals from the ionization probes. All signals are recorded by a personal computer and an output data file is automatically generated. The output data files include the dynamic pressure and its corresponding time.

Test procedure begins by evacuating the vessel and gas handling system using the vacuum pump. The chamber then is filled with JP8 vapor to the desired pressure and air is added. The vessel and the fuel tank are at the same temperature during the filling. After the chamber is filled with the proper mixture, several minutes are allowed for the system to become quiescent before it is ignited. This will prevent any turbulence inside the vessel. Six thermocouples on the liquid line are used to make sure that temperature along the filling line is never below the condensation temperature for JP8. At least three runs at each initial condition were made to provide a good statistical sample. Based on statistical

analysis, it was found that three runs are sufficient to achieve a 95% confidence level. Figure 1 shows the schematic of two combustion chambers.

Theoretical Model

The theoretical model used to calculate the burning speed from the pressure rise is based on one previously developed by Metghalchi and co-workers [1-5] and has been modified to include corrections for heat losses to electrodes and radiation from the burned gas to the wall as well as the temperature gradient in the preheat zone. It is assumed that gases in the combustion chamber can be divided into burned and unburned regions separated by a reaction layer of zero thickness as shown schematically in Figure 2. Burned gas in the center of chamber is divided into n number of shells where the number of shells is proportional to the combustion duration. Burned gas temperatures in shells are different from each other but burned gases are in chemical equilibrium in each shell at the given temperature. The burned gas is surrounded by the unburned gas in preheat zone (δ_{ph}) with variable temperature. Core unburned gas with uniform temperature surrounds the preheat zone gases. A boundary layer (δ_{bl}) separates core unburned gas from vessel wall. It is further assumed that: the burned and unburned gases are ideal, the unburned gas composition is frozen, the pressure throughout the chamber is uniform, compression of both burned and unburned gases is isentropic, and the heat flux due to the temperature gradient in the burned gas is negligible.

Radiation in the participating media is a well known area and has received a lot of attention in the past fifty years. The ideal approach to calculate radiative energy transfer through the hot gases in an enclosure is to use the relations for absorption, emission and scattering coefficients and their corresponding configuration factors. However, simple solutions for temperatures and heat flows are usually not possible for equations of radiative transfer combined with energy conservation relations including the correlations of participating media. For some conditions however, simplification can be made that will provide useful results. Among all different approaches, optically thin and thick approximation which their limits are examined in [6-7] has been predominantly used.

In our study it has been assumed that gases in the chamber are optically thin. This assumption is valid for the flames under study since even the species with largest

absorption coefficients do not play a major role in reabsorption. The reason is that, the product of the largest attenuation coefficient by the dimension of the combustion bomb is much less than unity. This argument has been also supported by Vranos and Hall [8] who has done a theoretical analysis on the effect of thermal radiation. They used gas band radiation description and allowed for reabsorption. Based on their detailed calculation, reabsorption becomes important only at very low strain rates and the correction for strain rates of 30 s^{-1} and below is less than 0.2%. The effect of radiation on temperature becomes more pronounced as strain rate decreases. In our experiments with different fuel/oxidizer mixtures strain rate at its lowest value is not less than 30 s^{-1} and hence the correction for reabsorption is very insignificant.

It is assumed that there is an energy transfer process from the mixture to the spark electrodes. Different spark electrodes have been tested with various thicknesses to investigate the effect of energy transfer on the burning speed but it was observed that it did not affect significantly. However, the energy transfer term to the electrodes is involved in the model. The thinnest electrodes have been used to reduce energy transfer.

For the conditions of interest in the present work, all these assumptions have been validated by numerous experiments in constant volume chambers and internal combustion engines carried out over the past several decades.

For spherical flames, the temperature distribution of the gases in the combustion chamber and the burned gas mass fraction can be determined from the measured pressure using the equations for conservation of volume and energy together with the ideal gas equation of state

$$pv = RT \quad (1)$$

where p is the pressure, v is the specific volume, R is the specific gas constant and T is the temperature.

The mass conservation equation is

$$m = m_b + m_u = \bar{\rho}_b V_b + \bar{\rho}_u V_u = p_i (V_c - V_e) / RT_i \quad (2)$$

where m is the mass of gas in the combustion chamber, m_b is the burned gas mass, m_u is the unburned gas mass, V_c is the volume of the combustion chamber, V_e is the electrode volume, and the subscript i denotes initial conditions. Subscripts b and u represent burned and unburned conditions respectively. $\bar{\rho}$ is average density and V is the volume of the gas.

The total volume of the gas in the combustion chamber is

$$V_i = V_c - V_e = V_b + V_u \quad (3)$$

The energy conservation equation is

$$E_i - Q_e - Q_w - Q_r = E_b + E_u \quad (4)$$

where E_i is the initial energy of the unburned gas, Q_w is the conduction heat loss to the wall, Q_e is the conduction heat loss to the electrodes, Q_r is the heat loss due to radiation from the burned gas.

In the case of rapidly increasing pressure such as that occurring during constant volume combustion, the terms representing compression work on the boundary layer may be neglected and the resulting equations are

$$Q_e = pV_{eb}/(\gamma_b - 1) = E_{eb} \quad (5)$$

$$Q_w = pV_{wb}/(\gamma_u - 1) = E_{wb} \quad (6)$$

The radiation heat loss from the burned gas was calculated using

$$Q_r = \int_0^t \dot{Q}_r(t') dt' = 4\alpha_p V_b \sigma T_b^4 \quad (7)$$

where α_p is the Planck mean absorption coefficient and σ is the Stefan- Boltzman constant.

Finally, we solve the following equations of volume and energy simultaneously

$$\int_0^{x_b} (v_{bs}(T', p) - v_{us}) dx' = v_i - v_{us} + (V_{eb} + V_{wb} + V_{ph})/m \quad (8)$$

$$\int_0^{x_b} (e_{bs}(T', p) - e_{us}) dx' = e_i - e_{us} + (pV_{ph}/(\gamma_u - 1) - Q_r)/m \quad (9)$$

where $v_i = (V_c - V_e)/m$ and $e_i = E_i/m$ are the initial specific volume and energy of the unburned gas in the chamber.

Equations 8 and 9 contain the three unknowns: p , $x_b(p)$, and $T_b(r,t)$. Using measured, $p(t)$, as a function of time, they can be solved numerically using the method of shells to obtain the burned mass fraction, $x_b(t)$, as a function of time and the radial temperature distribution $T(r,t)$. The mass burning rate, $\dot{m}_b = m\dot{x}_b$ can be obtained by numerical differentiation of $x_b(t)$. The thermodynamic properties of the burned and unburned used in the calculations were obtained from the JANAF Tables and STANJAN code.

If the specific heats of the burned and unburned gases are assumed constant we can simplify Eq. 9

$$p(v_{bs}/(\gamma_b - 1) - v_{us}/(\gamma_u - 1)) = h_{ub} + \frac{p(v_i - v_{us})}{(\gamma_u - 1)} + \left(\frac{pV_{ph}}{(\gamma_u - 1)} - Q_r \right) / m \quad (10)$$

where $h_{ub} = h_{fu} - h_{fb}$ is the difference between the enthalpies of formation of the unburned and burned gas at zero degrees Kelvin. Equations 8 and 10 are identical to those previously reported in last year's reports with correction for radiation heat loss, conduction heat loss to the electrodes, and the displacement thickness of the preheat zone added. Given the pressure, they can be solved analytically to obtain an excellent approximation for x_b and $(RT)_{bs} = pv_{bs}$. However, they do not give the temperature distribution in the burned gas. It is of interest to note that if the small correction terms for the preheat zone and the heat loss to the electrode are neglected, x_b and $(RT)_{bs} = pv_{bs}$ depend only on the pressure and are independent of the flame shape.

Burning speed may then be defined

$$S_b = \dot{m}_b / \rho_u A_b = m\dot{x} / \rho_u A_b \quad (11)$$

where A_b is the area of a sphere having a volume equal to that of the burned gas. This expression is valid for smooth, cracked, or wrinkled flames of any shape.

Experimental Results

A set of experiments were performed to study the structure of JP8-O₂-diluent premixed flames and ultimately calculate the burning speed of the laminar cases. Power law fits were developed for the laminar burning speeds by least square method. The performed experiments are:

- 1- JP8-Air experiments in equivalence ratio range of 0.8-1.2 and initial pressure range of 1-5 atm
 - 1-1: Burning speed is calculated and power law curve fit is developed by least square method for laminar cases. The laminar burning speed fit are for the range of $0.8 < \phi < 1.2$, $500 < T < 675$ K and $1 < P < 7$ atm.
 - 1-2: Pictures have been taken in those conditions.
- 2- JP8-O₂-He experiments in equivalence ratio range of 0.8-1 and initial pressure range of 1-7 atm

2-1: Burning speed is calculated both in laminar and non-laminar cases. Power law fit is developed for laminar for $0.8 < \phi < 1$, $500 < T < 800$ K, and $1 < P < 20$ atm.

2-2: by shadowgraph system a set of pictures have been taken in pressure range of 1-30 atm and equivalence ratio range of 0.8-1.

3- JP8- O_2 -Ar experiments:

3-1: set of flame propagation pictures are in range of 0.8-1.2 and pressure range of 1-23 atm.

4- Instability analysis:

Thermo-diffusive and hydrodynamic instability and cell formation analysis have been done for JP8 at different initial pressures, diluents and equivalence ratios. Some important properties of the flame have been calculated (flame thickness, thermal diffusion coefficient). The analyses show systematic and reproducible results.

5- Diesel Fuel experiment:

Burning speed of diesel-air mixtures is calculated for: $0.8 < \phi < 1$, $500 < T < 760$ K and $1 < P < 6$ atm. Flame pictures for atmospheric initial pressure have been taken.

6- JP-8/air autoignition experiments:

The autoignition and explosion limits of JP-8/air mixtures were tested by conducting high temperature and high pressure experiments in spherical vessel. The autoignition temperature and pressure of these mixtures were measured in various equivalence ratios.

JP8-Air experiments

JP8-air experiments have been performed to measure the burning speed and to study flame structures of those mixtures. Figure 3 shows the flame propagation of JP8-air mixtures at $\phi = 0.8$ and three different initial pressures which are $P_i = 1, 2.5$ and 5 atm. It is clear that as the pressure of the chamber increases the cells are formed. Figure 4 presents the flame propagation of JP8-air at $\phi = 0.9$ at the same initial pressures. Compared with $\phi = 0.8$ flames, the cells are formed earlier. The same result is obtained by looking the figures 5 and 6 for equivalence ratios of 1 and 1.2. Two major results are concluded in the pictures: instability, and ultimately turbulence, originates from cells in the flame which form with increasing pressure; cell formation develops earlier as the mixture gets richer.

Table 1 presents the cell formation pressures and temperatures. The critical pressure has been measured by the pressure transducer, and the critical temperature has been calculated by isentropic compression assumption of unburned gas zone.

$$T_{cr} = T_i \left(\frac{P_{cr}}{P_i} \right)^{\frac{\gamma}{\gamma-1}} \quad (12)$$

where T_{cr} and P_{cr} are cell formation temperature and pressure respectively and P_i and T_i are initial pressure and temperature respectively. γ is the ratio of constant pressure heat capacity to the constant volume heat capacity.

The same experiments were used to calculate the burning speed of JP8-air mixtures. Figure 7 show a typical pressure curve versus time. The black solid curve is the pressure and the colored lines are for the ionization probes sample. Ionization probes are located on spherical vessel walls to pinpoint the arrival of the flame. The discontinuous part of colored lines show the moment when the flame has touched the wall. If the discontinuity be observed at the same time, it is understood that the flame is symmetrical and buoyancy effects are negligible.

The laminar burning speed has been calculated and Figure 8 presents the laminar burning speed curves of the JP8-air mixtures at initial pressure of 1 atm. The burning speed data are plotted on isentropic lines versus unburned gas temperature. As it is expected in lean conditions the burning speed increases by increasing the equivalence ratio. Figure 9 and 10 show the laminar burning speed curves of the JP8-air mixtures at initial pressure of 2 and 5 atms. The same trend is observed but by increasing the pressure the burning speed of the mixture decreases. A power law fit has been developed by least square method to calculate the burning speed of JP8-air mixtures. The form of equation is:

$$S_b = S_{b0} (1 + a_1(1 - \phi) + a_2(1 - \phi)^2) \left[\frac{T_u}{T_{u0}} \right]^\alpha \left[\frac{P}{P_0} \right]^\beta \quad (13)$$

where S_{b0} is the burning speed at reference point ($P_0 = 1$ atm, $T_{u0} = 450$ K and $\phi = 1$) in cm/s, ϕ is the mixture equivalence ratio, T_u is the unburned gas temperature in K, T_{u0} is the reference temperature and equal to 450 K, P is the mixture pressure in atm and P_0 is the reference pressure and equal to 1 atm. The fitted constants, a_1 , a_2 , α and β are shown in table 2.

