Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

ENERGY & ENVIRONMENT DIVISION

COMBUSTION RESEARCH

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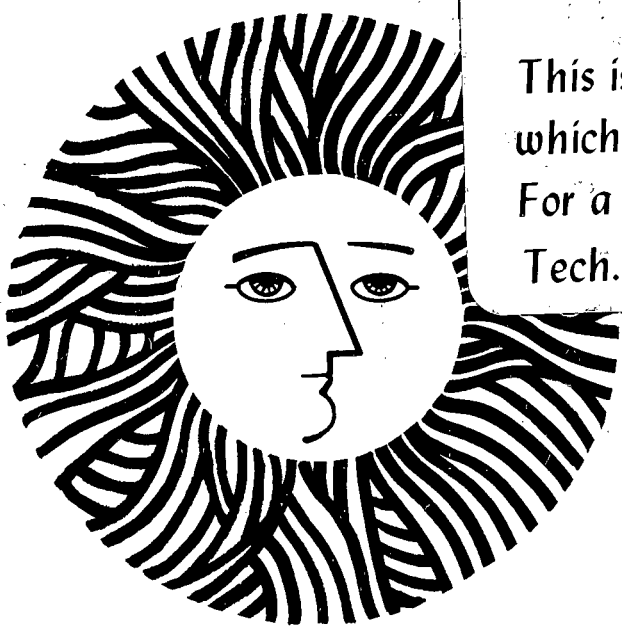

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DISCLAIMER

TABLE OF CONTENTS

COMBUSTION RESEARCH

Combustion Research

Introduction

Continued expansion of research on combustion processes has occurred both nationally and at Lawrence Berkeley Laboratory (LBL). The principal programmatic research goal is to reduce the level of pollutant emissions associated with the combustion of fossil fuels, while at the same time conserving our natural resources through high combustion efficiency and low capital investment.

The research programs described in the following are aimed at developing a better understanding of the various fluid mechanical and chemical processes which are thought to be of critical importance in reducing pollutant formation. The principal program areas are the interaction of fluid mechanical turbulence with combustion reactions, important phenomena and pollutant generating processes associated with internal combustion engines, fire safety and flame spread, and diagnostics and formation mechanisms associated with the generation of nitrogen containing pollutants. Most of these programs are closely associated with the University of California Department of Mechanical Engineering faculty, and the training of graduate students is an important aspect of the research.

Internal Combustion Engine Heat Transfer*

R. Greif, K. Chu, H. Heperkan, M. Nikanjam, and T. Namba

INTRODUCTION

The determination of the unsteady heat transfer in an internal combustion engine represents a problem that is of considerable practical importance as well as being one of fundamental interest. For example, heat transfer processes are critical to the quenching of wall reactions leading to high hydrocarbon emissions, the durability of engine components, the loss of energy leading to decreased efficiency, the reliability of calculations for cylinder pressure, etc. The transient, variable volume (moving surface), variable pressure aspects of the compression-expansion process result in complex phenomena that are difficult to appraise and predict.

ACCOMPLISHMENTS DURING 1978

In order to study reciprocating engine processes under well controlled laboratory conditions simulating the operation of a spark ignition engine, a single-pulse, compression-expansion apparatus was built by Oppenheim et al.[1] Measurements have been carried out in this system during the compression stroke (of a single pulse). In particular, experimental and theoretical studies have been completed of the unsteady wall heat transfer in nonreacting gases,[2,3] as discussed below.

The temporal variation of the pressure of the compressed gas was recorded by using a pressure transducer that was placed in one of the ports in the test section. The variable displacement of the piston was obtained by using a steel rack that moved with the piston and interrupted a magnetic pickup during the motion. The temperature of the wall was measured as a function of time by using a thin-film resistance thermometer. The resistance thermometer consisted of a thin platinum film on an insulated backing and was mounted flush with the wall to avoid disturbing the flow; it was connected as the active element in a d-c bridge. The increase in wall temperature during compression then caused a change in resistance of the platinum film which caused an unbalance in the bridge. The determination of the resistance versus time variation then yielded the desired variable wall temperature variation.

Based on the above measurements, the wall heat flux is obtained during piston compression. Specifically, the result is based on a solution of the conduction equation in the solid wall (insulated backing) subject to a variable surface temperature, and the heat flux is expressed as a Duhamel integral in terms of the variable surface temperature and the wall properties.[2]

An alternative approach for the determination of the wall heat flux is based on a solution of the conservation equations in the gas as applied to the thin boundary layer near the wall. Neglecting viscous dissipation and taking the pressure to be uniform yields the appropriate equations of continuity and energy. These equations have been solved to obtain a heat flux based on the gas properties.[2,3]

Typical results for the unsteady heat flux as determined from both the solution of the conduction equation in the solid and the solution of the laminar boundary layer conservation equations in the gas, are presented in Fig. 1. The results for the heat flux from these two

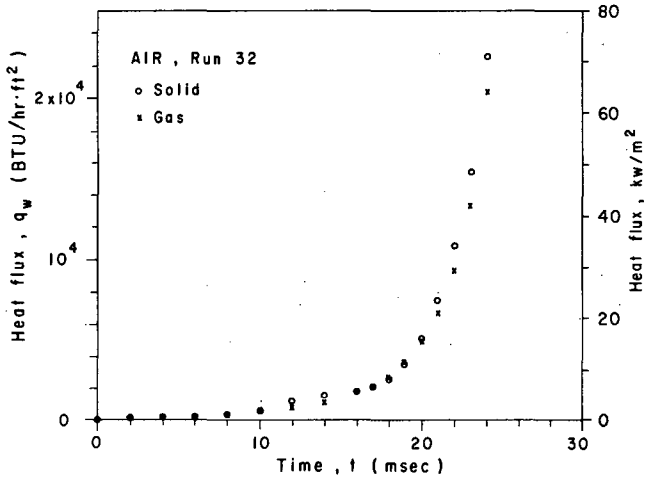

Fig. 1. Heat flux variation. (XBL 793-9047)

independent methods are seen to be in good agreement. Results for the heat transfer coefficient have also been obtained and exhibit a nonmonotonic variation. Detailed analyses have also been made of the thermal boundary layer thickness, the induced convective transport resulting from the drop in the gas temperature near the wall, and the conditions near both end and side walls.

In conclusion, note that the studies provide a rigorous and useful method for determining the heat transfer to a steel wall during piston compression (when there is no insulated backing present). Indeed such calculations have been carried out by solving simultaneously the conduction equation in the steel wall and the boundary layer equations in the gas subject to the required matching of the temperature and the heat flux at the surface.[3] The results should prove to be useful in a number of applications.

PLANNED ACTIVITIES FOR 1979

A basic effort in the next year will be the study of the heat transfer in the presence of reacting gases. This will also entail a contribution to the energy transport by thermal radiation. We also plan to carry out measurements in shock tubes since the transport in the wall region is directly related to the phenomena in the piston-cylinder configuration.

FOOTNOTES AND REFERENCES

*This work was supported by the Division of Fossil Fuel Utilization.

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2. M. Nikanjam and R. Greif, "Heat transfer during piston compression," Transactions of the ASME, J. of Heat Transfer, 100, p. 527, 1978 and Lawrence Berkeley Laboratory Report #LBL-7338.

3. R. Greif, T. Namba, and M. Nikanjam, "Heat transfer during piston compression including side wall and convection effects," International J. of Heat and Mass Transfer, accepted for publication, 1979.

Wall Quenching Processes

J. W. Daily

INTRODUCTION

Unburned hydrocarbons remain in an automobile engine due to incomplete chemical reactions within the cylinder, along the cylinder walls, and in any small gaps in the piston crevices where the flame quenches and the fuel is left unburned. The flow patterns within the engine cylinder that affect the combustion process are extremely complicated. Both the intake process and the compression stroke introduce turbulence into the flow field, the former by the jet action from the intake valve, and the latter due to the vortex roll-up phenomena and any other piston induced motion. The flame must propagate through this flow field, and the nature of the turbulence and its location within the cylinder can have a profound effect on the degree to which reactions are completed. In addition, flow changes near the spark plug have been postulated to be a major cause of cycle to cycle variations.

ACCOMPLISHMENTS DURING 1978

We have been studying the effect of engine configuration and operating conditions on unburned hydrocarbon emissions. The experiments have been conducted utilizing a pneumatically operated compression-expansion machine with square cross section and quartz side windows. Previous visualization experiments have been performed under conditions which allowed only a top view of the piston, whereas we are able to observe the combustion process from the side. Optical observations have been made by taking high speed schlieren movies of the test section. Hydrocarbons are measured by means of a gas chromatograph.

In a previous publication we have reported observations of unburned hydrocarbons for several piston configurations and have shown for our machine that the roll-up vortex and wall turbulence can play a critical role in determing combustion efficiency. The schlieren observations have shown a significant effect of piston shape and cycle timing on the flow field through which the flame must propagate. Even without the bulk turbulence that an intake process might introduce, wall turbulence can be generated during the compression stroke, both because of the roll-up vortex, and because of the unsteady boundary layers along the side walls. For complex piston shapes, large scale bulk motions are also induced.

The hydrocarbon measurements reveal a general trend of decreased combustion efficiency with retarded timing, and with total unburned fuel percentages much higher than that predicted by laminar quenching correlations.

PLANNED ACTIVITIES FOR 1979

Unfortunately, the gas chromatograph measurements provide no information about the dynamics of the quenching process. As the next stage in the investigation we would like to make spacially and time resolved optical measurements of methane concentration during the compression and expansion cycle. These measurements are to be performed by observing absorption of the HeNe 3.391 μ laser line by the methane. The square piston machine is ideally suited for such measurements.

Time and spacially resolved methane concentration measurements will allow identification of major hydrocarbon source areas and will enable comparison of measurements with appropriate theoretical models.

Lean Combustion in a Model I.C. Engine*

O. I. Smith,† R. F. Sawyer and C. K. Westbrook‡

INTRODUCTION

Requirements for the operation of internal combustion engines under conditions resulting in both high efficiency and low emissions of carbon monoxide, oxides of nitrogen and unburned hydrocarbons have resulted in increased interest in the combustion of very lean premixed gases. In general, lean combustion processes satisfy the first three criteria rather well; however, many studies show that unburned hydrocarbon emissions from internal combustion engines increase as the mixture is leaned from stoichiometric. This behavior may be attributed to three processes: misfire, wall quenching of the flame inside the thermal boundary layer, and quenching outside the thermal boundary layer (due to chamber expansion, for example), the so called "bulk quenching." Since the lean and rich flammability limits for premixed combustion approach stoichiometric values as the temperature and pressure of the unburned gas is lowered (due to adiabatic chamber expansion), it seems likely that the bulk quenching mechanism will assume increasing importance relative to wall quenching as the mixture approaches the lean flammability limit.

ACCOMPLISHMENTS DURING 1978

The experimental measurements have been carried out in a square-piston, single-pulse compression-expansion machine with schlieren quality glass side windows. The principal diagnostics for the present study were high-speed schlieren movies, and chemical analysis of the burned fuel mixture.

The results of the experimental investigations in premixed laminar methane-air flames have been described and compared with those of the corresponding theoretical investigations.[1,2] Both aspects of the studies were initiated in 1977. The experimental investigation allows one to estimate the role of bulk quenching in internal combustion systems, while the theoretical study provides an interpretation of the process on a molecular level.

The experimental studies have identified the two major contributions to bulk quenching as flame stretch, the process of flame kernel growth in a diverging (non-planar) geometry, and the magnitude (not the rate) of combustion chamber expansion.

The role of flame stretch in bulk quenching is well characterized by the Karlovitz number K, which serves as a measure of the net heat deficit due to divergent flame front propagation. The Karlovitz number depends on both mechanical properties (ignitor geometry) and the physical and chemical properties of the combustible mixture (specific heat, density, thermal conductivity and laminar flame speed) as well as the flame kernel diameter. For a laminar methane-air flame, flame stretch was found to play an important role if, at the beginning of chamber expansion, the flame kernel Karlovitz number is greater than 0.2. For $K < 0.2$, chamber expansion dominates and a one-dimensional (plane wave) model is likely to be satisfactory. Since K is inversely proportional to the flame kernel diameter, this principle indicates from a practical viewpoint that bulk quenching due to flame stretch will eventually become dominant as ignition timing is retarded. Further, within the limits of the Karlovitz number as a similarity variable, the condition for negligible flame stretch ($K < 0.2$) should apply to any combustible mixture, ignitor geometry, etc.

For bulk quenching processes where flame stretch is negligible, a one-dimensional theoretical analysis utilizing a 56 reaction chemical mechanism indicates that density decrease is ultimately responsible through its effect on both chemical and transport processes. Calculations indicate that bulk quenching occurs when H, O and OH radicals diffuse out of the flame zone faster than they can be consumed by the predominant chain propagation reactions. Volume expansion produces this effect because the rates of the bimolecular propagation reactions decrease quadratically with density while those of the diffusion processes decrease in proportion to the density. Thus this conclusion is in agreement with the experimentally observed correlation between amount of volume expansion and the point of bulk quenching, and suggests that for $K < 0.2$, simple heat loss models are unlikely to describe the process adequately. It also suggests that bulk quenching in I.C. engines should be much more sensitive to compression ratio than to engine speed.