JP8-O₂-Ar experiments

By looking at figures 3-6 it is understood that cells are formed in JP8-air mixtures early and due to this fact, developed power law fit for laminar flame can not cover a wide range of temperatures and pressures. It was planned to replace the diluent of the original mixture (Nitrogen) with Argon to see the effect. Figure 11 shows the comparison between the flame images of JP8-air and JP8-O₂-Ar mixtures. As it is seen in the pictures, Argon is not a stabilizing factor, causing cell formation earlier than Nitrogen

JP8-O₂-He experiments

The diluent was replaced with helium to see its effect on the structure of the flame. Figure 12 shows the JP8-O₂-He flames at three different equivalence ratios 0.8, 0.9, and 1 initial temperature of 463 K and initial pressure of 4 atm. The pictures demonstrate that helium as diluent can be a stabilizing factor compared with Nitrogen and Argon. It can be due to larger Lewis number and smaller expansion ratio of JP8-O₂-He mixtures. Table 3 presents the pressure and temperatures in which the cells were formed. The data show that the cells are formed at a specific pressure which is a function of equivalence ratio and diluent type. The cell formation temperature can be calculated by the equation (12). The same experiments were done in the spherical vessel to calculate the laminar burning speed of JP8-O₂-He. Figure 13 shows the laminar burning speeds of JP8-O₂-He mixtures at initial pressure of 1 atm versus unburned gas temperatures. As it is seen in the lean mixtures, laminar burning speed increases as the mixture becomes richer. Figure 14 presents the laminar burning speed at initial pressure of 2 atm, the same trend is observed without any significant difference from Figure 13. Figures 15, 16 and 17 are the laminar burning speed curves at initial pressures of 4, 5, 7 atms, respectively. Contrary to JP8-air mixtures, initial pressure does not play any role on the laminar burning speed of the mixture. A polynomial function has been fitted by least square method for the laminar burning speed of JP8-O₂-He mixtures. The form of the function is the same as equation (13). The corresponding

coefficients can be found at Table 4. As it can be seen the pressure exponent is almost zero making burning speed independent of pressure.

Instability analysis

A set of experiments were performed on JP8-O₂-diluent mixtures to detect the onset of instability and effective parameters in more detail. The strategy is to investigate the occurrence of instability by performing many experiments. The changing parameters are equivalence ratio, initial pressure and diluent type. The criterion for the instability is the formation and evaluation of small cells which develop by the propagation of the flame. Critical pressures and temperatures that cells are formed are tabulated in tables 5 and 6. It can be seen that the important factor in the cell formation and instability of the JP8-O₂-diluent flames are pressure and flame thickness. An estimation of flame thickness can be calculated by the following formula:

$$\delta \approx \frac{\alpha}{S_u} \quad (14)$$

where δ , α and S_u are flame thickness, thermal diffusivity and the burning speed of the mixture respectively. As it is seen, the cell formation pressure is independent of initial pressure and the instability temperature just depends on the pressure due to isentropic compression assumption. Another result is that in lean mixtures flame becomes more stable and the cell formation pressure increases. There is not any huge change in the flame thickness, but by non-dimensionalization of the flame thickness versus cell formation radius (R_{cr}), a systematic trend is observed which is the increasing δ/R_{cr} by the increasing of the equivalence ratio (δ/R_{cr} is the Peclet number).

The effect of diluent was investigated next. The diluent (N₂) was replaced with Helium to see the effect. It was observed that in the mixtures with helium as diluent, the cell formation was delayed because of higher instability pressure. Table 6 presents the results of these experiments.

The difference between mixtures with different diluents can be attributed to the heat conductivity. One of the most important factors in flame stabilization is the energy and mass transfer properties of the flame. Energy transfer is characterized by heat conduction

and mass transfer is specified by D_m , the mass diffusion coefficient. Combining both of these parameters produces the Lewis number:

$$Le = \frac{k}{\rho c_p D_m} \quad (15)$$

where k is the heat conductivity of the mixture, ρ is the density, c_p is the heat capacity, and D_m is the mass diffusion coefficient of deficient reactant in the mixture.

It is well established that mixtures with higher Lewis numbers are more thermo-diffusibly stable [9-12]. A FORTRAN program is developed which is joined with CHEMKIN to calculate the Lewis number of different mixtures. As there is not any released transport properties data for JP8 (which is needed as input for CHEMKIN), Lewis numbers of propane (C_3H_8) were calculated with different diluents at equal temperatures and pressures. It was seen that $Le_{C_3H_8-He} > Le_{C_3H_8-Ar} > Le_{C_3H_8-N_2}$ which roughly confirms the stability of JP8- O_2 -diluent mixtures. In addition, flame thickness of C_3H_8/O_2 /diluent flames has been calculated and it has been seen that $\delta_{C_3H_8-He} > \delta_{C_3H_8-N_2} > \delta_{C_3H_8-Ar}$. Earlier cell formation of JP8-Ar flames can be due to thinner flame thickness. Figure 18 shows the flame propagation pictures of JP8- O_2 mixtures with three different diluents and the analyses are confirmed. It is obvious that the mixtures with Argon as diluent are the most sensitive mixtures for cell formation due to thinner flame thickness compared to the other ones. The mixtures with Helium as diluent are the most stable ones due to higher Lewis number and thicker flames.

The reason for the mentioned phenomena is complex because of the involvement of both hydrodynamics and thermo-kinetics. The next task of this research is the calculation of some other important factors like expansion ratio and Lewis number of the mixtures to extract a rational trend.

Diesel Fuel Experiments

Diesel-air experiments have been performed at atmospheric initial pressure. Flame pictures demonstrate that cells are formed at early times after ignition. It shows that diesel-air mixtures are more sensitive to instabilities and cell formation than other kinds of flames.

The reason for this is not well understood, since the structure of diesel fuel is not defined yet. Figure 19 shows the flame propagation of diesel-air mixtures at atmospheric initial pressure, stoichiometric equivalence ratio and initial temperature of 463 K. It is obvious that the tolerance of diesel-air mixtures to instability is less than JP8-air mixtures. The advantage or disadvantage of turbulence occurrence in the flames depends on the application which is expected of the combustible device. Diesel fuel is going to be replaced with JP8 in some of machines. With respect to the application of the device, this should be seen whether lower cell formation tendency of JP8 is a positive sign or not.

The same experiments were performed in spherical vessel and burning speed of the mixture was calculated. Figure 20 shows the burning speeds of diesel/air mixtures at three different equivalence ratios and initial pressure of 1 atm. As expected this is seen that at lean conditions, by increasing the equivalence ratio burning speed increases.

JP-8/air autoignition experiments

The experiments have been performed at four initial pressure conditions of 8,9,10, and 11 atm respectively. The initial temperature was constant at 215 °C to ensure that it meets the boiling temperature of JP-8 [13], and the experiments were carried out using three equivalence ratios of 0.85,1, and 1.2.

The initial conditions are very important since these experiments are strongly equivalence ratio and temperature dependent. The procedure of these experiments are: 1- evacuate the vessel and the pipes by a vacuum pump to pressures lower than 80 millitorr; 2- assure that the temperature is uniform everywhere and fill the vessel with the liquid fuel. Then close the vessel valve. 3- Evacuate the pipes from liquid fuel; 4- fill the vessel with air; 5- wait at least for three minutes to let the mixture becomes homogeneous and uniform; 6- fire the vessel with ignition system and record the pressure; 7- vent the products to the atmosphere.

Results: The autoignition process in an unburned gas mixture is a very fast process with intense fluctuations. Abnormal pressure fluctuations can be a trace of autoignition in the unburned gas zone. One of the important issues about autoignition is its initiation process. In an ideally homogeneous mixture, it can be assumed that autoignition happens everywhere instantaneously with a specific ignition delay time corresponding to the

temperature, pressure, and equivalence ratio of the mixture. In these conditions, it is assumed that the mixture is perfectly uniform and there is no temperature, pressure or equivalence gradient in the mixture. In the practical combustors like internal combustion engines, it is hard to have homogeneous mixtures since there is a certain amount of temperature, pressure, and equivalence ratio gradients.

In this research, there are two different criteria for detecting autoignition. The first is done using the pressure signals and their rates. If an abrupt jump is observed in pressure data along with audible noise, it can be a trace of autoignition. The other method is by analyzing the ionization probes signal. If an ionization probe sends out highly oscillating signals (compared with normal combustion) it will be a sign of autoignition.

Figure 21a shows normal combustion and autoignition of JP-8/air mixture at two different initial conditions. It is seen that at normal combustion the pressure increases smoothly until it touches the vessel wall, reaches to equilibrium condition and then it decreases because of energy loss to the wall. The peak point of pressure is very close to the amounts calculated by the STANJAN equilibrium code. The ionization probes signals are normal and the discontinuity occurs at the same time, so the flame is symmetrical without any buoyancy. The other curve, presents the autoignition in which pressure has intense oscillations along with a very high peak pressure which is much higher than corresponding equilibrium pressure. In addition, it is observed that the ionization probes drive out very fluctuating signals, which indicate that the autoignition has occurred in the end gas zone.

Intense fluctuations in the ionization probes signals are due to autoignition in unburned gas zone and excitation of probes before flame arrival. Figure 21.b shows that the ionization signals occur almost at the same time. Therefore it indicates simultaneous autoignition all over the unburned gas zone. After repeating the experiments and ensuring that for reproducibility, the corresponding pressure and temperature should be measured to get the critical values. Therefore the point of the autoignition should be found to measure the corresponding temperature and pressure. This can be done with two different approaches. The first method is by analyzing the rate of pressure variations (dP/dt) values. If there is any abnormal variation in dP/dt values compared with normal combustion dP/dt 's, it can be autoignition trace. Figure 22 is the corresponding dP/dt curve of Figure 21b. It is

observed that dP/dt abrupt increase starts almost at $t = 44.84$ ms. At this time pressure increases along with oscillations that can be caused by acoustic pressure waves.

Figure 22 also shows the ionization probes. It indicates that the signals do not occur exactly at the same time that dP/dt starts to increase abnormally. The difference is about 0.4 ms. this event is reproducible in most cases. It can be explained due to the fact that in low temperatures the ignition process is in two stages [14-16]. In the first stage of ignition the pressure increases slightly. Then in the second part of the ignition where the main part of energy is released, pressure increases at a higher rate. The duration of these stages depends on the conditions of the mixtures, but in most of the conditions its order is in milliseconds [14-16].

As it is seen in Figure 23, the difference between the first peak of pressure and the other peaks are about 0.2-1 ms. Therefore ionization probes send out signals when there are sufficient radicals and products in the mixture to ionize the wires properly. Since the beginning of the ignition is from the start of the first stage, the autoignition temperatures and pressures are measured in that time.

Figure 24 shows the temperatures and pressures in which autoignition took place for three different equivalence ratios. The explosion temperature in a flame propagating combustor is the temperature where the ignition delay time of the unburned gas mixture is smaller than the time scale of flame propagation.

It can be seen that there is a specific range of temperature for the explosion of JP-8/air mixtures. It varies from 660K-710 K in a wide range of pressures and equivalence ratios. This figure shows the sensitivity of the mixture to temperature is much more than to pressure. The range of autoignition pressure is about 20 atm, but the range of temperature is just about 40 K. So it can be concluded that in an engine where JP-8 is used as the fuel the temperature does not exceed the temperature range presented in Figure 24.

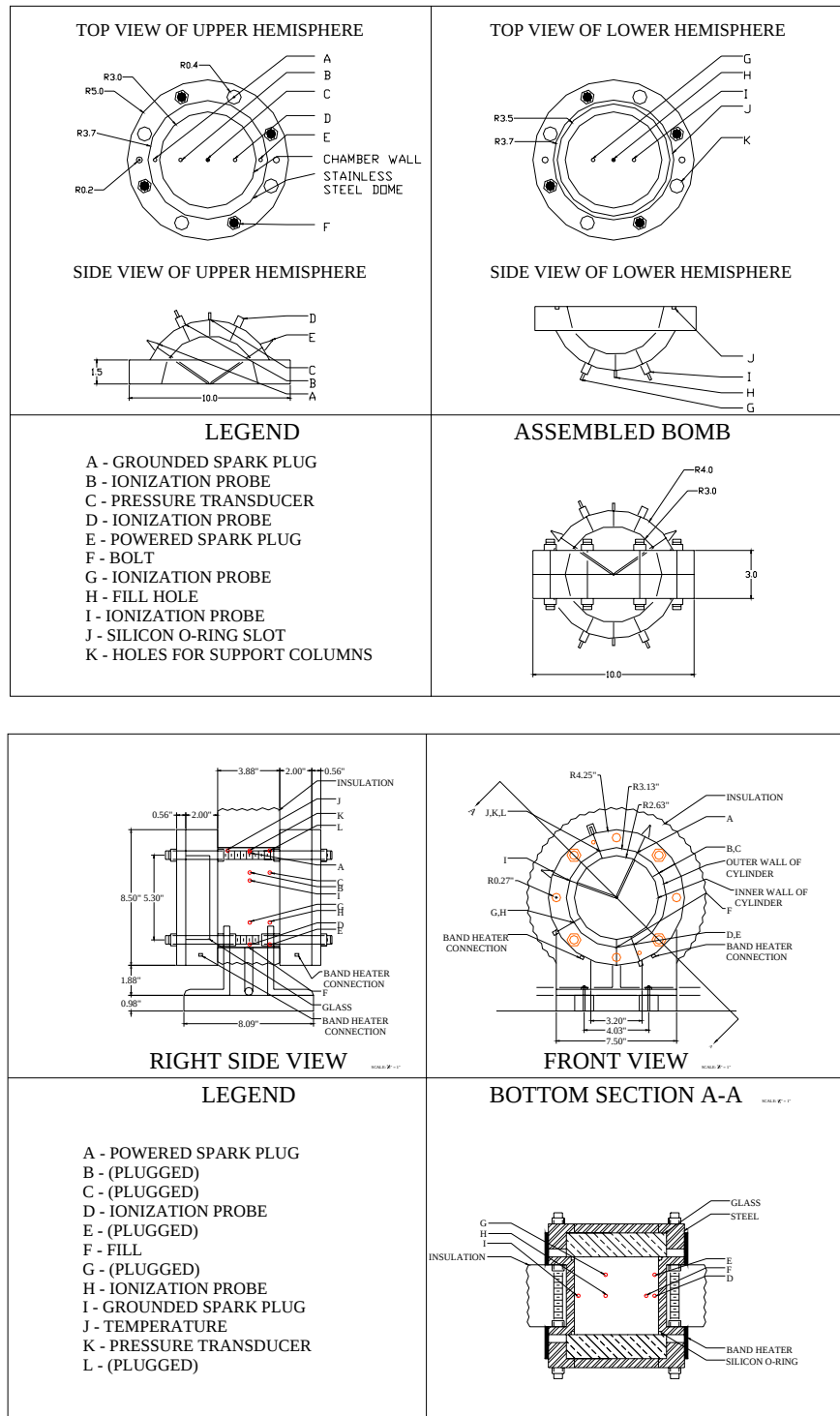


Figure 1a. (top) Schematic of 15.24 cm (6 inch) ID spherical combustion chamber and 1b. (bottom) 13.33 cm (5.25 inch) ID cylindrical combustion chamber, with aspect ratio of 1.

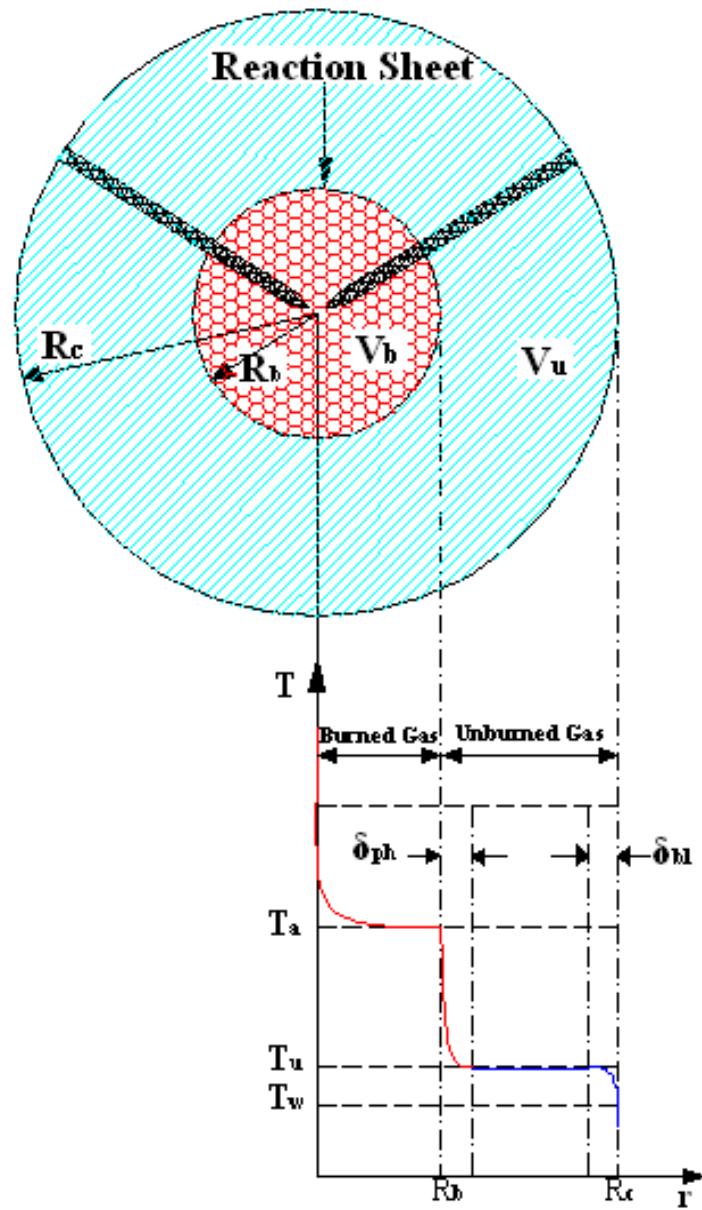


Figure 2. Three different regions of gases in combustion vessel

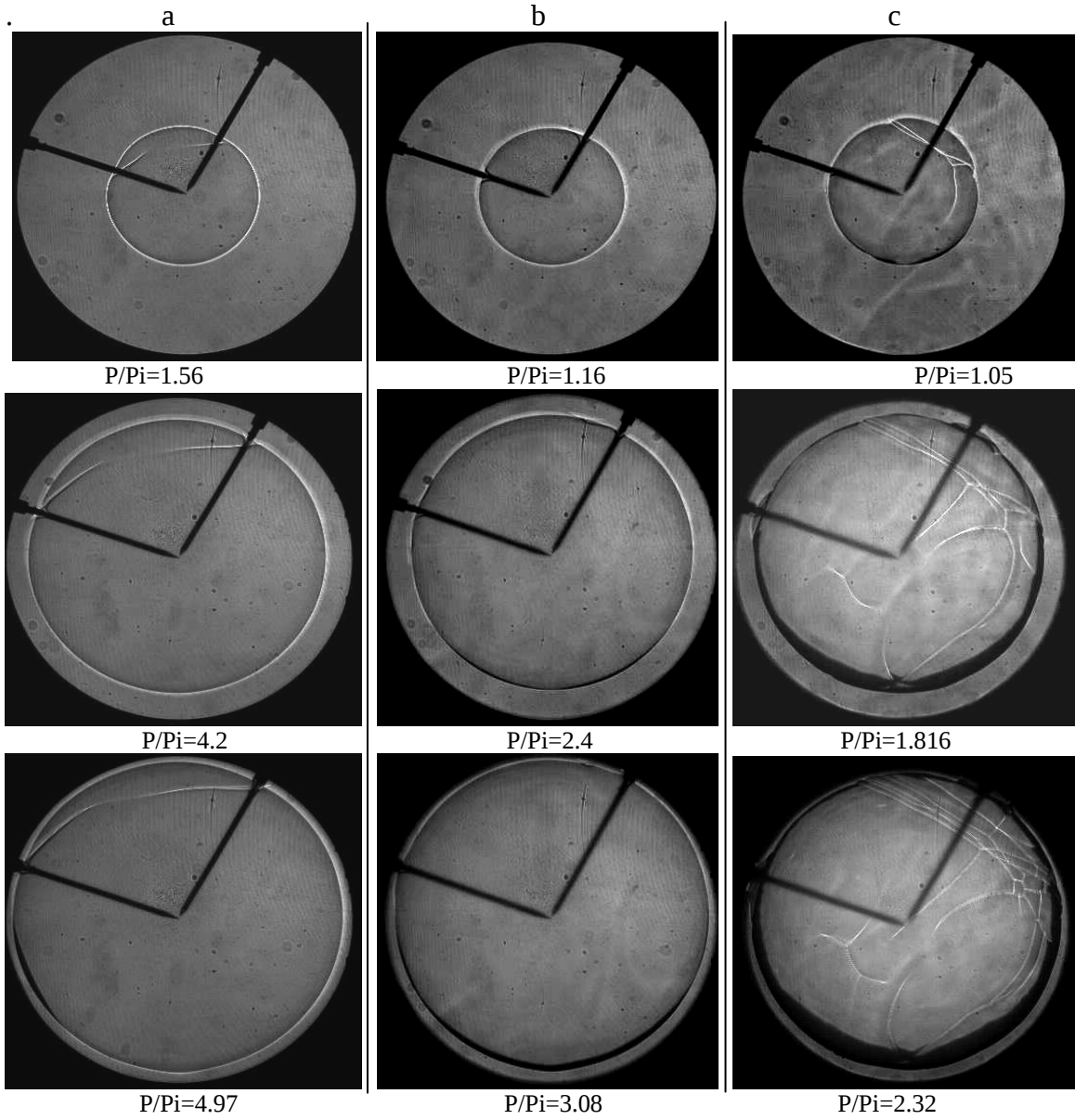


Figure 3: JP8/air mixture $\Phi=0.8$, $T_i=463$ K, a): $P_i=1$ atm, b): $P_i=2.5$ atm, c): $P_i=5$ atm

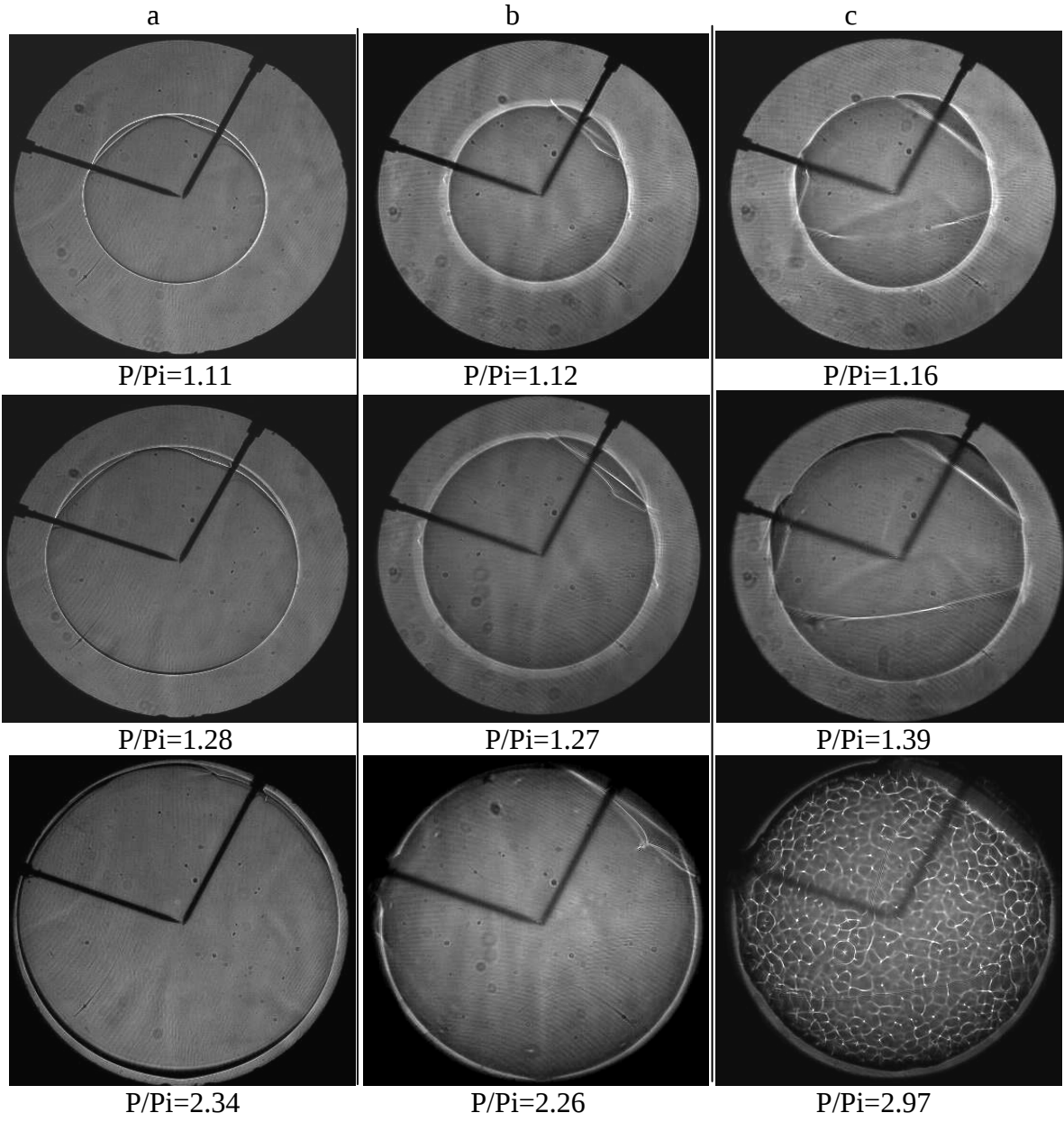


Figure 4: JP8/air mixture $\Phi=0.9$, $T_i=463$ K, a): $P_i=1$ atm, b): $P_i=2.5$ atm, c): $P_i=5$ atm