Although the experimental and theoretical work emphasized quenching in a flame propagating through a laminar flowfield, it was observed experimentally that turbulence, from whatever source, minimizes the effect of bulk quenching. In fact, bulk quenching was never observed once the flamefront had penetrated a turbulent flowfield. This limits the application of the conclusions discussed previously to practical I.C. engines since turbulence is always present from the intake valve and piston motion during the compression stroke.

PLANNED ACTIVITIES FOR 1979

No further work is planned in this area, although extension of the bulk quenching characterization to the turbulent regime (very difficult both experimentally and numerically) should be very useful to the design of lean burn I.C. engines. Other useful extensions involve development of correlations between bulk quenching and degree of volume expansion for more realistic fuels and experimental confirmation of our contention that the criterion for flame stretch influence ($K \sim 0.2$) applies to a wide range of different fuels, ignitor geometries, etc.

FOOTNOTES AND REFERENCES

*This work was supported by the Division of Fossil Fuel Utilization, Department of Energy.

†Chemical Engineering Department, University of California, Los Angeles.

‡Lawrence Livermore Laboratory

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Jet Ignition Studies*

A. K. Oppenheim, F. C. Hurlbut, F. A. Robben, K. Teichman, K. Hom, and H. E. Stewart

INTRODUCTION

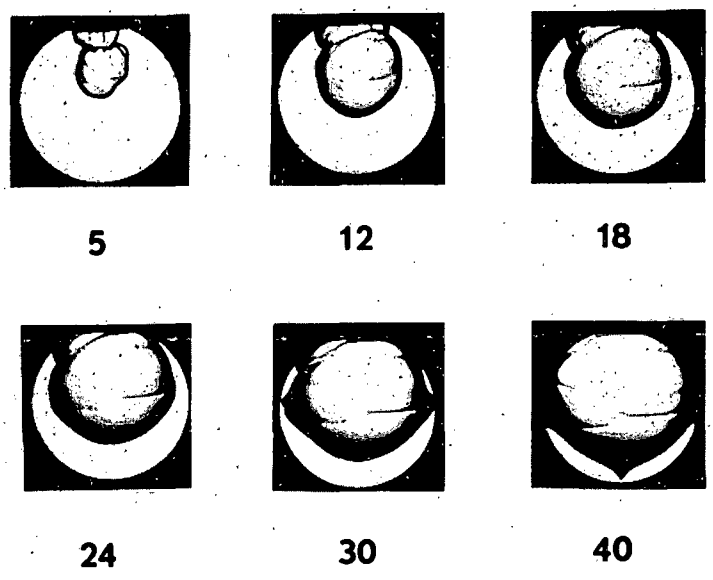
The goal of these studies is to explore the fundamental features of the process of ignition of lean gaseous fuel-air mixtures using jets of radicals. The jets are generated either by an electric discharge, creating a plasma, or by combustion in a small prechamber producing a non-equilibrium mixture of products. The results of the study are of particular importance to the development of internal combustion engines operating on lean mixtures. Such engines should have the attributes of high efficiency and at the same time relatively clean exhaust gases.

ACCOMPLISHMENTS DURING 1978

The major effort was directed towards the investigation of the effectiveness of various seed gases in the plasma jet ignition system. This was accomplished by introducing different gases into the plasma jet generator cavity. In order to insure reliable data, main chamber methane-air mixtures of an equivalence ratio $\phi = 0.6$ were used, while the orifice diameter of the plasma jet generator was kept at 2.4 mm. This work has resulted in a Ph.D. thesis[1] now being edited for publication as an LBL Report. As an illustration of the results obtained in the course of this study, some practical aspects are described below.

Figures 1, 2, and 3 are excerpts from high speed schlieren movies and pressure transducer records taken at the same time for three plasma jet igniter cases--methane seed, no seed, and nitrogen seed respectively. The time interval indicated under each print is the delay after discharge in the igniter, expressed in milliseconds. The pressure and time scales for each oscillogram are 10 psi per division and 20 msec per division, respectively.

Figure 4 shows the evolution of the volume of gas burned determined from the cinematographic records, while Fig. 5 compares the pressure



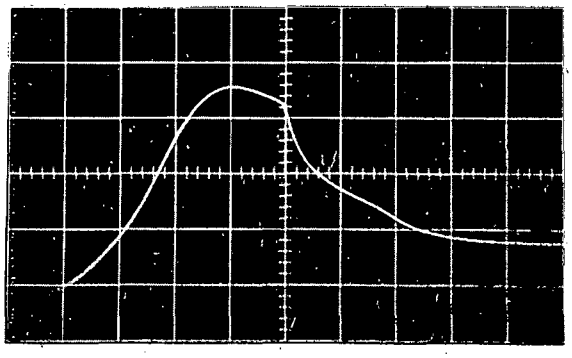
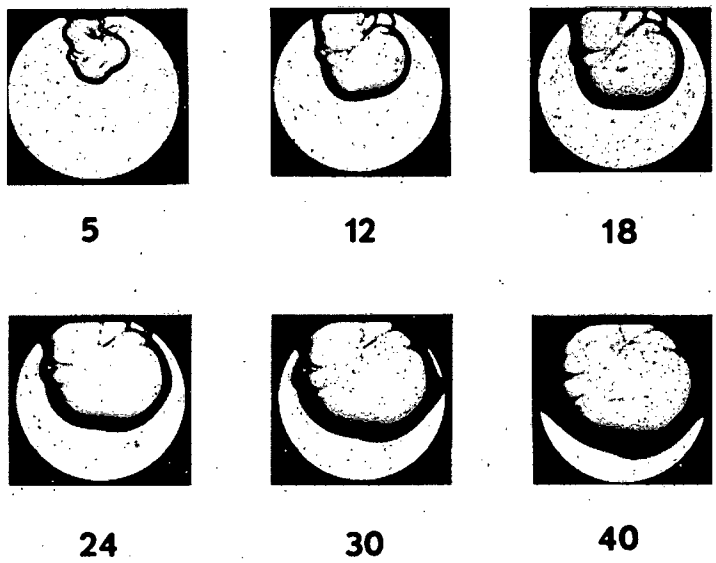


Fig. 1. Cinematographic schlieren photographs and pressure transducer record for plasma jet ignition ($\phi = 0.6$) -- CH_4 seed. (XBL 793-1047)



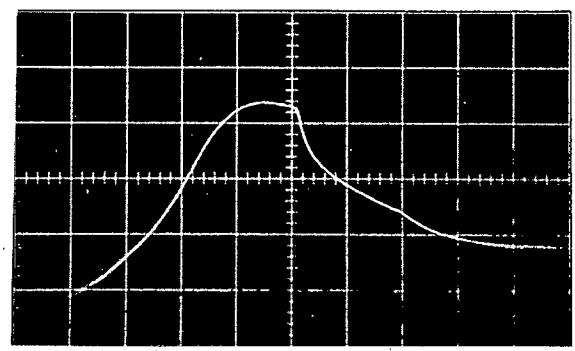
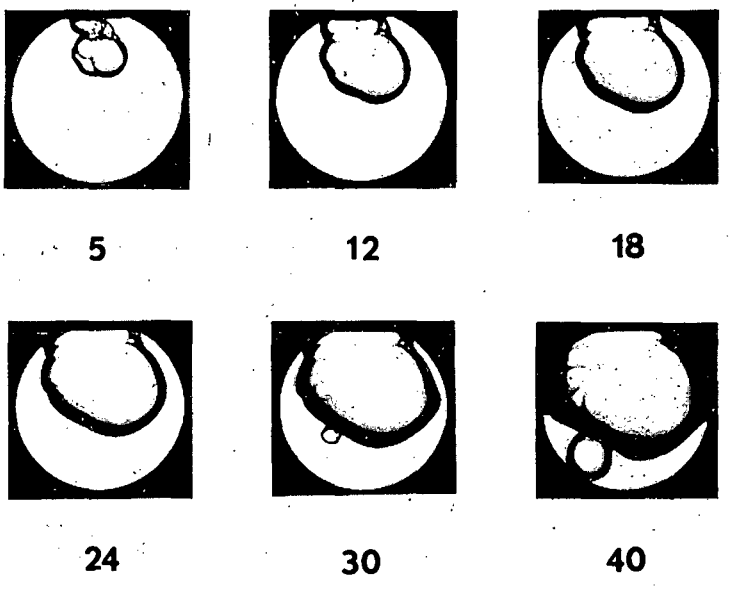


Fig. 2. Cinematographic schlieren photographs and pressure transducer record for plasma jet ignition (ϕ = 0.6) -- no seed. (XBL 794-1046)



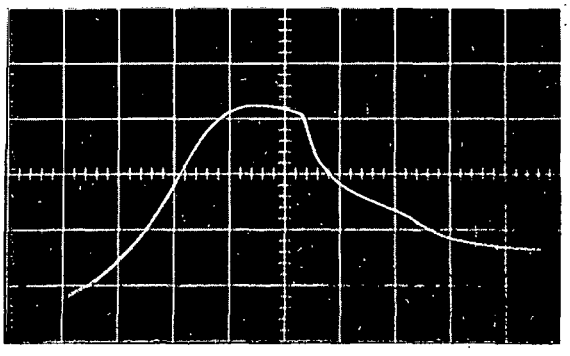


Fig. 3. Cinematographic schlieren photographs and pressure transducer record for plasma jet ignition (ϕ = 0.6) -- N_2 seed. (XBL 794-1045)

in the explosion vessel as a function of time for the three plasma jet igniter cases. These results demonstrate clearly the superiority of methane seed over the others. The evolution of the mass burned in the explosion vessel evaluated from these data is displayed in Fig. 6, while the variation of the corresponding mass averaged flame speed, S_u, is shown in Fig. 7. In all three cases, the maximum value for S_u occurs at 4 msec (the starting point for the computations) and decreases continuously. The maximum value of S_u for the methane seeded case is 34.7 cm/sec, while those for the no seed case and nitrogen case are respectively 33.4 cm/sec and 33 cm/sec, all significantly higher than the classical laminar flame speed of 8 cm/sec for a methane-air mixture at room temperature and an equivalence ratio of 0.6. This indicates conclusively the positive effects due to turbulence created by the jets in the enhancement of the combustion process they are capable of initiating.

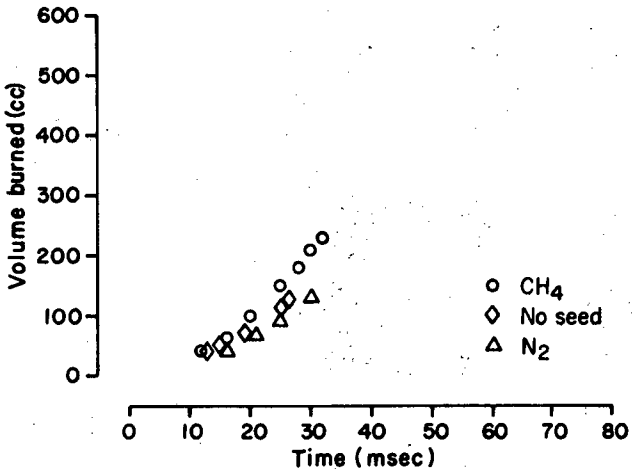


Fig. 4. Volume burned as a function of time for three cases of plasma jet ignition -- CH_4 seed, no seed, and N_2 seed. (XBL 7812-13316)

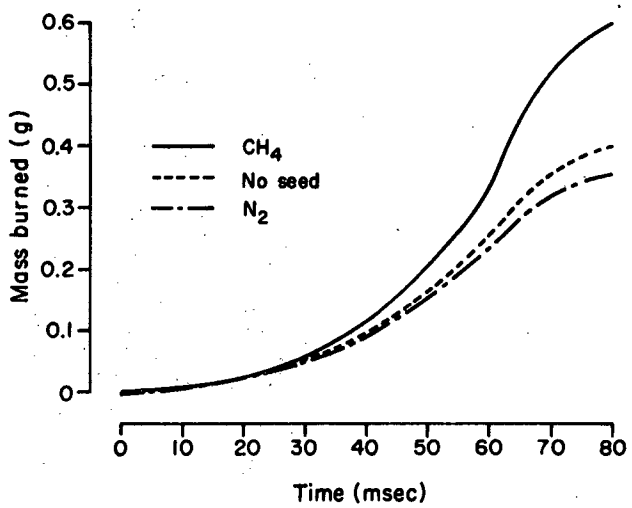


Fig. 6. Mass burned as a function of time for three cases of plasma jet ignition -- CH_4 seed, no seed, and N_2 seed. (XBL 7812-13326)

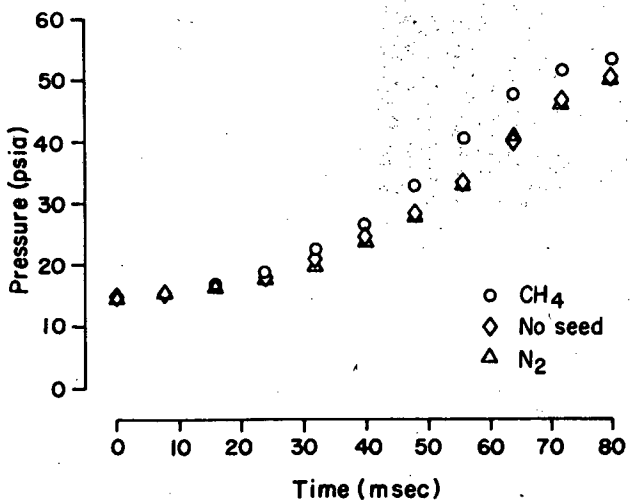


Fig. 5. Pressure as a function of time for three cases of plasma jet ignition -- CH_4 seed, no seed, N_2 seed. (XBL 7812-13315)

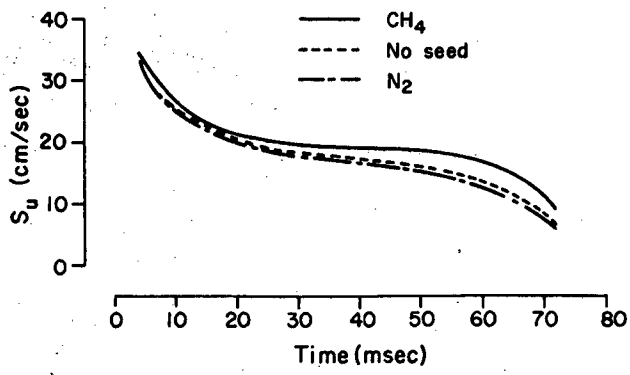


Fig. 7. Mass averaged flame speeds as a function of time for three cases of plasma jet ignition -- CH_4 seed, no seed, N_2 seed. (XBL 7812-13328)

PLANNED ACTIVITIES FOR 1979

With results of our preliminary investigation providing the necessary background, we intend to concentrate upon the basic features of the processes involved in the generation of free and active radicals and their performance as multi-point ignition sources. This will be accomplished by two parallel and closely related programs+ of study. One, under the direction of Professor F.C. Hurlbut, will be concerned mainly with the measurement of time resolved local concentration of chemical species in the jets using a molecular beam sampling technique with a quadrupole mass spectrometer serving as the primary sensing element. The other, under the direction of Dr. F. A. Robben, will concentrate upon non-intrusive optical measurements using at first conventional emission and absorption spectroscopy and later, as they become available, laser induced florescence and scattering techniques. This strategy is based upon the premise that the most appropriate research tools for this purpose, laser-based instruments, are not yet developed to a point where they could provide a reliable means for studying the chemical reactions of these ignition processes. Hopefully they will become available in time to make a contribution to our experiments.

FOOTNOTES AND REFERENCES

*This work was supported by the Division of Fossil Fuel Utilization, Department of Energy.

+Future research to be supported by the Division of Basic Energy Sciences, Department of Energy.

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Flame Propagation in a Turbulent Flow*

R. G. Bill, Jr., I. Namer, F. A. Robben, and L. Talbot

INTRODUCTION

The inability of classical techniques of analysis to resolve problems in turbulence may, to a large extent, be interpreted as a result of the wide spectrum of length scales that are associated with these flows. The importance of the scale of turbulence in turbulent flame propagation is attested to by numerous studies in which flame speed is correlated with the scale and intensity of turbulence. Recent reviews of such studies were given by Andrews et al[2] and Abdel-Gayed and Bradley.[1] Despite the large number of studies devoted to this problem, few studies exist for which sufficient measurements of turbulent parameters have been reported to provide a clear understanding of the effect of turbulence on flame propagation.

Smith and Gouldin[4,5] investigated the effects of turbulence on the flame speed of unconfined V-shaped, stabilized methane-air flames in a flow with a grid generated turbulence. Local flame speeds were measured employing hot film and laser anemometry as well as fine-wire thermocouples. Over a narrow range of test conditions, flame speeds were found to increase with increased macroscale and rms. velocity fluctuation level. Unfortunately, due to instrumentation difficulties, only relatively cool regions of the flame were investigated. Although the studies demonstrated the importance of local measurements of flame speed in turbulent flows, more measurements over the entire flow field are needed to expand our knowledge of the effect of turbulence on flame propagation.

We are presently investigating V-shaped, stabilized, propane-air flames using Rayleigh scattering and laser Doppler anemometry for two upstream flow conditions: 1) flow with grid generated turbulence and 2) flow in which a cylinder generates a Kármán vortex street in an otherwise laminar flow. Our objective in the first experiment will be to compare our measurements of flame speed to correlations with the turbulent Reynolds number based upon integral scales or Taylor microscales. The evolution of length scales upstream and through the flame front will help to quantify the effect of eddy size on the transition of the wrinkled laminar flame to a disrupted flame sheet and on the production of turbulent kinetic energy. Development of probability density functions should be helpful in determining the effect of eddy size on the mixing of burnt and unburnt gases. Furthermore, the shape of these distributions may give some insight into conditional sampling techniques necessary to isolate coherent structures in the flame propagation process.

In the second experiment, the regularity of the Kármán vortex street will enable us to use phase locked signal averaging to obtain the density and flow fields associated with the disturbed flame. For this purpose a reference hot wire probe is used in the wake of the cylinder to monitor the oscillatory patterns of the Kármán vortex street.

ACCOMPLISHMENTS DURING 1978

A computerized data acquisition system has been completed based upon a Digital Equipment Corporation (DEC) PDP 11/10 computer with 28 K words of memory. The computer system is run under a DEC RT-11 operating system using an RK05 disk with 1.25 million words of storage. Eight channels of 12 bit A/D conversion are

available. Samples may be acquired at a constant sampling rate through clock control (the maximum clock frequency being 1 MH) or individual samples may be initiated by a separate control voltage input by the user. In the latter mode, the time between samples is continuously monitored by the clock. In addition to these data acquisition capabilities, an interface has been added to the PDP 11/10 to provide for control of stepping motors to be used to move flow field positions through the laser optical path for Rayleigh scattering and laser anemometry measurements. The stepping motor controls have been completed and tested under computer control.

In order to overcome previous problems encountered in making Rayleigh scattering measurements (Namer et al[3]), a coaxial combustor was built and tested. The flow of the combustible mixture is limited to the inner jet while air flow in the outer jet shields the flow from mixing associated with interaction with the stagnant surroundings. The wake formed behind the wall of the inner nozzle is smoothed using #200 mesh screen.

The use of conventional hot wire probes and probe supports in the second experiment would introduce disturbances in the flow similar to that of the Kármán vortex street; hence, these probes can not be employed. A hot wire probe design was constructed which incorporated a cylindrical tube both as the probe holder and as a wake generator. The wire sensor, 0.02 mm diameter gold plated tungsten, is welded to 0.5 mm diameter platinum wire supports 6 mm apart. The sensor position is fixed at 1 cm above the cylinder and offset to the side by one cylinder radius.

PLANNED ACTIVITIES FOR 1979

Rayleigh scattering and laser anemometry measurements will be used to measure mean and fluctuating values of density and velocity in the turbulent flow with a V-shaped, stabilized flame. Parameters to be varied will include flow velocity equivalence ratio and grid mesh size. The combustor to be used is that described above, adapted for use with grid-induced turbulence. Flame speed and flow divergence will be locally determined at the flame front. Distributions of length scale as indicated by autocorrelation functions and power spectra will be computed. Probability density functions will be calculated to give insight into mixing processes both before and after the flame front.

The development of the Kármán vortex street as it moves downstream in the flow will initially be mapped in detail using a hot wire anemometer. The hot wire will also be used to test and verify the computer algorithm used for signal averaging measurements of the vortex street. Following this, Rayleigh scattering and laser anemometry measurements will be used to analyze the interaction of the vortex with the V-shaped stabilized flame. In particular, the distortion of the flame front by the vortex, and the intensity of the vortex after passing through the flame front, will be carefully investigated.

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*This work was supported by the Air Force Office of Scientific Research through the University of California, Berkeley, Campus Research Office.

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Combustion in a Turbulent Boundary Layer*

R. K. Cheng, R. G. Bill, Jr., F. Robben, L. Talbot

INTRODUCTION

The interaction of turbulence with the combustion process is an important element of almost all practical combustion systems. The combustion intensity, the degree of completion of combustion, and the generation of gaseous pollutants are profoundly affected by the nature and degree of turbulence. Considerable progress has been made recently in numerically modeling turbulence, and the results have been applied to turbulent combustion with varying degrees of success. In order to assist in the formulation of suitable approximations for turbulent combustion, and to critically evaluate the results of these numerical models, laboratory scale experiments are required on suitable turbulent combustion geometries capable of detailed diagnostic studies. In this program we study a heated flat plate boundary layer with induced turbulence in which premixed combustion can occur.

This classical geometry was chosen because of the extent of theoretical and experimental work dealing with laminar and turbulent boundary layers. A heated boundary layer is well suited for the study of combustion for it can support combustion under a wide range of equivalence ratios ranging from stoichiometric to very lean by proper control of the wall temperature and free stream velocity. The change in the scale and intensity of turbulence as a result of combustion heat release can be investigated over a much wider range of conditions than in conventional combustion systems such as flames. Furthermore, the combustion heat release can be adjusted to occur throughout the boundary layer permitting detailed study of the evolution of turbulence through each stage of the exothermic process.

ACCOMPLISHMENTS IN 1978

Several pieces of experimental equipment have been completed and tested in the last year. An existing PDP 11/10 computer with an LPS 11 peripheral system was expanded so as to have 28 K of memory, a programmable clock, 4 channels of buffered analog inputs, an RK 01 hard disc, Tektronix 4025 terminal, Telecorporation line printer and a communication link to a central PDP 11/45 computer. Two three axis stepping motor drives for the 2.5 cm and 10 cm channel combustion tunnels were constructed and interfaced to the computer. Software has been developed and is operational for program development, file management, and operation of the experiment to take laser Doppler velocimeter and Rayleigh scattering data. This includes plotting of the data on the terminal and calculation of simple statistical parameters.

A device to generate approximately 2 micron particles for LDV measurements has been constructed, tested and found to be reasonably satisfactory. It is based on the burning of magnesium ribbon to form MgO particles.

A 2.5 cm square channel, 10 cm long, has been built to fit onto an existing stagnation chamber and traversing mechanism. One wall of this channel consists of thin strips of Kanthal, a high temperature iron based heating alloy, over which combustion takes place. It is being used for initial measurements and as a prototype for the 10 cm combustion channel.

Construction is nearly complete on a tunnel which will give 20 m/s velocity of combustible gas in a 10 cm square channel up to 1 m long. This combustion tunnel is driven by a centrifugal pump and is mounted on a 3-axis stepping motor controlled traverse mechanism.

All results to date have been obtained in the 2.5 cm square channel, which gives a Reynolds number of approximately 3×10^5 at the channel exit at the maximum flow velocity of 22 m/s. This is too low for a fully developed turbulent boundary layer, but high enough for transition type disturbances created by an obstacle or by a non-uniform surface. The initial design of the heated surface, using Kanthal strips, is rather uneven and thus we find a fairly high degree of unsteady motion in the boundary layer. Fairly extensive measurements have been made in this channel using a hot wire anemometer with an unheated wall, laser Doppler velocimetry for an unheated and heated wall, and Rayleigh scattering for a heated wall. Further, interferograms of the integrated density across the channel have been made using differential interferometry.

The development of combustion in the boundary layer as a function of surface temperature, fuel equivalence ratio and flow velocity has been qualitatively determined from the interferograms. Some judgment on the intensity of the turbulence can also be made; it appears that the introduction of combustion, with all other factors remaining approximately the same, results in a decrease in the turbulent intensity. Detailed statistical measurements of the velocity and density fields have had to await the completion of computer controlled data acquisition, and at present new data has been recorded but not yet analyzed.[1]

The primary measurement techniques, laser Doppler velocimetry and Rayleigh scattering, have considerable inherent fluctuation, or noise, and methods for extracting the turbulent flow fluctuations from these signals have not yet been treated properly in the literature, if at all. The corrections for root-mean-square fluctuation, and the auto-correlation and power spectral density appear fairly straightforward, while the corrections for the probability density function are more complex. We have developed a model for this purpose which has yet to be

implemented and verified. These are important problems in the analysis of turbulent flow data, and advances are valuable in a broad area of research.

The motion of small (2 micron) particles in a thermal boundary layer has been studied in some detail. It was found necessary to investigate this problem in order to properly apply the laser Doppler velocimeter technique to thermal boundary layers, and the end result is a significant contribution to the field of thermophoretic motion of particles as well as to laser Doppler velocimetry. Our data, taken at much larger thermal gradients than previous studies, is quite precise, and is analyzed by full consideration of the fluid mechanics and particle trajectories. From the results we are able to distinguish between several theories of thermophoretic motion; presentation of our results with a review of other measurements and theoretical results is in draft form.