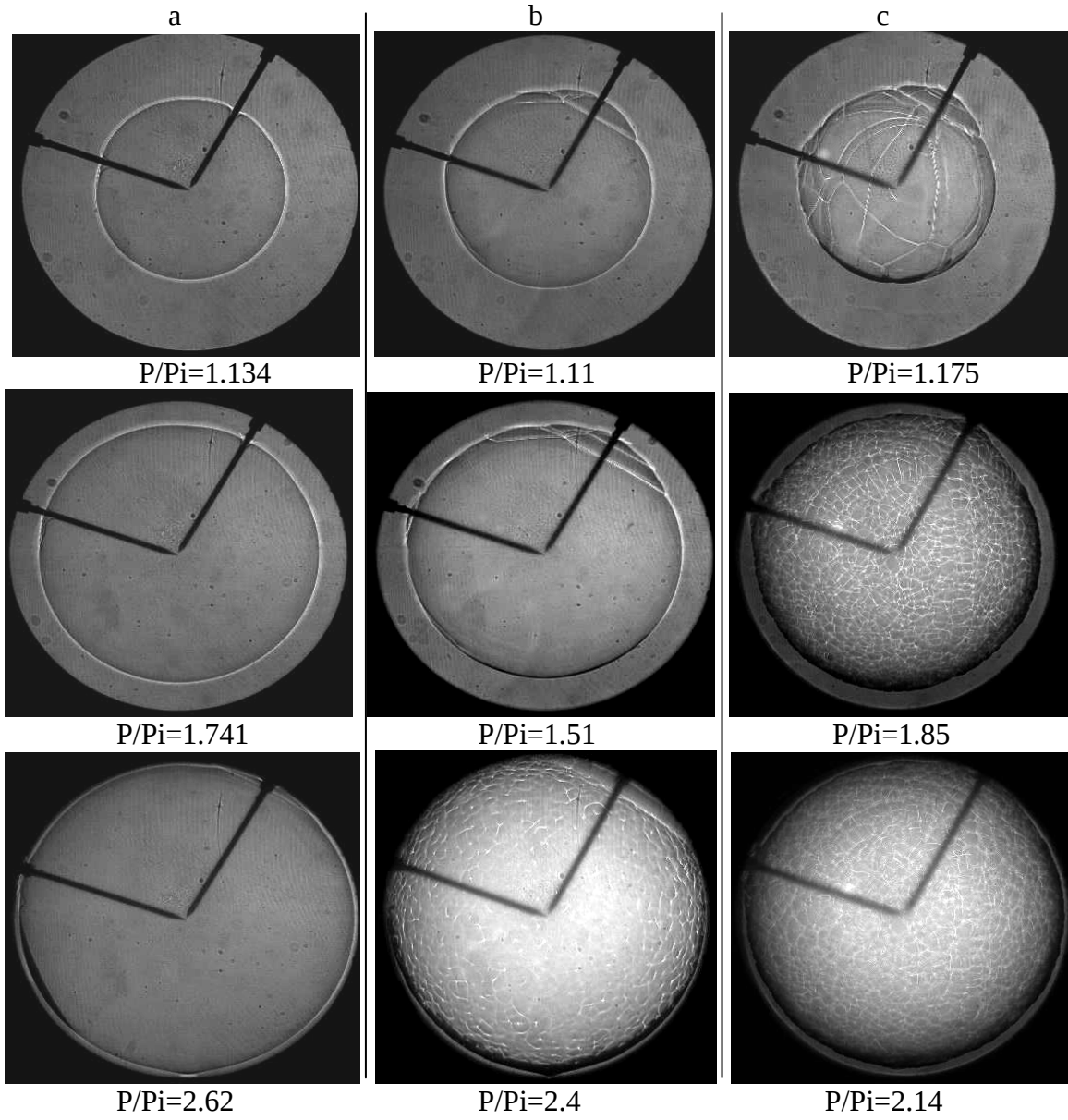


Figure 5: JP8-air mixture $\Phi=1$, $T_i=463$ K, a): $P_i=1$ atm, b): $P_i=2.5$ atm, c): $P_i=5$ atm

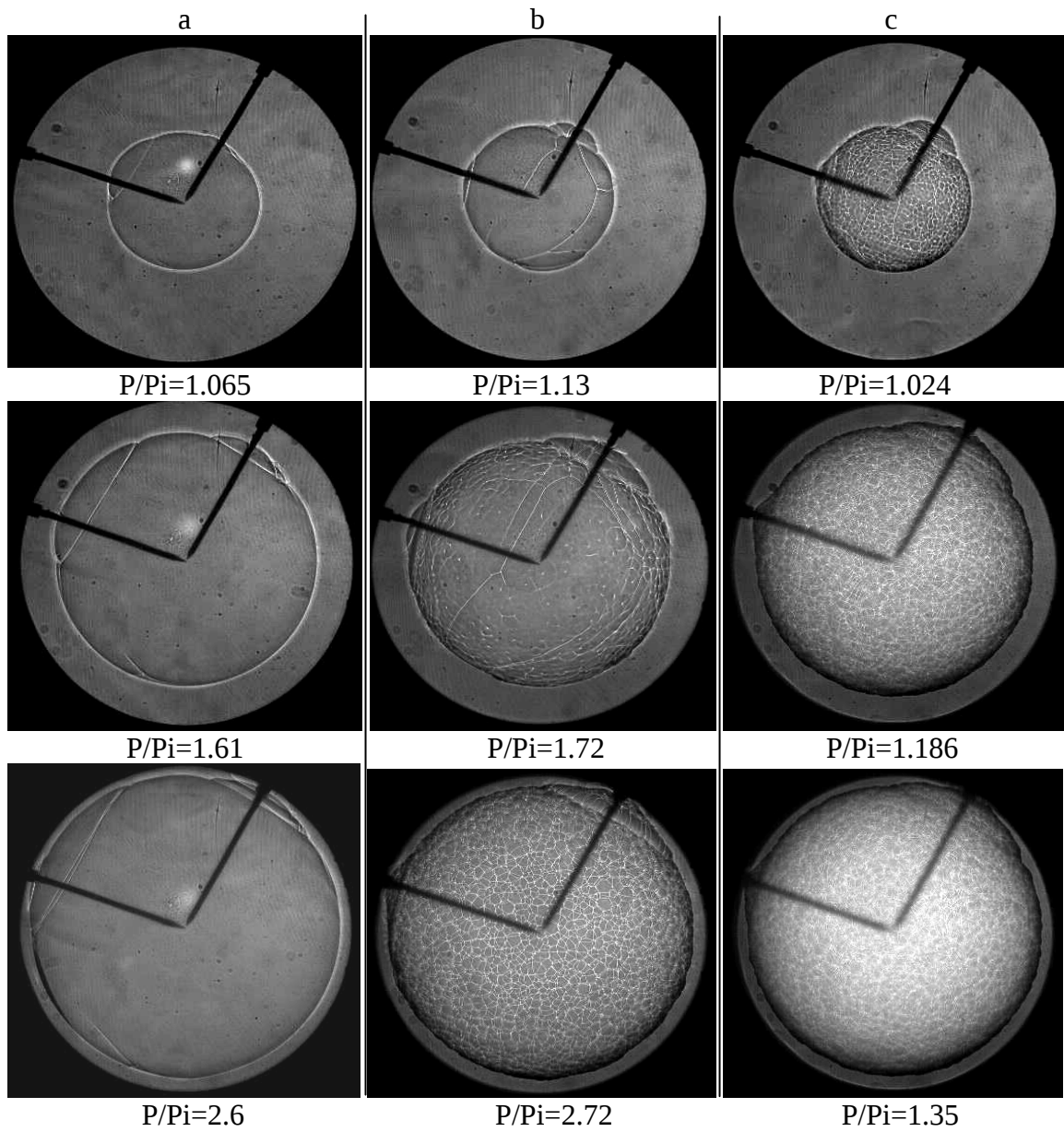


Figure 6: JP8-air mixture $\Phi=1.2$, $T_i=463$ K, a): $P_i=1$ atm, b): $P_i=2.5$ atm, c): $P_i=5$ atm

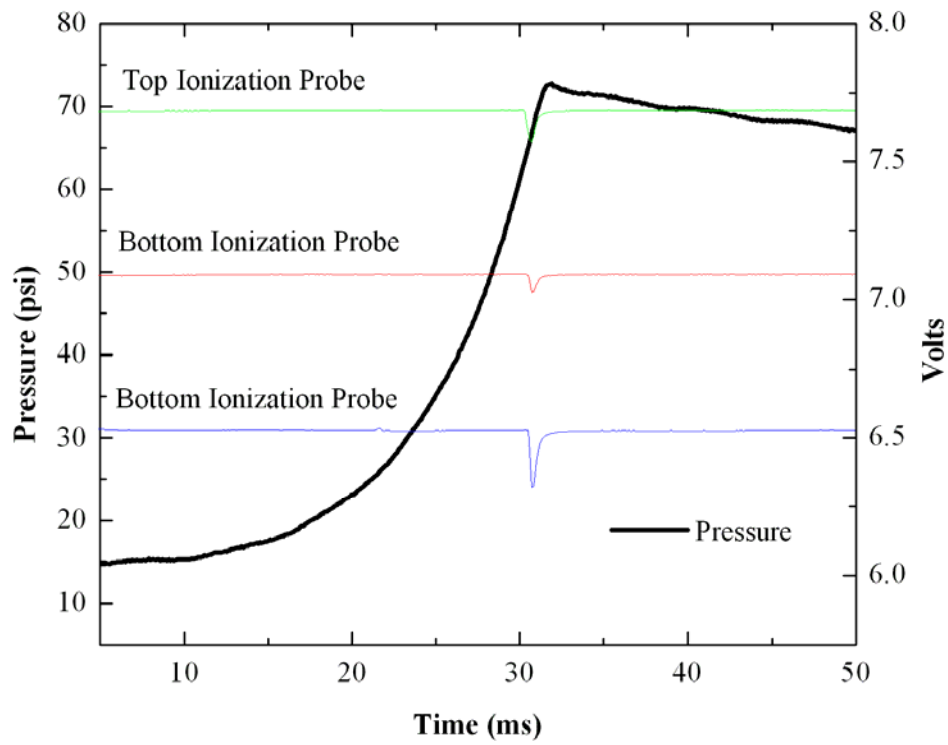


Figure 7: The pressure data versus time for JP8-air mixture, $P_i=1$ atm, $T_i=463$ K

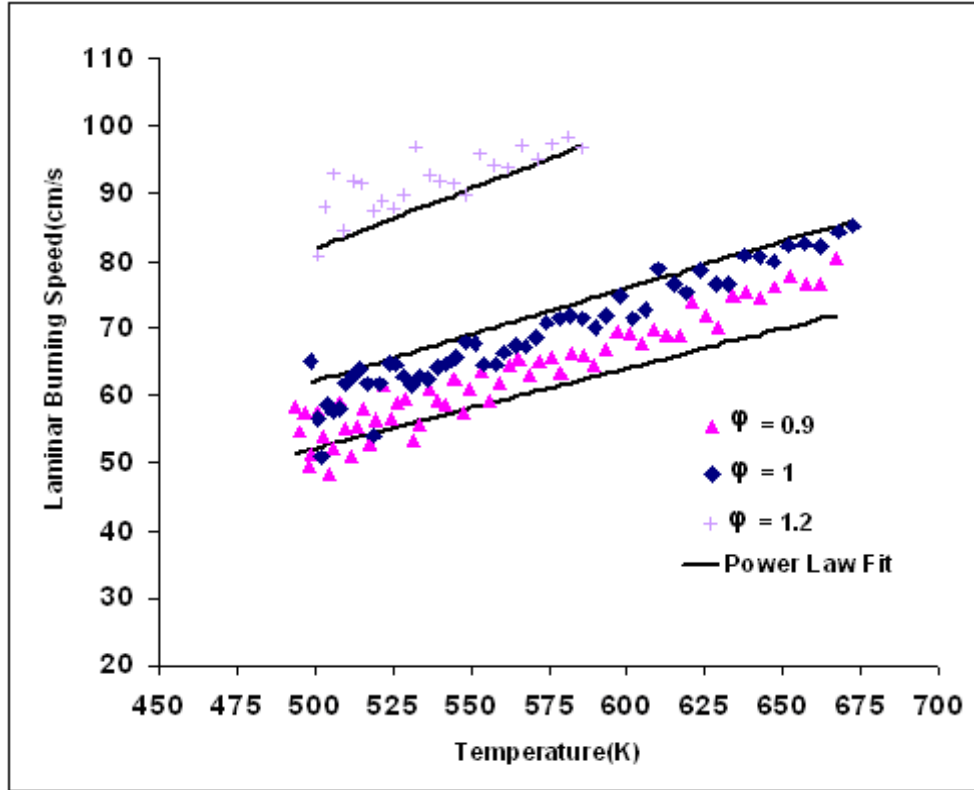


Figure 8: JP8-air mixture laminar burning speed at different equivalence ratios, $T_i=463$ K, $P_i=1$ atm

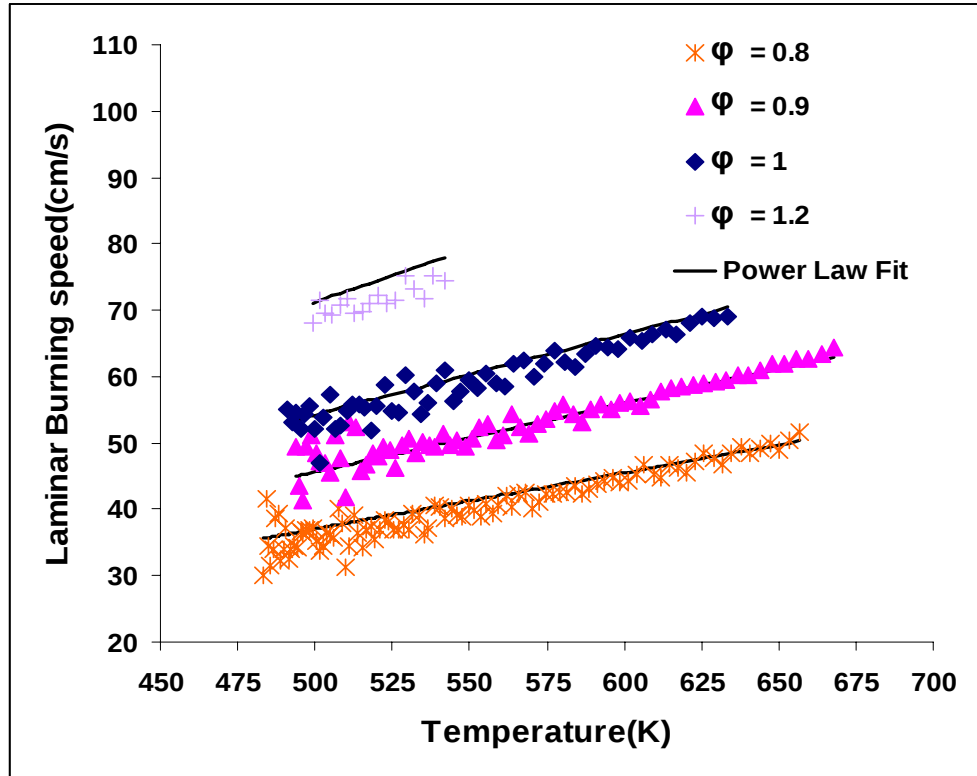


Figure 9: JP8-air mixture laminar burning speed at different equivalence ratios, $T_i=463$ K, $P_i=2$ atm

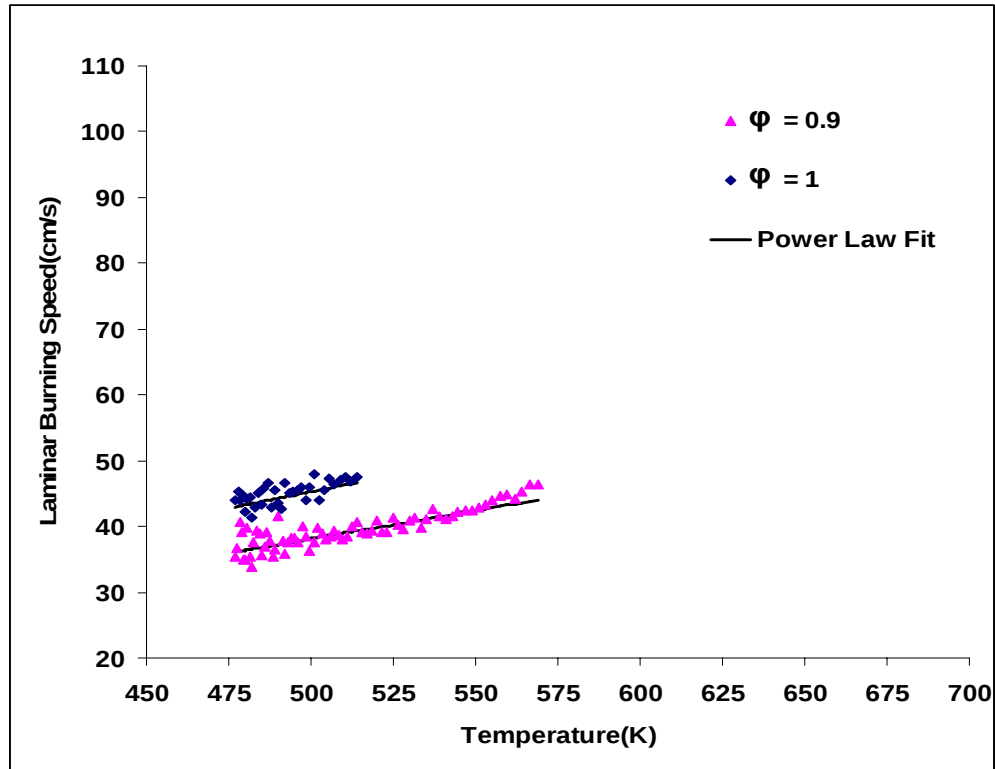
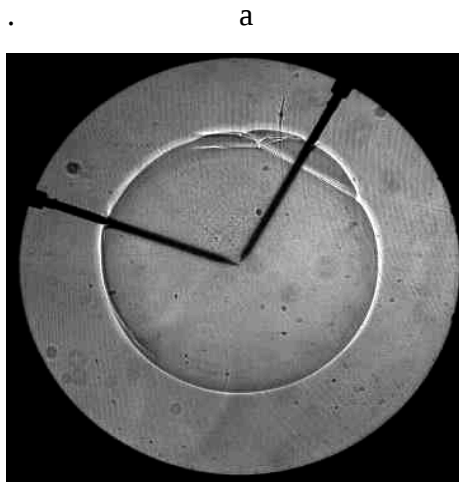
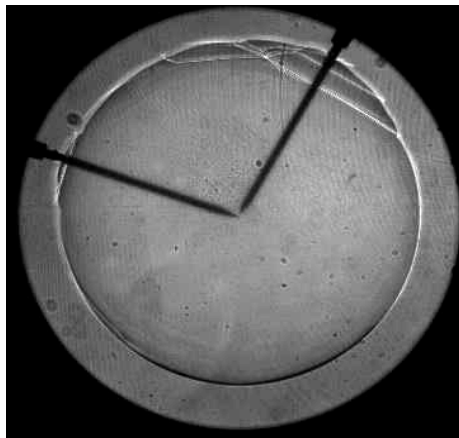


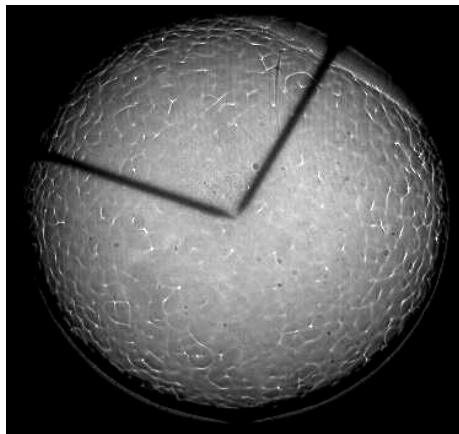
Figure 10: JP8-air mixture laminar burning speed at different equivalence ratios, $T_i=463$ K, $P_i=5$ atm



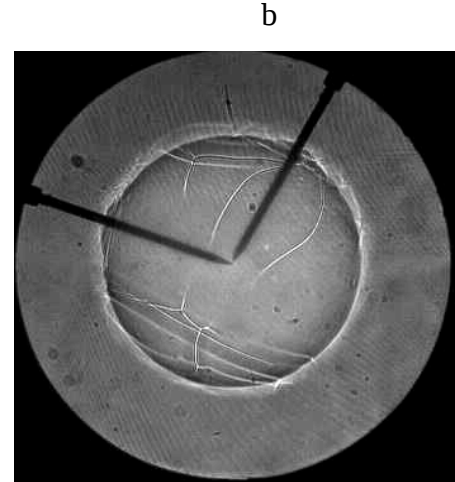
$P/P_i=1.21$



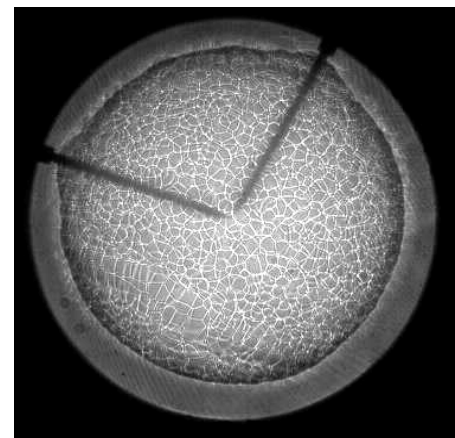
$P/P_i=1.53$



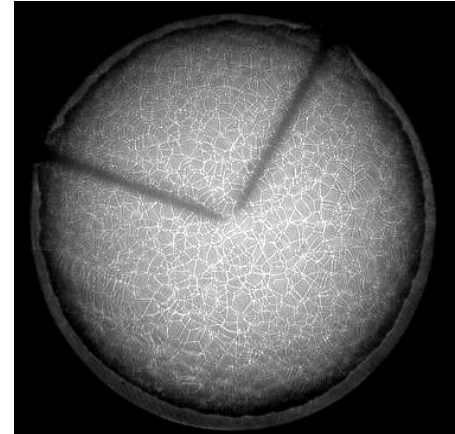
$P/P_i=2.47$



$P/P_i=1.22$



$P/P_i=1.69$



$P/P_i=2.52$

Figure 11: JP8-O₂-diluent mixture $\Phi=1$, $T_i=463$ K, $P_i=2.5$ atm, a): with N₂, b): with Argon