PLANNED ACTIVITIES FOR 1979

Final analysis of the results obtained from the 2.5 cm square channel will be made. This will require the development of proper methods for extracting the probability density and the power spectral density of the fluid from the data. This analysis will characterize the turbulence properties in the disturbed boundary layer, and give the effect of boundary layer combustion upon these properties.

Measurements in the 10 cm square channel will initially concentrate on the same statistical turbulence properties (density and velocity) as measured in the small channel. Both larger Reynolds numbers and lower flow velocities will be investigated, and the effect of combustion in the boundary layer on these properties will be determined. The experimental results will be compared with available numerical modeling results, and extension of present numerical modeling techniques to heated boundary layer combustion will be undertaken.

There are considerable uncertainties in the use of the laser Doppler velocimeter technique for fluctuating velocities, and investigation will be necessary in order that the quality of our measurements can be assured. There are problems with control over the size and rate of particle seeding, with thermophoretic motion of particles in the heated boundary layer, and with the processing of the Doppler bursts to give the velocity.

At least one of several possible extensions of the diagnostic measurements will be undertaken. Simultaneous measurement of two components of velocity is relatively straightforward and will enable the evaluation of the mean Reynolds stress in the fluid. The introduction of a periodic disturbance into the boundary layer will enable phase-locked measurements to be made of the coherent disturbance. This could be a very powerful technique to assess the effect of combustion on a coherent disturbance in the boundary layer. The other contemplated diagnostic extensions involve simultaneous measurement of velocity and density at one point and simultaneous measurements of either velocity or density at two different points. The first of these measurements allows evaluation of ρv correlations and the use of Favre averaging; the second establishes the spatial correlation functions and the spatial scale of the turbulent fluctuations.

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Turbulence Modeling of Heat and Momentum Transport Processes

B. E. Launder

Research in 1978 proceeded on two principal fronts. One of these was the development and testing of a second-order closure for heat and momentum transport processes in two- and three-dimensional flows. The work has been fully documented,[1] while journal articles on the research are under review[2] and in preparation. This work has, we believe, carried forward closures based on transport equations for the turbulent heat fluxes as far as is practical without introducing independent turbulent time scales for the velocity and temperature fluctuations. Indeed, devising a workable and reliable scheme for obtaining the thermal-turbulent time scale is a major goal of the writer's research work during the present year and the next.

The thermal-time-scale work will be aided by studies currently underway aimed at devising models for momentum transport (not heat transport) that adopt multiple independent time scales. This is the second of the fronts mentioned above. The modeling consists of dividing the Reynolds stress spectrum into more than one slice and devising characteristic time scales for each part. The work, still in its development stages, has nevertheless succeeded in widening the range of flows that can be predicted with a single set of equations and coefficients. Chief among these is the round jet in stagnant surroundings for which single-time-scale models usually predict a rate of spread that is 50% too large.

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Chemically Reacting Turbulent Free Shear Layer*

B. Pitz, J. Keller, M. Houser, and J. W. Daily

OBJECTIVES

Most flames of industrial interest today burn in a free shear layer that is turbulent. Premixed flames are stabilized by heat recirculation involving the recycling of hot combustion products which are mixed with the cold reactants in a free shear layer. Diffusion flames are controlled by the rate at which fuel and oxidizer mix in a free shear layer. Free shear layers play such a controlling role in the development and propagation of flames that it is important to understand them in detail.

Because of the strong current interest in prevaporized/premixed combustion caused by the NOx air pollution problem, we have been conducting a study of the premixed flame stabilized by mixing of cold reactants with hot combustion products in a turbulent free shear layer. This flow is typical of that occurring in the stabilization region of premixed combustors, and knowledge of its characteristics is needed to establish stability and flame spread rates.

Although there has been extensive and thorough research on turbulent flame propagation and stability in the past,[1,2] investigation of these processes in light of recent research on large eddy structures in turbulent shear flows has given a new direction to studies in this field.[3-7] The basic findings of such studies have established the importance of coherent large scale structures in turbulent shear flows. This leads to a deterministic approach to the description of the flow field, according to which large eddies are formed first in quasi-orderly fashion and then are carried through the mixing layer, growing by coalescence and engulfment. Fine mixing inside the eddies occurs by the action of small scale turbulence and viscosity.[7] These structures have been observed in geometrically simple, nonreacting flows; primarily two dimensional free shear layers and round jets, with some evidence of their existence in boundary layers and wakes.

RECENT WORK AND ACCOMPLISHMENTS

Our studies have been conducted in a two dimension premixed burner equipped with fused quartz windows on the side and top for optical access to the combustion zone. Preliminary work by Gangi and Sawyer[8] shows that although long exposure schlieren photographs illustrate apparently well defined regions of flame propagation and recirculation, in fact both are controlled by the dynamics of large scale eddies. High

speed schlieren movies confirm a pattern of large scale structures in the form of rolled up eddies and reveal the eddy formation rate, growth rate, coalescence and intermittent intrusion into the recirculation zone.

Given the qualitative nature of the flow field, we have made detailed measurements of conventional turbulence parameters and used these in conjunction with the schlieren movies to increase understanding of the interaction between the fluid mechanics and combustion process.

The measurements include:

(1) Hot wire anemometry measurements of the inlet flow field, including mean and rms fluctuating velocities, autocorrelations, power spectral, and probability distribution functions.

(2) Laser anemometry measurements in the body of the flow field with the same quantities obtained as in (1) above.

(3) Rayleigh scattering total density measurements in the body of the flow field, including mean and rms fluctuating density, auto-correlations, power spectra, and probability density distribution functions.

(4) Laser schlieren power spectra.

(5) Schlieren movies of the entire flow field.

The measurements have been used to study the effect of inlet velocity, temperature, and turbulence state on the shear layer structure.

The measurements reveal a number of interesting trends including:

(1) There is strong acoustic coupling between the combustor configuration and the shear layer behavior.

(2) Temperature affects the shear layer stability as expected through a variation in sonic velocity and transport properties.

(3) The beautiful two-dimension nature of the shear layer is lost when the incoming boundary layer becomes turbulent although the large structures do not disappear.

(4) The effect of combustion on the shear layer structure is surprisingly small.

PLANS FOR THE COMING YEAR

The current combustor stabilized the flame on a rearward facing step. In the coming year we will install a two stream free shear layer combustor and continue our studies with this new configuration.

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Fundamental Features of Lean Premixed Prevaporized Combustion*

J. W. Daily, A. R. Ganji, A. K. Oppenheim,
L. J. Parker, R. W. Pitz, and R. F. Sawyer

INTRODUCTION

An experimental study of lean, premixed turbulent flames has been undertaken in recognition that basic understanding of the fluid dynamics and chemistry of these types of flames is a major step in the application of premixed prevaporized combustion to gas turbines.

The use of lean, premixed combustion is one possible approach for the reduction of oxides of nitrogen and particulate emissions, and for the improvement of turbine inlet temperature patterns. On the other hand, some related problems including stability, flashback, and auto ignition must be solved before the application of the concept to the gas turbine combustor becomes feasible. The advantages and problems for the application of premixed combustion to gas turbine combustors have been discussed in detail in Ref. 1.

Although there has been extensive and thorough research on turbulent flame propagation and stability,[2,3] investigation of these processes in light of new findings in turbulent flow research has attained renewed interest. Recent research on large eddy structures in turbulent shear flows has led to a new direction to fluid mechanics research in this field.[4-8] This work has established the concept of coherent large scale structures in turbulent flows. This results in a rather deterministic approach to the description of turbulent flow, according to which large eddies formed first in quasi-orderly fashion are then carried through the mixing layer and grow through coalescence and engulfment. Fine mixing inside the eddies occurs by the action of small scale turbulence and viscosity.[8] Such structures have been observed in geometrically simple, nonreacting flows, primarily two dimensional free shear layers and round jets, with some evidence in boundary layers and wakes.

The problem of turbulent combustion in shear layers is far more complicated in the sense that fluid dynamics and chemical reaction are coupled phenomena governing the propagation and growth of the flame. In order to clarify some fundamental aspects of this problem, a unique experimental facility has been constructed in our laboratory. Its primary function is to provide a two dimensional premixed burner 17.3 cm wide, 5.1 cm high, and 22 cm long equipped with fused quartz windows on the sides for optical access to the combustion zone. The flame is stabilized behind a step which is streamlined in the upstream direction and has a blockage ratio of 0.5. Uniform mixing of propane and air and uniform velocity are attained by the time the flow reaches the entrance to the test section. The flame is initiated at the edge of the holder and propagates toward the top of the combustion chamber, while a "recirculation zone" is established behind the step, and extends to the bottom of the combustor. The experimental apparatus is shwon in Fig. 1.

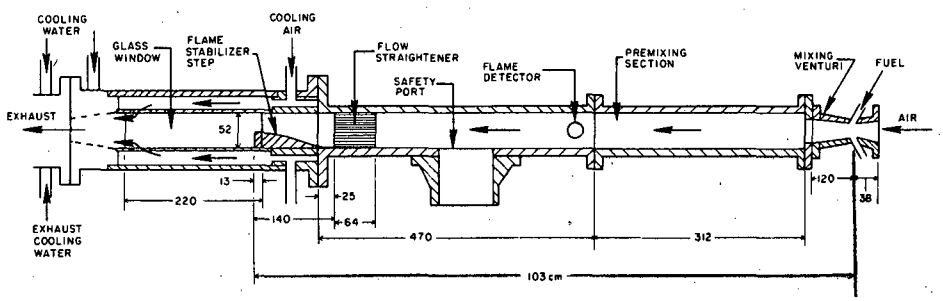
ACCOMPLISHMENTS DURING 1978

Work carried out last year was concerned primarily with the following two aspects of experimental investigations.[9]

1) Flow field visualization and characterization for both the stable mode of operation of the burner and for the unsteady processes of flashback and blowout.

2) Pollutant formation processes through the use of conventional probe techniques.

A schlieren system was used for taking both still photographs and high speed (6500 frames per second) motion pictures (in black-and-white as well as in color). Pt/Pt-Rd fine wire (.076 mm)



EXPERIMENTAL APPARATUS

Fig. 1. Two dimensional combustor test section. (XBL 794-9131)

thermocouples and aerodynamically quenched quartz microprobes were used to measure the space resolved (but time averaged) temperature and species concentrations inside the flame. Pointwise combustion efficiency was determined from these measurements.

Reynolds numbers based on the reference flow velocity have been in the range of 0.5×10^4/cm to 1.5×10^4/cm corresponding to reference flow velocities of 7.5 to 22.5 m/sec at ambient temperature. Studies have been conducted for equivalence ratios of 0.40 to 0.67 at atmospheric pressure and inlet temperatures of 300 K to 600 K.

The system has a narrow range of stability between lean blowout and lean flashback, compared to results presented in Refs. 2 and 3. Flashback occurs when the equivalence ratio is increased above a certain value (depending on initial velocity and inlet temperature). It leads to "chugging" --a non-steady mode of operation manifested by cyclic flow variation associated with a static pressure oscillation inside the chamber. Temperature measurements show a sharp drop across the flame close to the edge of the step while the corresponding change from fully reacting to nonreacting fluid a few centimeters downstream of the step is quite gradual, demonstrating that the apparent sharp flame front observed in conventional (long exposure time) pictures of the flame does not actually exist; instead the flow field is dominated by large scale turbulent mixing which obliterates the effects of sharp flame fronts.

Analysis of the still pictures and high speed motion pictures reveal the following features of the flow field:

1) Long exposure (20 msec) schlieren pictures show a well defined region immediately behind the step (commonly referred to as a recirculation zone) and a well defined region of flame propagation (usually associated with the shear mixing layer).

2) Short exposure time ($< 1\,\mu$sec) shadowgraph and schlieren pictures show a pattern of large eddies which grow downstream to a size of the order of the chamber height and intrude into the recirculation zone (see Fig. 2).

3) High speed schlieren movies confirm the pattern of large scale structures in the form of roll up eddies as observed in the still pictures and reveal additional details, both qualitative and quantitative, including the formation of eddies, their shedding frequency spectrum, shedding position spectrum, convection velocity, growth rate, coalescence, and intermittent intrusion into the recirculation zone. The above phenomena have been investigated for different operating conditions (equivalence ratio, entrance velocity, and inlet temperature) for both reacting and nonreacting flows.

Fig. 2. Spark shadowgraph of the flame (exposure time $< 1\,\mu$sec). The flow is from left to right and the flame is stabilized at the edge of the step (left). (Experimental conditions: reference velocity = 13.3 m/sec, equivalence ratio = 0.6, inlet temperature = 300 K).

4) Schlieren movies show that the process of flashback corresponds to overgrowth of the eddies behind the step until the flame is lifted from the edge of the step and enters the throat above the step. Flashback leads to a "chugging" mode generated by the growth of a single eddy behind the step until it fills out the test section and is subsequently blown out. The reactants are then again reignited by the products of combustion in the recirculation zone behind the step and the process repeats itself.