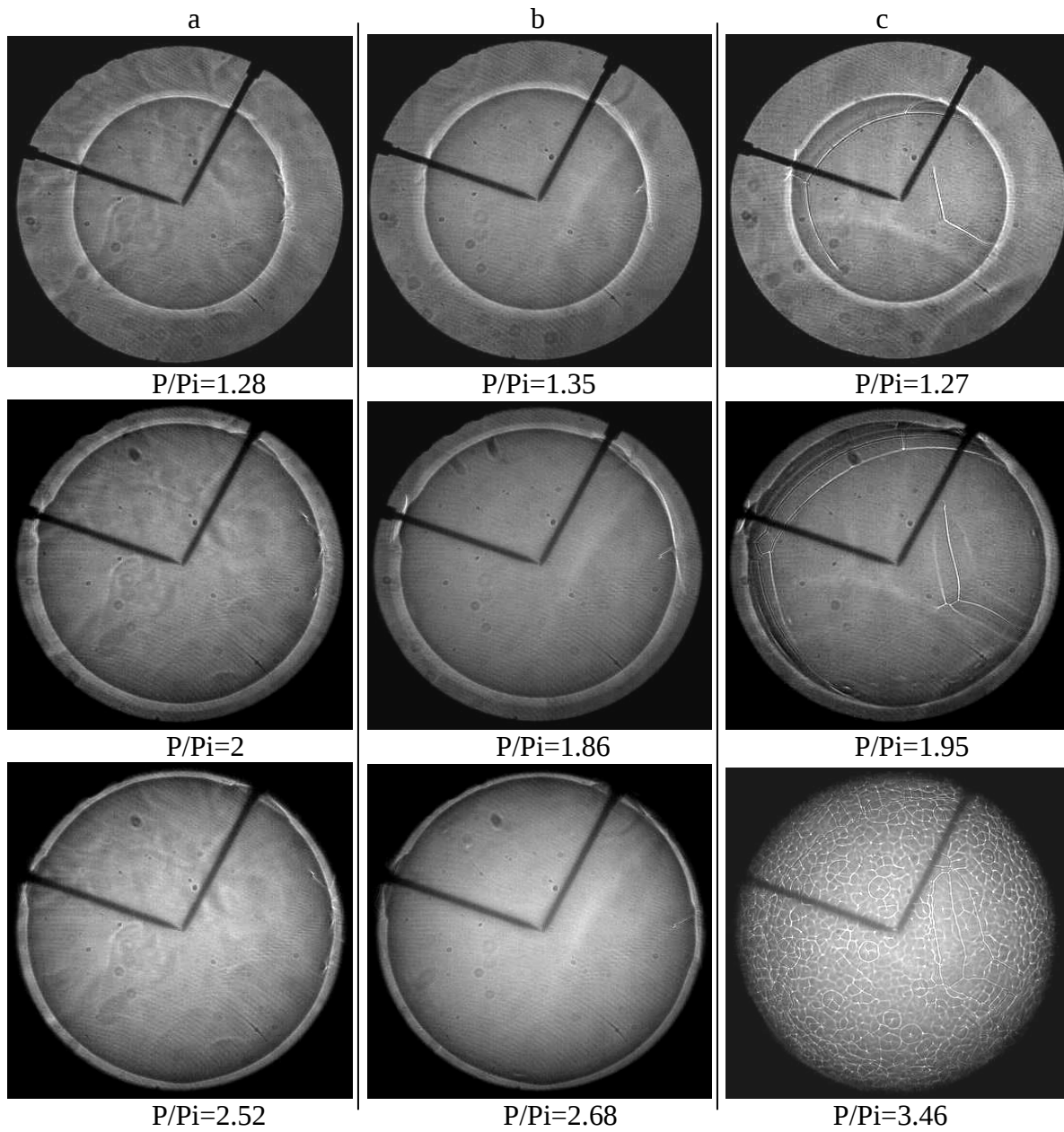


Figure 12: JP8-O₂-He mixtures, $T_i=463$ K, $P_i=4$ atm a): $\Phi=0.8$, b): $\Phi=0.9$, c): $\Phi=1$

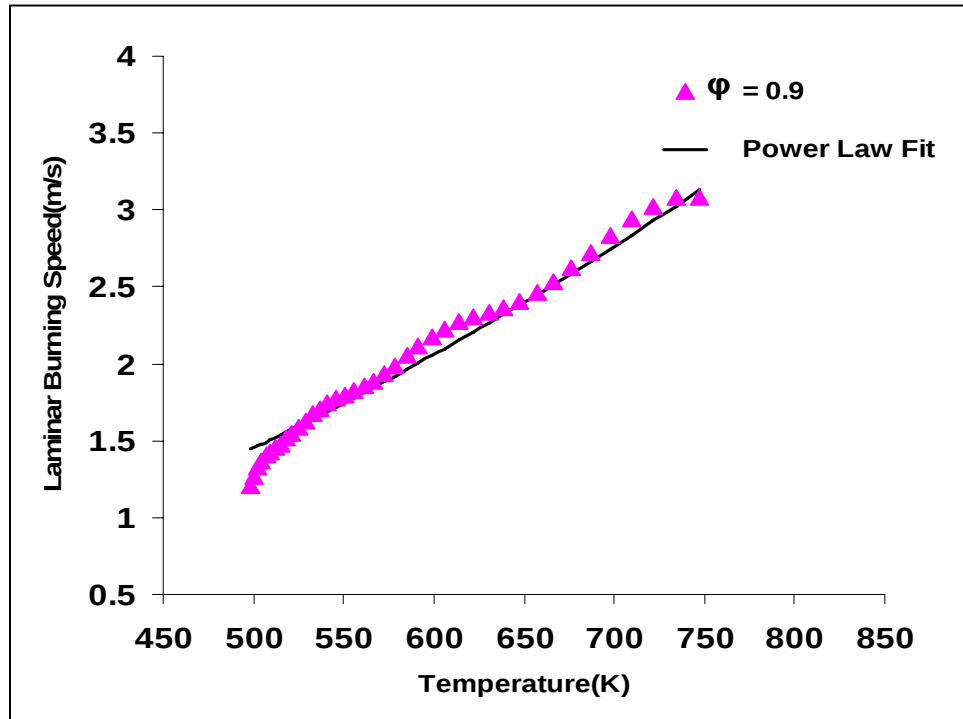


Figure 13: JP8-O₂-He mixture laminar burning speed, $T_i=463$ K, $P_i=1$ atm

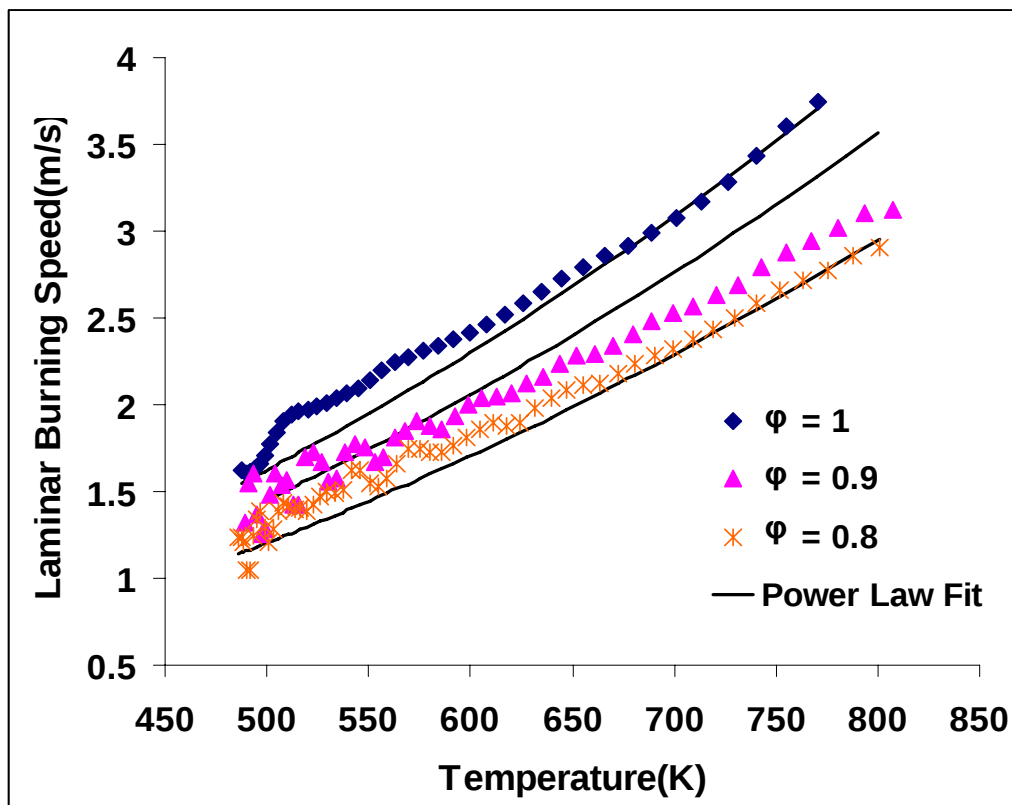


Figure 14: JP8-O₂-He mixture laminar burning speed, $T_i=463$ K, $P_i=2$ atm

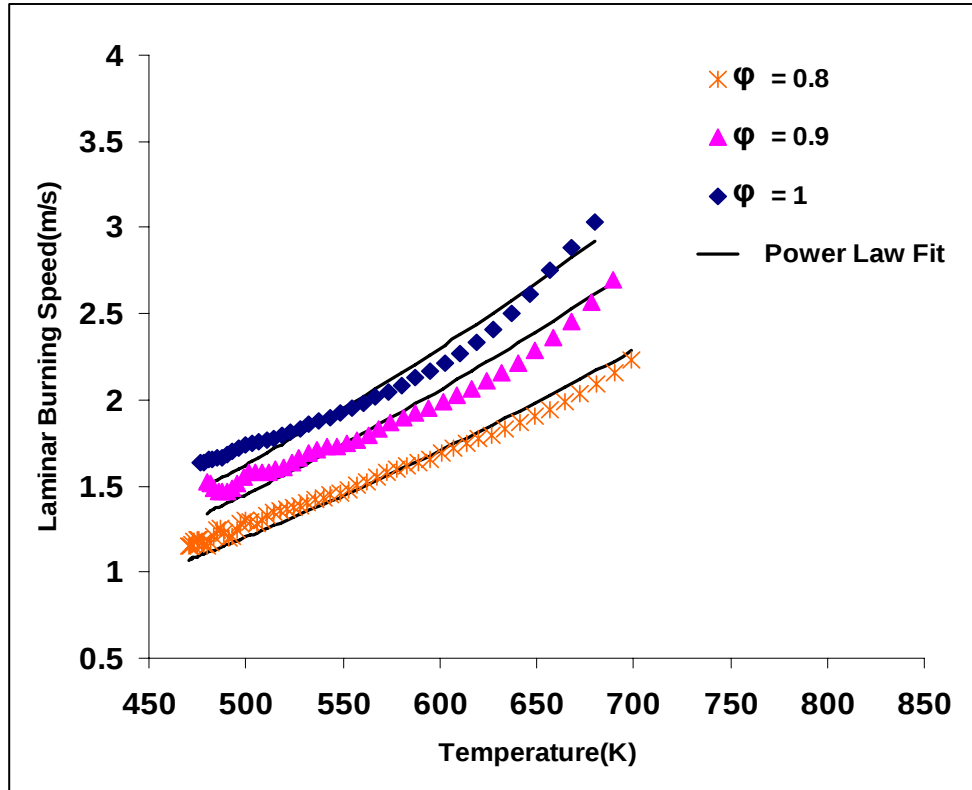


Figure 15: JP8-O₂-He mixture laminar burning speed, $T_i=463$ K, $P_i=4$ atm

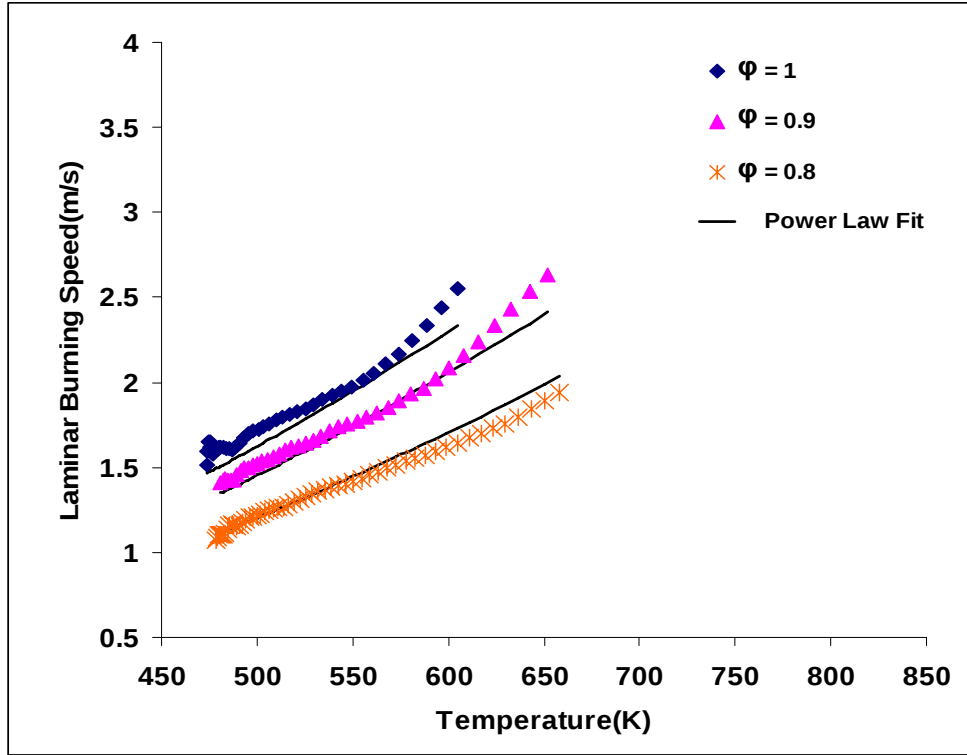


Figure 16: JP8-O₂-He mixture laminar burning speed, $T_i=463$ K, $P_i=5$ atm

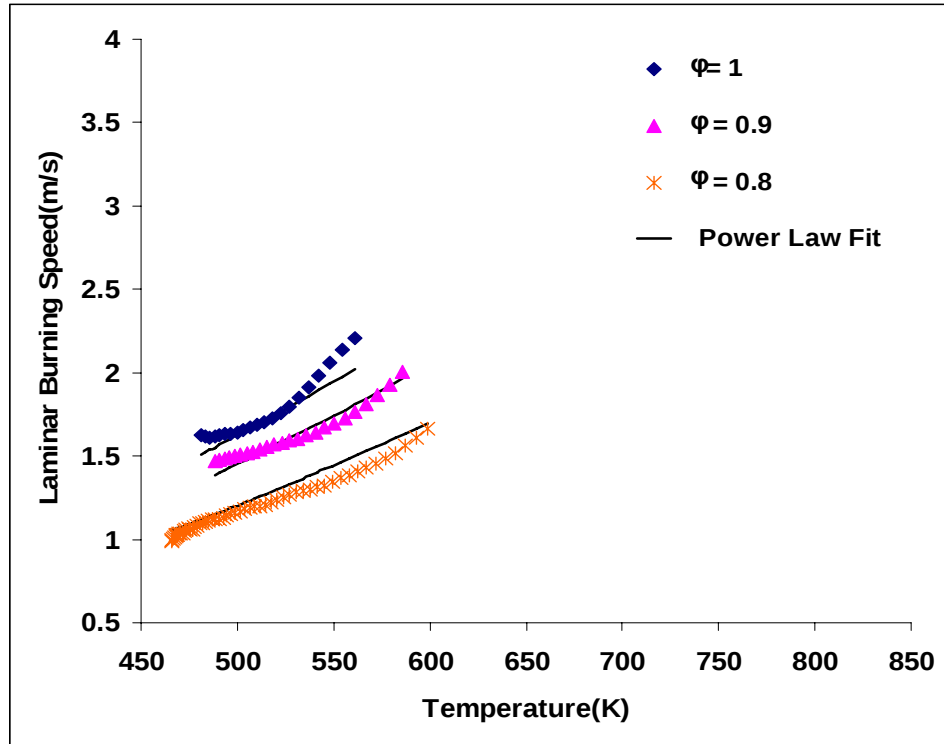


Figure 17: JP8-O₂-He mixture laminar burning speed, $T_i=463$ K, $P_i=7$ atm

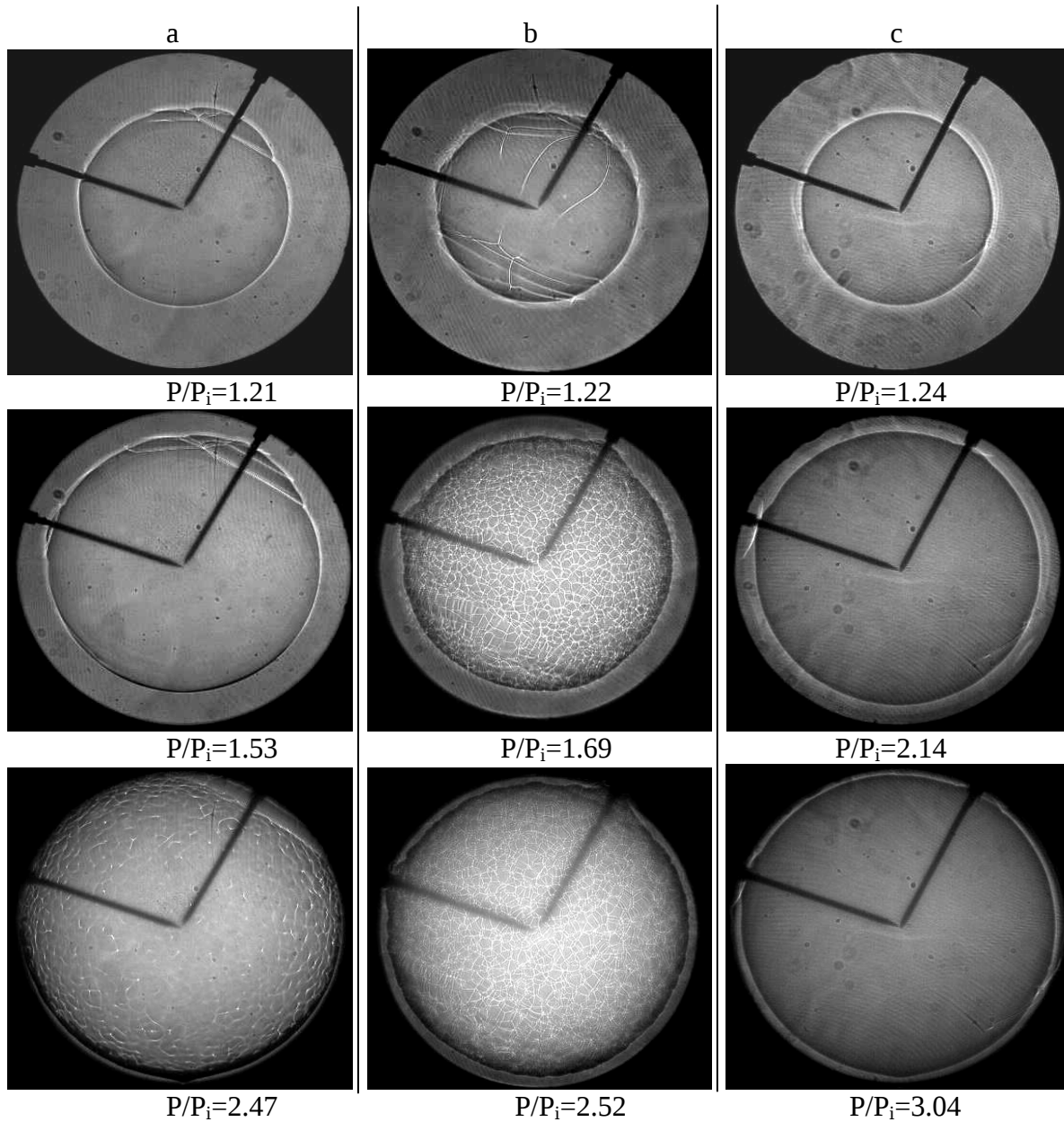


Figure 18: JP8-O₂-diluent mixture $\Phi = 1$, $T_i = 463$ K, $P_i = 2.5$ atm, a) with N₂, b) with Argon, c) with Helium

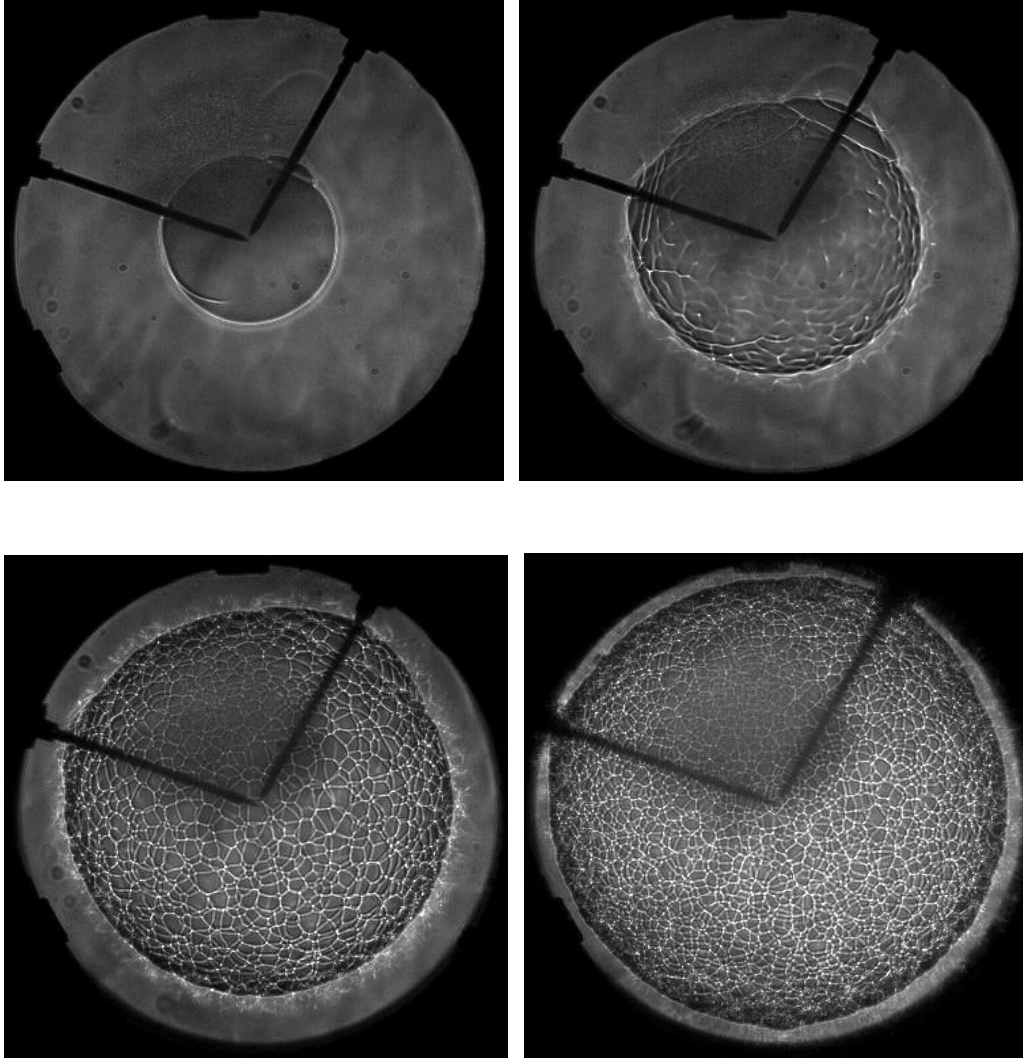


Figure 19: Diesel/air mixture $\phi = 1$, $T_i=463$ K, $P_i=1$ atm

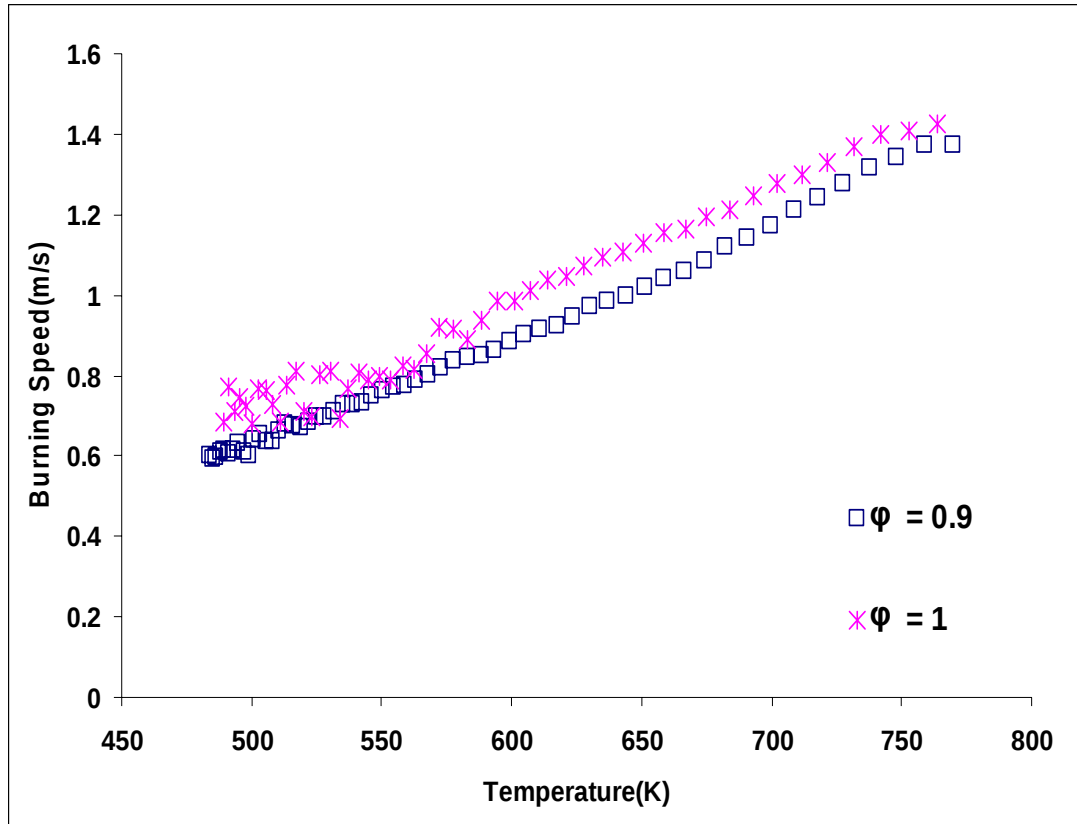
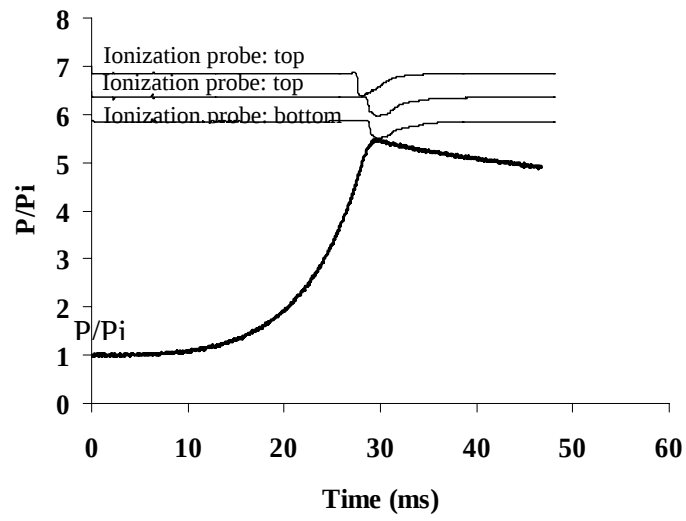
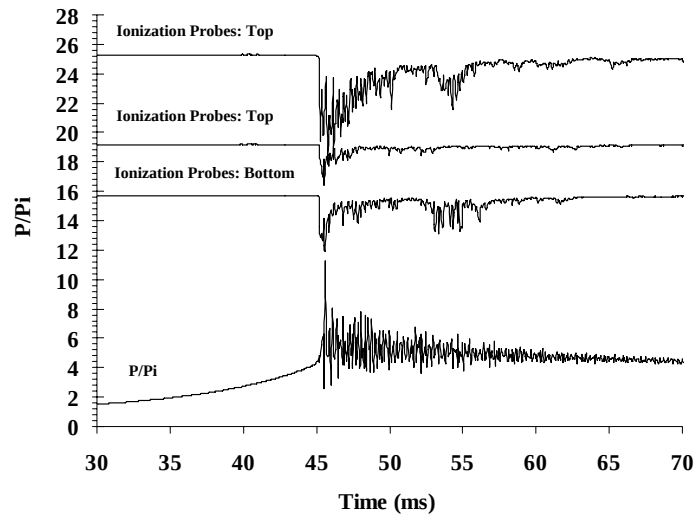