The primary accomplishments and conclusions of this research are:

1) Demonstration of a two dimensional facility for the study of premixed turbulent combustion processes with surprisingly high optical quality.

2) Confirmation that the quasi-orderly large scale eddy structures which have been observed in simple, nonreacting flows also exist in nonreacting and reacting flows behind a step.

3) Establishment of the fact that combustion is confined to these large structures and that the "flame front" and the "recirculation zone" are intermittent in character, being dominated by the transport of large scale eddies.

4) Attainment of optical records of turbulent combustion, and the processes of flashback and blowout which provide new insights for the modeling of turbulent combustion.

5) Evaluation of stability, efficiency, temperature, NO, NO_2, CO, and HC concentrations inside the above described flames.

PLANNED ACTIVITIES FOR 1979

The program of work to be carried out next year consists of the following items:

1) Establishment of the turbulent properties of the flow fields based on point measurements of density and velocity fluctuations using Rayleigh scattering, hot wire anemometry, and laser Doppler velocimetry (under the direction of J.W. Daily).

2) Experimental study of the mechanism of flashback and the non-steady chugging mode of combustion it triggers (under the direction of A.K. Oppenheim).

3) Computational analysis of the non-steady flow phenomena associated with a flashback and chugging (under the direction of A.K. Oppenheim).

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Blast Wave Studies*

A. F. Ghoniem, R. H. Guirguis, S. A. Berger, and A. K. Oppenheim

INTRODUCTION

Explosions are manifested by blast waves: the non-steady flow fields generated at the center by an explosive source and bounded on the periphery by a shock front. The effects of the latter are readily observable. The objective of our studies is to elucidate the evolution of the driving force at the source as these effects are produced. This can be attained only by theoretical analysis, for experimental insight into processes occurring at the center is practically impossible. One has to develop proper techniques for an analytical insight into the structure of blast waves, furnishing information about the link between the processes occurring at the center with the motion of the wave front.

So far the only means available for this purpose have been numerical computations based on finite difference techniques. Besides their inherent limitation to a single specific example at a time, and a relatively high cost, these techniques are deficient for three fundamental reasons:

1) The results are fuzzy since the data have to be smoothed out over a number of computational cells so that information on discontinuities, which are the essential elements of the structure, are lost.

2) The effects of transport phenomena cannot be assessed because they are obscured by those of the numerical diffusivity.

3) The conditions at the center cannot be properly evaluated for, as a rule, they are at a singularity which has to be avoided in order to assure convergence of the numerical scheme.

ACCOMPLISHMENTS DURING 1978

We have developed an analytical technique, the Phase Space Method, that is capable of treating conditions at singularities in the center with great precision. An analysis based on this method is applicable to point, line, or plane symmetrical blast waves, yielding an asymptotic solution; that is, one permitting exact results to be approached as closely as one wishes depending on the number of steps taken in their evaluation.

We have derived analytical solutions for a complete class of self-similar blast waves driven by the deposition of variable energy at the front. Of particular interest is the clarification of non-unique type of solutions that may have locally either sonic or supersonic flow immediately behind the front. Such situations can arise in the case of laser-driven explosions.

Some results of our studies have been reported in Ref. 1-3; results described in Refs. 4 and 5 are in press, while the remainder of our results are being prepared for publication in the form of Ref. 6-8.

No work is planned in this area in 1979.

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Numerical Analysis of Flow Fields Generated by Accelerating Flames*

J. Kurylo, H. A. Dwyer, and A. K. Oppenheim

INTRODUCTION

This research program concerns the evaluation of the gasdynamic effects in explosive clouds--a subject which is of particular interest today in connection with the transportation of large quantities of LNG, as exemplified by a number of papers presented at the last Combustion Symposium.[1,2,3] The particular question to which the study has been addressed can be stated as follows: A flame emanating from the center of the cloud at a steady velocity has been established. At a given moment its speed increases abruptly due to some turbulent disturbances. One is interested to find out the consequences of this event.

ACCOMPLISHMENTS DURING 1978

The planned analysis of this problem has been completed and publishd in an LBL Report,[4] and the main aspects of the work have been described in a paper presented at an AIAA meeting.[5]

Specific results have been obtained for the following case representing conditions typical of a hydrocarbon-air mixture close to its stoichiometric composition:

Specific volume ratio at initial pressure:
$\nu_F = 7$
Specific heat ratio of unburned medium:
$\Delta_u = 1.3$
Specific heat ratio of burned gases:
$\Delta_b = 1.2$
Ambient pressure:
$p_a = 1$ atm
Velocity of sound at ambient conditions:
$a_a = 331$ m/sec

The flame burning speed S_u, is expressed in terms of a law based on experimental evidence,[6-10]

$$S_u = S_o\left(\frac{p}{p_a}\right)^{0.5}\left(\frac{a}{a_a}\right)^{4.6}$$

where subscript o denotes the initial flame speed, while subscript a refers to conditions of the ambient atmosphere into which the flame propagates initially.

The initial conditions for the computations are provided by the solution of the pressure wave generated by a flame propagating with constant burning speed, S_o.[11] When the flame is at a radius X = 1, its speed is suddenly increased by a finite increment, ΔS. The ensuing development of the process is determined using our computational technique.

A time-space wave diagram of the solution is presented in Fig. 1. Here we have S_o = 9.6 m/sec and ΔS = 14.6 m/sec, while the flow was considered to be plane symmetrical (j = 0). A solution obtained under similar circumstances for the same initial flame speed but with ΔS = 19.0 m/sec is displayed in Fig. 2. On both diagrams dashed thick lines represent the trajectories of deflagrations, solid lines refer to shocks, the thick solid line corresponds to detonation, and the thin broken lines indicate the particle paths.

In the first case, the imploding shock, generated when the flame speed was suddenly increased at $x = x_o$, was reduced to a sound wave after eight reflections from the center and interactions with the deflagration. In the meantime the progagation speed of the deflagration increased to 37.2 m/sec while the Mach number of the shock at the front of the pressure wave was augmented from 1.1 to 1.4. The process took about 240 x_o m/sec while the deflagration traveled a distance of 53 x_o meters, where x_o is expressed in meters. Thereupon the whole wave system settled to a steady state corresponding to a self-similar solution obtained for the final propagation speed of the deflagration.

In the second case, however, as demonstrated in Fig. 2, the process escalated to detonation propagating finally at a speed of 2250 m/sec. Its onset occurred at a radius of 20.3 x_o meters and the time of 76 x_o milliseconds. Associated with this was the generation of a retonation wave traveling at a speed of 1250 m/sec, corresponding to a local Mach number of 1.29, into the burned medium.

Details of the wave interaction processes associated with the onset of the detonation and retonation waves are shown in Fig. 3. This is, in effect, an enlargement of a part of the solution delineated by a small rectangle on Fig. 2. Added here for clarity of exposition are the characteristics. As it appears here, the onset of detonation is associated also with the formation of a centered rarefaction wave. Its front edge is at the Chapman-Jouguet state propagating with the detonation front, while its trailing edge is identified on the diagram by a chain-double-dotted line.

There are thus two possibilities: a steady solution culminated by a constant velocity flame driving a pressure wave or an unsteady solution associated with transition to detona-

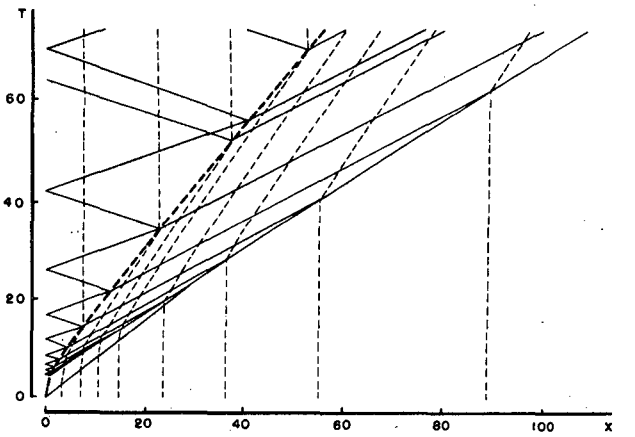

Fig. 1. Wave diagram of stable solution obtained in the case of subcritical burning speed increment. (XBL 781-6814)

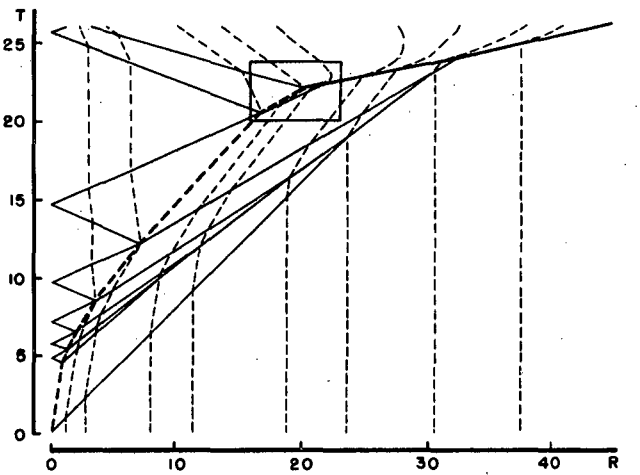

Fig. 2. Wave diagram of unstable solution obtained in the case of supercritical burning speed increment. (XBL 781-6815)

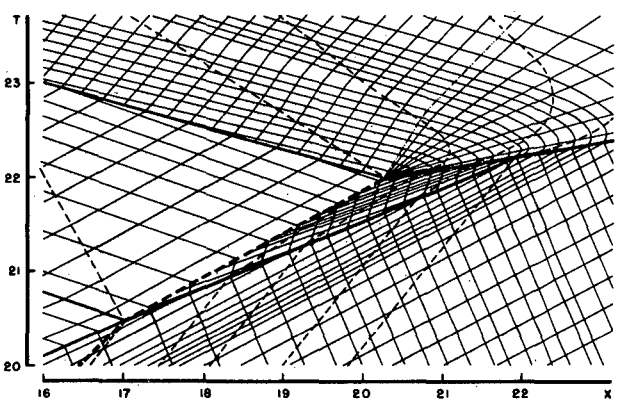

Fig. 3. Details of solution presented by Fig. 2 depicting the onset of detonation. (XBL 781-6816)

tion. The distinction between the two is governed solely by the value of the initial flame speed and the flame speed increment. The demarcation line between the two regimes of these parameters is presented in Fig. 4. For initial conditions corresponding to a point below the line, a stable solution, like that of Fig. 1, is obtained; for points above the line the solutions are unstable as exemplified by Fig. 2.

For stable cases similar solutions to that of Fig. 1 were obtained by our Cloud Code[12] -- a Lagrangian computational scheme for blast waves employing the von Neumann-Richtmyer artificial viscosity with Wilkins' modification. However, when the unstable conditions associated with transition to detonation were approached, the computations became excessively unstable. This feature manifested itself so distinctly that it was actually exploited to check the demarcation line of Fig. 4. With the use of the Cloud Code such lines were determined by spherical as well as planar flow fields. The difference between them turned out to be so small that the line presented in Fig. 4 could be considered to be valid irrespectively of the geometry of the flow field.

Noted on the diagram are a number of specific points marked by crosses. That indicated by S corresponds to the solution of Fig. 1; the point denoted by U specifies initial conditions for the solution presented in Figs. 2-3. Points indicated by W refer to experimental results obtained by Dörge et al.[13] with the use of acetylene-air mixtures. Subscript S denotes cases when the flame, after passing the screen barrier, settled to a new steady propagation velocity. Subscript U refers to the unstable case associated with transition to detonation which was observed when air was enriched with oxygen. The numerals in the subscripts indicate

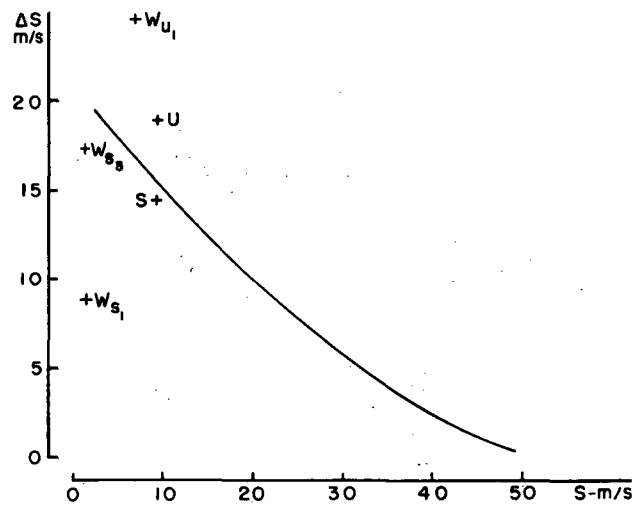

Fig. 4. Regimes of initial conditions for stable and unstable solutions.
(XBL 781-6821)

the number of turbulence generating screens used in the experiment. As it appears the increase in flame burning speed could be practically doubled by the use of three screens instead of one. However, the addition of oxygen to air was so effective in triggering the transition to detonation that evidently one screen was in this case quite sufficient.

PLANNED ACTIVITIES FOR 1979

No work is planned in this area in 1979.

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Catalytic Combustion in a Boundary Layer*

R. Schefer, R. K. Cheng, and F. Robben

INTRODUCTION

Interest in the use of catalytic surfaces to promote combustion reactions has increased greatly over the past several years due to the potential improvements in combustor efficiency and the greatly reduced pollutant levels which have been demonstrated. Much of the work to date has involved parametric investigations of prototype catalytic combustor configurations. Such work is necessary to the development of practical catalytic combustors and the results have been quite promising. However, such studies are somewhat limited in terms of obtaining a more fundamental understanding of catalytically supported combustion. Two such areas where a greater knowledge would be desirable are the role of internal heat and mass transfer in the catalytic combustion process, and the role of homogeneous as opposed to catalytic surface reactions. An understanding of these and related processes such as pollutant generation is necessary for the optimum evaluation and application of the surface catalysis concept to practical combustion system design.

The approach of the present investigation has been to examine catalytically supported combustion in a well characterized system in which most of the important physical and chemical processes found in larger scale catalytic combustors are present. The geometry chosen consists of combustion in the boundary layer of a heated catalytic flat plate. This system provides a suitable geometry for both experimental and numerical modeling studies. The operation of such a system under a suitably selected range of conditions greatly facilitates determination of the roles of the various processes involved. The parallel development of a numerical modeling program has aided considerably in the analysis of the experimental results and will provide a means with which to extend these results to more practical combustion systems.

Since initiation in 1976 the experimental system has been constructed and several measurement techniques have been developed. These include optical pyrometry to measure surface temperature, Rayleigh scattering and differential interferometry to measure gas temperatures in the boundary layer, and the measurement of surface energy release rates from plate heating strip power inputs. A numerical finite difference scheme was also developed for boundary layer flows which includes detailed gas phase kinetics and realistic transport properties. A simplified model was proposed for surface reaction based on the limiting case of an equilibrium surface condition.

ACCOMPLISHMENTS DURING 1978

A detailed study was completed of boundary layer behavior under combustion conditions for lean H_2/air mixtures flowing over a platinum catalytic surface.[1,2] Regions were identified in which only surface reaction was present and, at higher equivalence ratios and surface temperatures, in which both surface reaction and stable boundary layer combustion occurred simultaneously. At the highest equivalence ratios and surface temperatures, the combustion zone moved upstream toward the plate leading edge where the primary reaction zone developed into a flamelike structure characterized by steep temperature gradients which extended well out into the free stream. These results are summarized in Fig. 1.

Surface energy release rates were measured over a range of conditions for both H_2/air[3] and C_3H_8/air mixtures. Under all conditions investigated the surface reactions rapidly became diffusion limited downstream of the plate leading edge, thus limiting the catalyst reaction rate. From the data it was possible to derive expressions for the surface reaction rate based on simplified surface reaction mechanisms. The determination of high temperature surface reaction rate data such as this is necessary for the development of future catalytic combustor design criteria.

A more realistic model was developed for catalytic surface reactions which included surface oxidation of H_2 to H_2O and radical recombination at the plate surface. The H_2 surface oxidation rate was based on experimentally measured values and the rates for

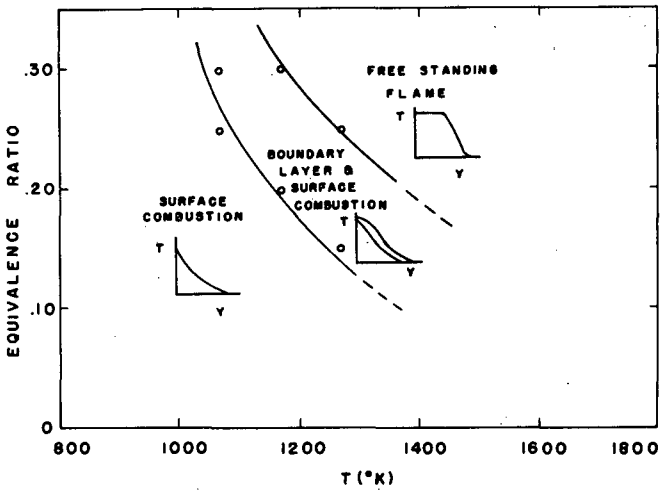

Fig. 1. Combustion regions for H_2/air mixtures over a heated platinum plate. U_∞ = 1.5 m/s, T_∞ = 293K. (XBL 784-7918)

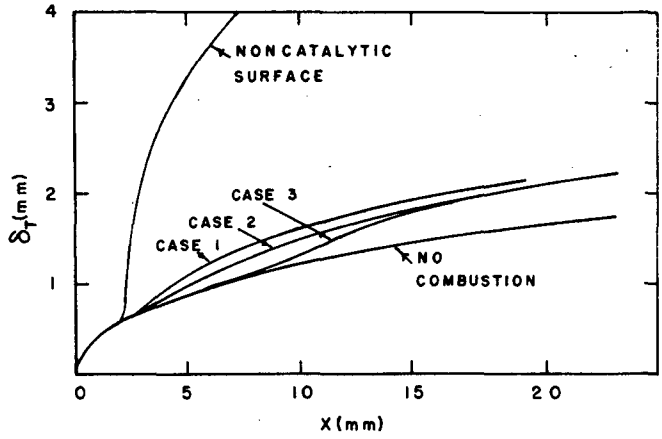

Fig. 2. The effect of surface boundary condition on thermal boundary layer thickness. H_2/air combustion. ϕ = 0.1, T_S = 1100K, U_∞ = 3.17 m/s. Case 1. Total equilibrium surface; Case 2. Surface oxidation of H_2; Case 3. Surface oxidation of H_2 and radical recombustion. (XBL 792-8363)

radical recombination were derived from a kinetic theory surface collision model assuming a reaction probability of unity for each collision.

The effect of various surface reaction models on the combustion process was investigated for lean H_2/air mixtures. The surface boundary conditions considered were based on 1) the limiting case of an equilibrium surface at which species concentrations are driven instantaneously to their equilibrium values, 2) a condition which includes finite rate surface oxidation of H_2 to H_2O, and 3) a condition which includes radical recombination at the plate surface in addition to surface oxidation of H_2. A detailed reaction mechanism for gas phase combustion which included 13 reactions and 8 species was used in the calculations. A comparison of the above models for a catalytic surface with results for a noncatalytic plate is presented in Fig. 2 where the thermal boundary layer thickness, δ_T, is shown as a function of distance along the plate. An increase in δ_T over that found for the case of no combustion indicates the presence of gas phase heat release. These results show the strong quenching effect that surface reaction has on the initiation of gas phase combustion in the boundary layer, due to the depletion of H_2 near the plate surface and the quenching of radical species generated in the gas phase. This results in a significant reduction in gas phase heat release rates over that found with a noncatalytic plate surface.

The numerical calculations for a catalytic plate surface predicted higher gas phase heat release rates than were found experimentally for lean H_2/air mixtures flowing over a platinum plate. Possible causes for this descrepancy are uncertainties in the surface reaction model and uncertainties in the gas phase kinetic mechanism. A series of sensitivity tests were carried out which indicated that uncertainties in the gas phase kinetic mechanism are the most likely cause of the high predicted heat release rates.

PLANNED ACTIVITIES FOR 1979

The above work in catalytic combustion is currently being extended into several areas. Studies similar to that done for H_2 will be conducted for typical hydrocarbon fuels. These studies will include mapping out the various combustion zones for these fuels over a variety of catalyst materials, obtaining surface reaction rate data, and developing models for surface and gas phase reactions. Data over a noncatalytic plate would improve our understanding of the effect of surface reaction on gas phase combustion. An area of particular interest with respect to catalytic combustion is the burning of fuels with a high fuel bound nitrogen content since future energy needs will require an increasing reliance on fuels of this type. Preliminary results indicate that catalytic combustor operation under fuel rich conditions could be very effective in reducing the conversion of fuel bound nitrogen to NO_x. Our studies to date have concentrated on fuel lean operation. During the coming year catalyst operation under fuel rich conditions will be investigated with the emphasis on soot formation characteristics and its effect on catalyst performance.

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Characterization of NOx Removal Through Ammonia Addition*

N. J. Brown, R. F. Sawyer, T. S. Eitzen, K. Basden, G. Georgalas, A. Gordon

INTRODUCTION

Control of nitrogen oxides emissions is most desirable since these compounds result in atmospheric nitrogen dioxide, photochemical smog formation, nitrate formation and perhaps other compounds whose role in air pollution is less well defined. Combustion sources both of the mobile and stationary types are recognized as the primary sources of the oxides of nitrogen. The two principal sources of nitrogen oxides in the combustion of conventional fuels are oxidation of atmospheric molecular nitrogen (thermal NO_x) and oxidation of nitrogen containing compounds in the fuel (fuel nitrogen NO_x). The latter classification of NO_x increases with the nitrogen content of the fuel and may account for more than half of the nitrogen oxides emitted from the combustion of high nitrogen content oil or coal in power plants. While the formation mechanism of thermal NO_x is quite well understood, the mechanism of fuel NO_x formation is not understood. Fuel NO_x production appears favored under conditions different from those which enhance thermal NO_x production. Consequently, the various control strategies used in the United States to meet NO_x emission standards, namely the modification of the combustion processes to reduce thermal NO_x production, are ineffective in reducing fuel NO_x.

A new NO_x control technology has been patented by Exxon Research and Engineering Company which selectively removes NO_x from combustion effluent gases through homogeneous reaction with ammonia and oxygen. This process is distinctly different from other technologies in that it does not prevent or limit NO_x formation but rather removes the NO_x through reaction after its formation. Thus, the process offers the possibility of removing both thermal and fuel NO_x. This process has been proposed for the control of oxides of nitrogen from stationary sources in California. It is of major importance to assess its potential for secondary pollutant formation, especially at operating conditions different from those which are considered optimal for reduction of oxides of nitrogen.

In recognition that NO_x removal through NH_3 addition appears to be a viable control strategy, the California Air Resources Board is sponsoring a research program at the Lawrence Berkeley Laboratory. This research is directed toward characterizing the NH_3 addition/NO_x removal process for secondary pollutant potential, and providing a framework to assist the California Air Resources Board in assessing utilization of this control process. This research is being conducted in a laboratory scale combustion tunnel which is a well controlled experimental environment. Experimental variables which are being considered are: 1) equivalence ratio, 2) temperature of the combustion products prior to ammonia addition, 3) ammonia concentration, 4) NO_x concentration, and 5) type of fuel nitrogen added. Propane is being used as a fuel and nirogen addition is being used to control the gas temperature at the point of ammonia addition.

ACCOMPLISHMENTS DURING 1978

A stainless steel combustion tunnel has been constructed and characterized to ascertain that the performance is consistent with that required to evaluate the NH_3 addition/NO_x control process. Composition and temperature measurements have been performed at various radial and axial positions downstream of combustion under various operating conditions. Temperatures are measured with thermocouples and radiation corrections are made with suction pyrometry; CO and CO_2 concentrations are measured with non-dispersive infra-red analyzers and NO and NO_2 are measured using a chemiluminescent analyzer. Figure 1 is an illustrative plot of CO_2 concentration as a function of radial position downstream of the NH_3 injector. Agreement among the measurements at the various points is indicative of good mixing and completeness of combustion. Analysis of the various measurements indicate that stable, steady state and reproducible combustion occurs in the tunnel over a range of experimental variables, and that mixing lengths are relatively short. Since the quantity of ammonia injected into the product combustion gases is an important

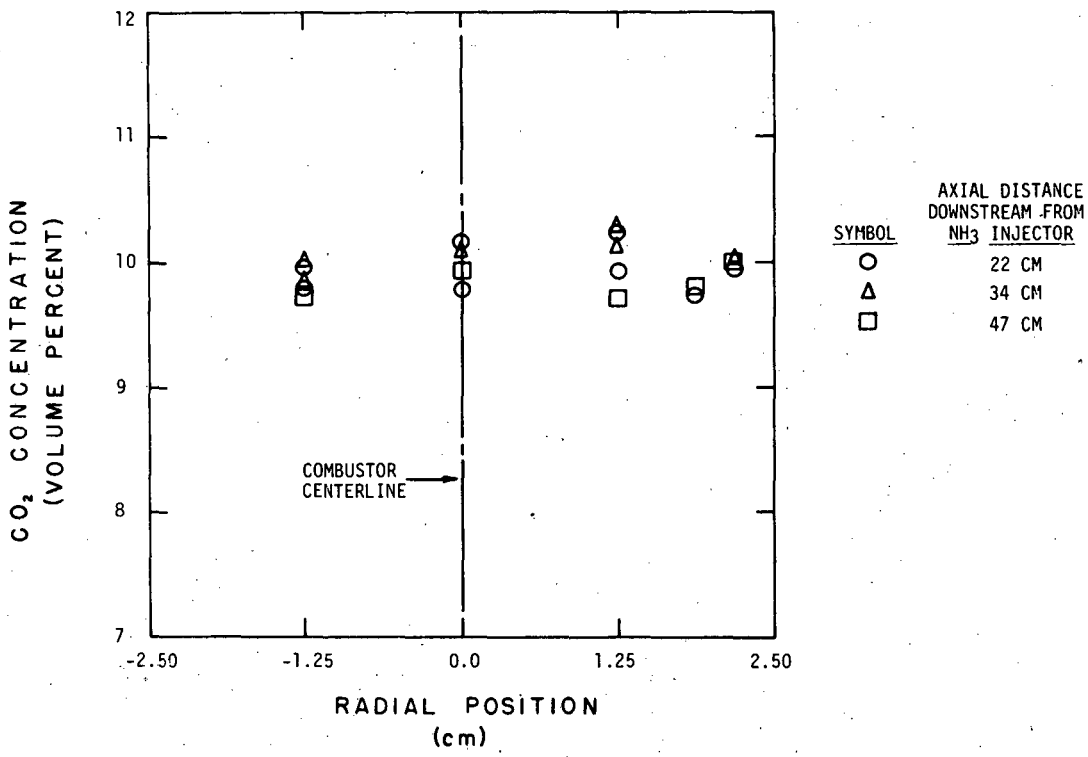

Fig. 1. Spatial variation in dry CO_2 concentration for propane/air combustion at an equivalence ratio of 0.8. (XBL 794-9135)

experimental parameter, a series of experiments has been performed to determine a satisfactory ammonia injection technique. Ammonia was found to decompose catalytically in a stainless steel inlet system at elevated temperatures; however, a quartz injector system was found satisfactory.