Figure 20: Burning speed of diesel/air mixtures, $P_i=1$ atm, $T_i=450$ K



(a)



(b)

Figure 21: Pressure and ionization probes data of JP-8/air, $\Phi = 1$, $T_i = 483$ K, a: $P_i = 1$ atm, b: $P_i = 10$ atm

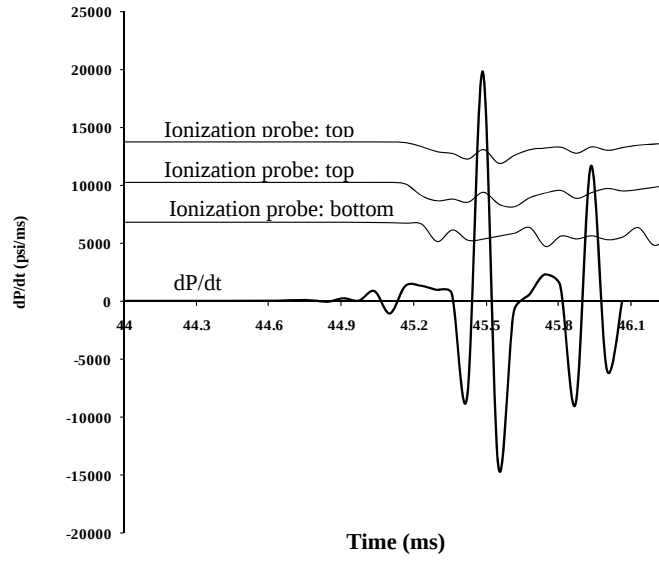


Figure 22: Pressure rate JP-8/air, $\Phi = 1$, $P_i = 10\text{atm}$, $T_i = 483\text{ K}$

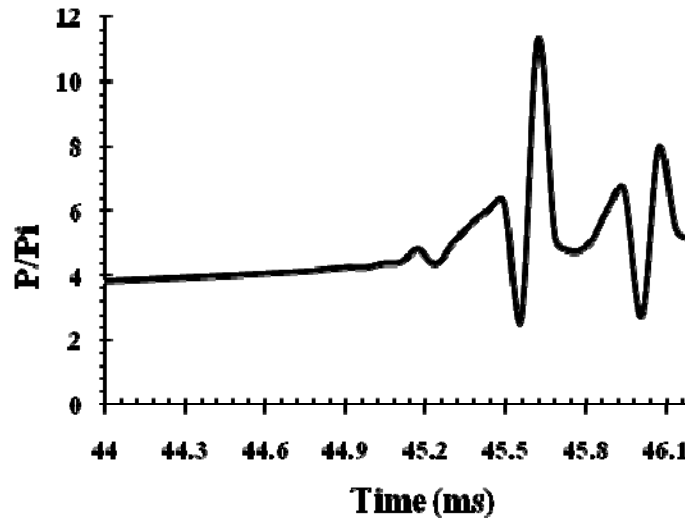


Figure 23: Focused pressure of JP-8/air, $\Phi = 1$, $P_i = 10\text{atm}$, $T_i = 483\text{ K}$

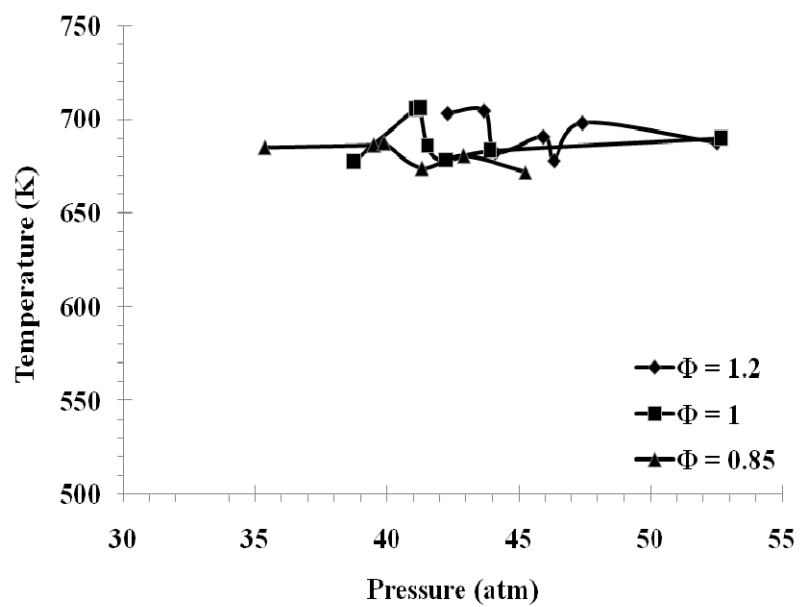


Figure 24: Explosion temperature versus pressure of JP-8/air mixtures

Table1: Laminar and non-laminar conditions of JP8-air flames

ϕ	Pi=1 atm	Pi=2.5 atm	Pi=5 atm
0.8	Non-Cellular	Non-Cellular	$P_{cr}=16.2$ atm
			$T_{cr}=643$ K
0.9	Non-Cellular	$P_{cr}=10.2$ atm	$P_{cr}=11.2$ atm
		$T_{cr}=672$ K	$T_{cr}=565$ K
1	Non-Cellular	$P_{cr}=7.48$ atm	$P_{cr}=7.89$ atm
		$T_{cr}=621$ K	$T_{cr}=504$ K
1.2	$P_{cr}=2.78$	$P_{cr}=3.87$ atm	From the beginning
	$T_{cr}=594$ K	$T_{cr}=541$ K	

Table 2: power law fit function coefficients of JP8-air mixture

S_{b0}	a_1	a_2	α	β
53.46m/s	-1.58	-0.006	1.94	-0.19

Table 3: Cell formation analysis of JP8-O₂-He mixtures

ϕ	Pi=2.5 atm	Pi=4 atm
0.8	P _{cr} =16.05 atm	P _{cr} =19.31 atm
	T _{cr} =832 K	T _{cr} =760 K
0.9	P _{cr} =15.17 atm	P _{cr} =15.71 atm
	T _{cr} =817 K	T _{cr} =716 K
1	P _{cr} =13.8 atm	P _{cr} =13.3 atm
	T _{cr} =797 K	T _{cr} =621 K

Table 4: power law fit function coefficients of JP8-O₂-He mixture

S_{b0}	a_1	a_2	α	β
1.328 m/s	-0.815	-2.395	1.91	-0.0004

Table 5: Cell formation and Instability Analyses for JP8-air mixtures

ϕ	Pi = 1 atm	Pi = 2.5 atm	Pi = 5 atm
0.8	Stable	Stable	T = 643 K
			P _{cr} = 20.2 atm
			$\alpha = 0.00000245 \text{ m}^2/\text{s}$
			$\delta = 0.00529 \text{ mm}$
1	Stable	T = 621 K	T = 504 K
		P _{cr} = 8.57 atm	P _{cr} = 8.12 atm
		$\alpha = 0.00000561 \text{ m}^2/\text{s}$	$\alpha = 0.00000478 \text{ m}^2/\text{s}$
		$\delta = 0.0079 \text{ mm}$	$\delta = 0.01 \text{ mm}$
1.2	T = 699 K	T = 554 K	Unstable from the beginning
	P _{cr} =2.78	P _{cr} =3.87 atm	
	$\alpha = 0.00000922 \text{ m}^2/\text{s}$	$\alpha = 0.00000775 \text{ m}^2/\text{s}$	
	$\delta = 0.0071 \text{ mm}$	$\delta = 0.00933 \text{ mm}$	

Table 6: Cell formation and Instability Analyses for JP8-O₂-He mixtures

ϕ	Pi = 2.5 atm	Pi = 4 atm
0.8	T = 832 K	T = 760 K
	P = 16.05 atm	P = 19.34 atm
	$\alpha = 0.0000395 \text{ m}^2/\text{s}$	$\alpha = 0.0000278 \text{ m}^2/\text{s}$
	$\delta = 0.0124\text{mm}$	$\delta = 0.01\text{mm}$
0.9	T = 817 K	T = 716 K
	P = 223.855 psi	P = 231 psi
	$\alpha = 0.0000405 \text{ m}^2/\text{s}$	$\alpha = 0.0000312 \text{ m}^2/\text{s}$
	$\delta = 0.01 \text{ mm}$	$\delta = 0.01 \text{ mm}$
1	T=797 K	T=665 K
	P=203 psi	P=181 psi
	$\alpha = 0.000043 \text{ m}^2/\text{s}$	$\alpha = .000035 \text{ m}^2/\text{s}$
	$\delta = 0.01 \text{ mm}$	$\delta = 0.0125 \text{ mm}$

Biographical Sketch

NAME: Mohamad (Hameed) Metghalchi

POSITION TITLE: Professor, Mechanical and Industrial Engineering Department Chair

Research and Professional Experience:

Mohamad (Hameed) Metghalchi received his Bachelor of Science in Mechanical Engineering from Oklahoma University in 1975. He received Masters and Doctor of Science Degree in Mechanical Engineering from Massachusetts Institute of Technology in 1977 and 1980 respectively. In fall of 1979, he joined department of Mechanical Engineering at Northeastern University. Professor Metghalchi is Chair of Mechanical and Industrial Engineering Department.

Professor Metghalchi is an active member of national societies, such as, the American Society of Mechanical Engineers, the American Society of Engineering Education, the Society of Automotive Engineers and the Combustion Institute. He is a Fellow of ASME and past chair of ASME Advanced Energy System Division. He is an Associate Editor of ASME Journal of Energy Resources Technology. He is a member of the Editorial Board of the International Journal of Exergy. He is also a member of the Scientific Council of International Center for Applied Thermodynamics. He has been proposal and scientific paper reviewer for the National Science Foundation, Army Research Office, Combustion Science Technology, Combustion Institute, Combustion and Flame, ASME Journal of Energy Resources Technology, ASME Journal of Engineering for Gas Turbine and Power, Biotechnology and American Chemical Society- the Petroleum Research Fund.

Professor Metghalchi's research is in the area of thermofluids dealing with scientific issues in Combustion, fluid mechanics, thermodynamics, heat transfer and chemical reactions. Professor Metghalchi has supervised 10 Ph.D. theses and 19 M. Sc. theses at Northeastern University. Currently, six graduate students are working under his supervision. Professor Metghalchi has published extensively in education and research in the last twenty five years.

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B. List of persons, other than those cited in the publication list, who have collaborated on a project or a book, article, report or paper within the last 4 years. Negative reports should be indicated.

Collaborator: None

C. Names of graduate and Post graduate advisors and advisees.

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