The literature associated with currently used NO_x reduction techniques has been surveyed and a report[1] summarizing the findings has been written. In addition the literature associated with combustion sources of nitrogen compounds has been reviewed and a paper[2] has been written which describes potential sources of non-criteria nitrogeneous pollutants.

PLANNED ACTIVITIES FOR 1979

This work is to be completed during 1979. A series of measurements will be performed to determine NO_x reduction levels under conditions deemed optimum for NO_x removal through NH_3 addition and for a set of conditions that are less than optimum. Gas chromatography and mass spectroscopy will be used to determine possible nitrogen-containing by-products. CO/CO_2 will be monitored over the range of experimental variables. A light distillate oil containing nitrogen will be substituted for propane and a series of characterization studies will be performed.

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* This work was supported by the California Air Resources Board.

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Characterization of Emissions from the Combustion of Alternative Fuels

N. J. Brown, W. K. Chin, T. Hadeishi, A. S. Newton, R. F. Sawyer, and R. W. Schefer

INTRODUCTION

Increased reliance on heavier alternate and fossil fuels derived from coal and shale to supply future energy requirements has associated environmental impacts of potentially serious consequences. One of the more serious problems associated with utilization of these fuels is pollution formation resulting from their combustion. Alternative and fossil fuels pose a substantially more serious threat to air quality than natural gas and distillate oils since they contain nitrogen and sulfur chemically bound to hydrocarbon chains and aromatic rings of the fuel. While sulfur removal via fuel pretreatment or product scrubbing appears to be an economical solution to the sulfur emissions problem, analogous removal procedures do not appear promising for nitrogen chemically bound in the fuel. Thus initial stages of this proposed research will be concerned with the characterization of nitrogen emissions from alternative and fossil fuels. This is important since it is a crucial step in the sequence which leads to the determination of source emissions and an assessment of health effects of pollutant species.

To date consideration of nitrogen compounds as air pollutants has focused upon the nitrogen oxides, NO and NO_2, with occasional interest in ammonia. The so-called technology for assessing nitrogen emissions reflects this in that it is specialized with regard to NO_x and even more specifically to the NO_x evolved from the oxidation of atmospheric nitrogen (thermal NO_x). It now appears that fuel nitrogen will become a significant and even dominant source of NO_x with combustion of alternative and fossil fuels. Moreover, a potentially more dangerous and difficult problem exists since combustion processes involving these fuels are likely to emit, in addition to oxides, a host of other nitrogen compounds (e.g.: ammonia, hydrogen cyanide, amines, nitriles, isocyanides, cyanates, isocyanates).

The importance of the potentially serious fuel nitrogen pollution problem associated with increased alternative and fossil fuel utilization has not been assessed since all the nitrogen containing combustion products have neither been identified nor quantified. It is, however, reasonable to assume that these compounds are at least as reactive as oxides of nitrogen and should be of similar concern on an equal mass basis. The major problem associated with assessing and controlling the nitrogen containing combustion products is lack of suitable analytical techniques. The analyses are complicated by adsorption and reactions in sampling systems and interferences from other species.

A coordinated research program is underway to determine measurement techniques suitable for nitrogen compound quantification in combustion environments. This effort involves the close collaboration of researchers in combustion, pollution chemistry, mass spectrometry and modern laser spectroscopy, and consists of the following four tasks:

Task 1: Measurement of nitrogeneous emissions from prototype alternative fuels in premixed laminar flat flames.

Task 2: In situ detection of nitrogen and sulfur compounds from alternative and fossil fuel combustion.

Task 3: The identification and quantitative determination of nitrogen containing combustion products by mass spectroscopy and GC/MS.

Task 4: Analysis of nitrogen compound emissions from coal and coal derived fuels using the opposed flow diffusion burner.

ACCOMPLISHMENTS DURING 1978

A flat flame apparatus has been constructed and characterization experiments have been performed to determine which portions of the flame are suitable for comparative diagnostic measurements. Hot wire anemometry has been used to determine velocity profiles of cold gases flowing through the burner and temperature profiles have been determined for stoichiometric, methane/air flames at various heights above the burner surfaces. Figure 1 is an illustrative plot of the maximum temperature measured at a fixed axial distance above the burner as a function of radial distance from the centerline to burner edge. Characterization studies indicate that the current apparatus is suitable for diagnostic measurements in the post-flame zone. A chemiluminescent analyzer, suitable for NO and NO_x measurements has been constructed.

An optical technique has recently been developed at Lawrence Berkeley Laboratory which is suitable for the quantitative determination of trace amounts of small molecular species. An atomic line source (e.g. cadmium) is placed in a variable magnetic field, and through utilization of the Zeeman effect, two closely spaced atomic emission lines, a σ^+ and σ^- component, are obtained which can be tuned by varying the field strength so that one component corresponds to an absorption line of the species to be measured. The differential absorption between the two components is then proportional to the concentration of that species and is very insensitive to most other disturbances. Calibration experiments have been conducted so that the technique can be used to measure NO and NO_2 in a mixture of combustion gases.

Work is underway to determine suitable separation techniques for qualitative and quantitative analyses of low molecular weight nitrogen compounds from combustion environments. A sampling system

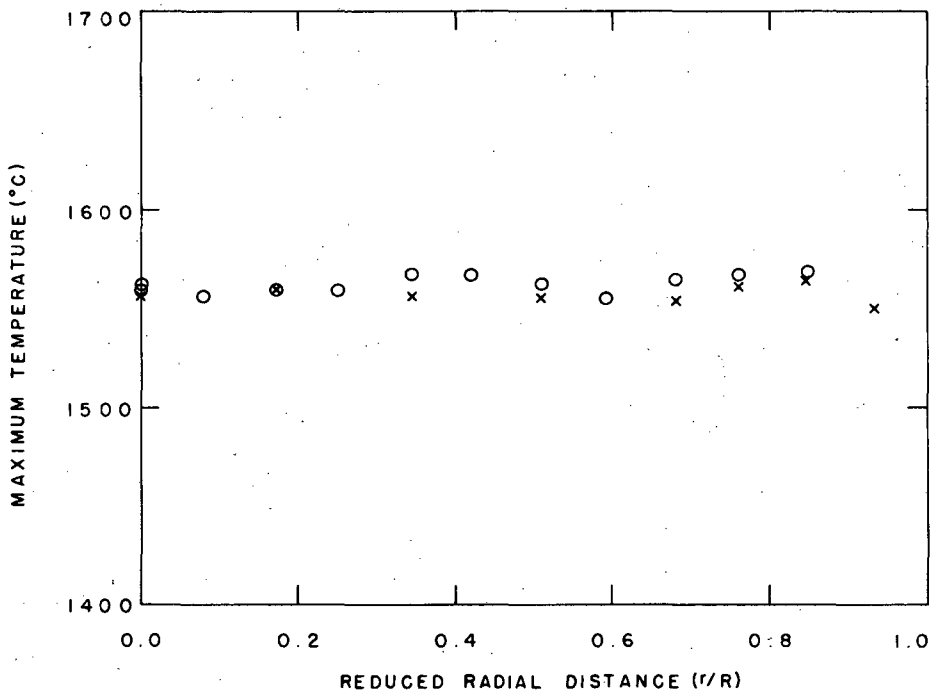

Fig. 1. Maximum temperature as a function of reduced radial distance (r/R), R = 29.5 mm, measured from burner centerline, at the axial position corresponding to the maximum temperature of a premixed stoichiometric methane/air flame. Flame velocity at the burner surface is 117.9 mm/sec and x and o designate different radii. (XBL 794-9136)

has been constructed to probe the nitrogen containing products of combustion from the test section of a combustion tunnel. In addition, a sampling system has been designed for sample extraction from the products of coal combustion, produced in the opposed flow diffusion burning of nitrogen containing coals.

PLANNED ACTIVITIES FOR 1979

Various diagnostics will be used to measure NO and NO_2 produced in premixed laminar flames. Experimental variables will be: 1) fuel type 2) equivalence ratio, and 3) fuel nitrogen concentration. Samples will be: 1) extracted with different probe types and measured with chemiluminescent analysis, 2) extracted with different probe types and measured spectroscopically in an absorption cell, and 3) measured in situ spectroscopically. A new burner will be constructed which gives proper one dimensional behavior in the pre-flame and flame zones. Effects of probe disturbances to the flames will be characterized.

Analysis schemes for chromatographic separation of low molecular weight nitrogen compounds present in combustion gases will be devised for use under a variety of experimental conditions. These techniques will be used for nitrogen compound measurement in coal combustion, in premixed flame experiments with prototype alternative fuels, and is assessing non-criteria nitrogen pollutants formed in the NH_3 addition/NO_x reduction process. Measurements of low molecular weight nitrogen compounds formed in the combustion of coal in the opposed flow diffusion flame will be conducted for a variety of coal types.

Application of Unimolecular Rate Theory to Combustion Science

N. J. Brown

INTRODUCTION

Combustion science is concerned with chemistry and fluid mechanics and the coupling between them. Our ability to understand the multistep chemical mechanisms characteristic of combustion processes is made difficult since they are of the chain type and individual reactions are difficult to isolate for experimental study. Relative to the considerable experimental effort, the application of theory to the kinetics of combustion chemistry has been rather limited. Applications of theory can be used to eliminate potential reaction steps in a proposed chemical mechanism. Theory is also useful in evaluating rate coefficients, predicting reaction pathways, and in experimental interpretation of rate data. In addition it should find considerable use in predicting non-Arrenhius behavior and in minimizing errors in the extrapolation of low temperature data to the high temperature regime germane to combustion. One such theory that has benefitted from recent progress is that associated with unimolecular reactions. Unimolecular rate theory can be applied to dissociation, recombination and isomerization reactions. These reactions play an important role in combustion initiation, fuel pyrolysis, radical quenching, and pollutant formation and destruction reactions. Unimolecular reactions are governed by a complex competition between collisional energy transfer and intramolecular energy redistribution. The kinetics are of the second-order type at low pressure where collisional intermolecular energy transfer is rate controlling and first order in the high pressure regime which is rate limited by intramolecular energy transfer. Between the high and low pressure limits, the kinetics are complicated by the coupling between the intermolecular and intramolecular processes, and this intermediate area is termed the fall-off regime.

This research program which was initiated in mid 1978 is concerned with formally extending current theories of unimolecular reactions. These extensions will then be applied to generate kinetic data for reactions that are important in combustion processes.

ACCOMPLISHMENTS DURING 1978

Work associated with the remaining two parts of a four part study of the $H_2 + D_2$ bimolecular exchange reaction was completed. Three potential energy surfaces were computed using valence bond theory to generate simple model wavefunction. A semi-empirical evaluation of the various electronic integrals was undertaken to obtain a tractable analytical form for the H_4 potential surface and its derivatives. A parametrization of the integrals was chosen to give proper asymptotic limits. The remaining parameters governing the repulsive four-atom effects are chosen to give agreement with ab initio calculations of the H_4 potential. The similarities and differences among these three surfaces and their comparison with ab initio results are discussed in a paper[1] soon to be presented for publication. A paper[2] summarizing the results of a comparative scattering study investigating reactivity and energy transfer on the three valence bond surfaces and on a London surface has been written and will soon be submitted for publication.

The current scientific literature associated with unimolecular reaction-rate theory has been reviewed.

PLANNED ACTIVITIES FOR 1979

An improved description of centrifugal effects will be sought for small molecule reactions. Bond fission reactions occurring at or near the high pressure limit will be investigated and fully rotationally averaged rate coefficients will be determined.

PUBLICATIONS IN PREPARATION

1. D.M. Silver and N.J. Brown, "Valence bond model potential energy surfaces for H_4."

2. N.J. Brown and D.M. Silver, "Comparison of reactive and inelastic scattering of $H_2 + D_2$ using four semi-empirical potential energy surfaces."

Laser-Induced Fluorescence Spectroscopy Applied to Turbulent Combustion Flow*

J. W. Daily and C. Chan

INTRODUCTION

Due to large fluorescence cross-sections, laser induced fluorescence spectroscopy has been shown to be a very promising diagnostic technique for combustion systems. The method consists of illuminating the gas with a laser source tuned to an absorption line of the species of interest. The molecules are excited and then reradiated spontaneously, and the resulting fluorescence is measured. The beam diameter and the collection optics define the spatial resolution which may be as fine as 0.1 to 0.5 mm.

ACCOMPLISHMENTS DURING 1978

The primary difficulty with using laser induced fluorescence spectroscopy to make species density measurements has been that collisional de-excitation of the excited state completely dominates radiative de-excitation, causing fluorescence quenching. For atomic species like sodium, we have demonstrated that this difficulty can be overcome by using a laser source of sufficient intensity to saturate the exciting transition. A linear curve of growth for sodium atom concentration has been obtained. The dynamic range of the measurement is approximately two orders of magnitude, limited at low number densities by detectability limit considerations and at high densities by radiative trapping. For diatomic molecules the more complex molecular structure means that the intensity required to saturate is several orders of magnitude higher than that for atomic species. If one cannot attain saturation conditions, the quenching rate must be known in order to interpret the fluorescence signal.

The quenching of OH under flame conditions has been studied and a detailed model of rotational relaxation and quenching for the excited molecules has been developed. The success of this model is reflected in the comparison between the predicted fluorescence spectrum and experimental results. A typical comparison between the computed spectrum and the experimental results is shown in Fig. 1. One of the adjustable parameters for the model is the quenching rate which can be obtained through an iterative procedure. The quenching rate of OH is found to be about 5.0×10^{-9} sec^{-1} for a methane/air premixed flame at an equivalence ratio of 1.03. We are presently studying the dependence of the quenching rates on temperature, equivalence ratio and diluent ratio.

As mentioned above, one problem that exists for atomic fluorescence spectroscopy is that fluorescence trapping severely limits the dynamic range. One method for overcoming this limitation is to observe the enhanced Rayleigh scattering near resonance, rather than the fluorescence signal itself. If the laser is detuned from resonance slightly, then the spectrum of the scattered light consists of a Rayleigh scattering line at the laser frequency, a fluorescent signal which is caused by collisional redistribution of energy to the resonant state, and perhaps a three photon signal if the laser intensity is sufficiently large. We have observed the Rayleigh and the resonance peaks in sodium in flames. We have demonstrated that the Rayleigh component is not significantly trapped at number densities much higher than that for which fluorescence trapping becomes important.

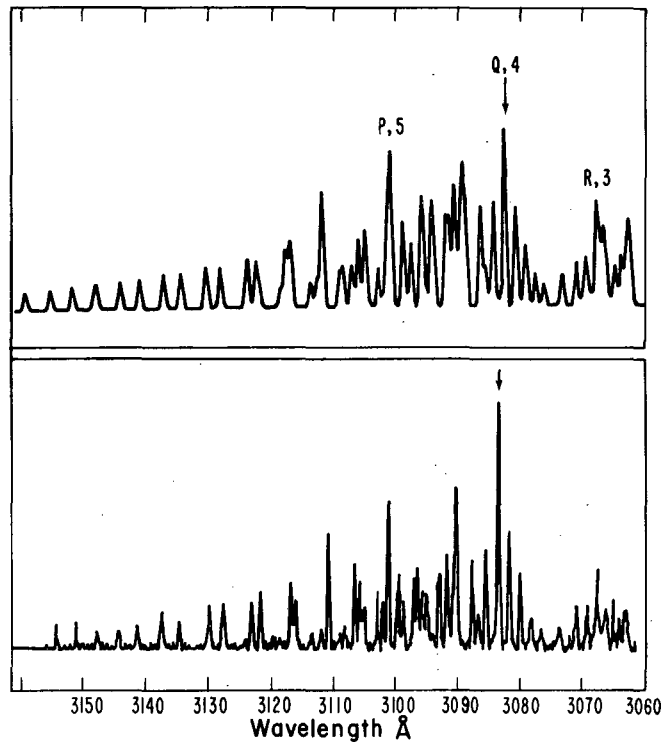

Fig. 1. A comparison between computed spectrum (top) and experimental results (bottom). (XBL 794-1143)

Other useful information can also be obtained by laser induced fluorescence spectroscopy. If the characteristic decay time of the excited species is of comparable length to the exciting pulse, chemical decay may be observed directly. We have observed and made measurements of such decay on sodium for a range of flame conditions.

FOOTNOTE

* This work was supported by the Air Force Office of Scientific Research through the Engineering Office of Research Services, University of California, Berkeley.

Combustion of Coal and Coal Related Fuels in an Opposed Flow Diffusion Flame*

W. K. Chin and R. F. Sawyer

INTRODUCTION

The growing and renewed importance of coal as a primary energy source has motivated our study of of the fundamental combustion characteristics of coal and coal derived fuels. Initiated in Fall 1976, this project is based upon utilization of an existing opposed flow diffusion flame (OFDF) burner for experimental investigation on burning characteristics of coal and coal related fuels (solvent refined coal [SRC], coke, carbon and graphite). Research has included: comparison studies among these five fuels, determination of the relative importance of O_2 and CO_2 on surface oxidation, measurement of pollutant formation, and extraction of physical properties under burning conditions.

The utility of the OFDF apparatus for laboratory study of the combustion of gaseous, liquid, and polymer fuels has been demonstrated by a number of researchers. We have employed this configuration to study the steady state combustion of graphite, pulverized coal, and SRC in an opposed flow of oxygen/nitrogen or oxygen/argon. The advantages of this geometry lie primarily in the ability to observe the combustion of coal and coal related fuels in a particularly well controlled environment. While the heating rates, which are known to be important to the pyrolysis and combustion of coal, are considerably less than is typical of the burning of pulverized coal, they are in the range of applicability to the in-situ, fluidized bed, and possibly stoker fed combustion of coal. Moreover, this experimental technique provides a means of observing the combustion of these fuels under comparable combustion conditions. In previously completed work, the experimental program has demonstrated the suitability of the OFDF technique to the study of the combustion of graphite and pressed pulverized coal samples, even in cases where there is a substantial ash fraction, 6% by weight. Porosimeter measurements indicate void and pore characteristics in the pressed samples which are consistent with reported properties of the pulverized coal. Regression rate under steady state condition was measured and solid phase temperature distribution in coal and SRC were obtained by an imbedded fine thermocouple.

ACCOMPLISHMENTS DURING 1978

The OFDF apparatus is contained in a 10 cm diameter pyrex cross to eliminate external disturbances, Fig. 1. The oxidizer is metered through the rotometer and enters the nozzle above the sample. A He-Ne laser and a photodiode is used to sense the sample surface, providing a signal to a stepping motor which automatically positions the fuel sample. Linear regression rate measurements are obtained directly from an electronic counter.

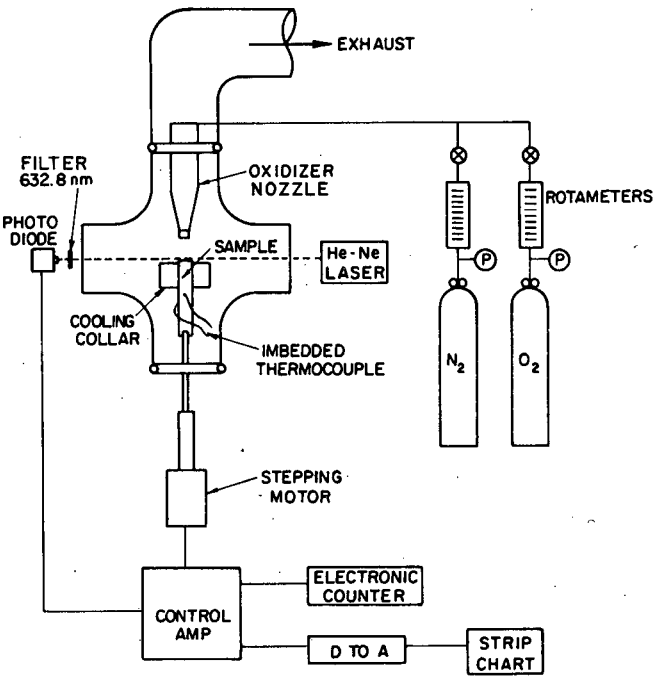

Fig. 1. Opposed flow diffusion flame apparatus. (XBL 784-7996)

The burning characteristics of pulverized coal and SRC in the OFDF were investigated by measuring the regression rate dependence on oxygen concentration and oxidizer flow velocity. Both fuels have shown roughly the same power dependence on oxygen mole fraction at oxidizer velocity of 3.81 m/s. This similarity of burning characteristics suggests that the rate limiting process for both may be established by char oxidation.

To investigate the relative importance of carbon dioxide and oxygen on surface oxidation, pulverized char was obtained by heating pulverized coal at the rate of 28°C/min to 700°C in an oven purged with nitrogen gas. Coke samples were pressed into cylindrical rods.

Carbon electrodes also have been studied. The regression rates in mixtures of oxygen and nitrogen and in mixtures of oxygen, carbon dioxide and argon were compared. No clear indication of the effect of carbon dioxide on regression rate has yet been observed.

PLANNED ACTIVITIES FOR 1979

The relative importance of CO_2 and O_2 on surface oxidation will be investigated further. Gas phase product composition will be measured and gas phase

temperature profiles determined. Experimental results will be analyzed to provide a comparison of the combustion of the several fuels studied and a final report of this phase of work will be completed.

FOOTNOTE

* This work was supported by the LBL Director's Office Fund. Lawrence Berkeley Laboratory, Berkeley, California.

Condensation of Ash and Trace Metals from Pulverized Coal Combustion*

R. Greif, J. Pennucci, F. Robben, and P. Sherman

INTRODUCTION

All indications point to a greater use of pulverized coal and in all probability greater use of coal of lower quality. This trend enlarges the concern in recent years over the environmental effects of the particulates emitted by coal combustion. The effects on the atmosphere of new power plants, even with improvements in clean-up devices, such as electrostatic precipitators, remains a serious problem. New regulations for particulates from power plants provide an added incentive for exploring new and more efficient ways of decreasing emissions.

It had been thought that the very small (<.5μ) particles emitted during coal combustion were neither prevalent nor detrimental. However, more recent studies show that there are indeed many submicron particles[1] and furthermore, that the smallest particles are the ones which are deposited in the pulmonary region of the respiratory system. In addition, there are indications that toxic trace elements are concentrated in the smaller particles[1,2] and these are particularly hazardous when ingested. There now are also indications that crops may be affected by the particulate emissions; further, the way in which the smaller particles effect the formation of larger ones to create "smoke" is just being investigated.

Although the submicron particulates may represent only a small fraction of the total mass of particulates emitted, they do represent a large fraction of the total number of particulates emitted. Cleanup devices remove the larger particles most easily; cleanup of the smaller particles is much more costly.

It is clear that it would be preferable to generate a smaller number of larger particles instead of a larger number of smaller particles. One possibility for doing this is by modifying the combustion process. Variations in the combustion process, such as changes in temporal and spatial temperature histories, have a profound effect on the combustion products. It is therefore of interest to consider the feasibility of controlling the generation of small (50Å to 5000Å) particulates from pulverized coal combustion by varying the combustion and heat transfer parameters. This work initiated last year is directed toward investigating that possibility.

ACCOMPLISHMENTS DURING 1978

A preliminary laboratory arrangement has been designed and built. For convenience and simplicity a Bunsen burner type of arrangement was chosen to burn the pulverized fuel. Provision was made for auxiliary gaseous fuel, oxygen and air for support combustion. (Stoichiometric methane-air temperature is 2236°K while stoichiometric methane-oxygen temperature is 3053°K.) The gaseous fuel, oxygen and air are injected radially at the bottom of a 1/2" diameter mixing tube. The coal/air mixture is delivered through a 1/8" diameter tube and injected vertically on the center line of the mixing tube. The main disadvantage of the burner arrangement is the flow velocity limitation due to flash back. However, reasonable velocity limits can be found using methane, air, and oxygen keeping an equivalence ratio well below 1.0. The limits using hydrogen are more restrictive.

Emphasis of the program is on particulates in the 50Å to 1000Å range. An appropriate sampling device should therefore collect and disaggregate the small particles for examination. It must also eliminate any larger particles which may obscure the small ones. Sampling can be done isokinetically, using an impacting surface, using a sonic orifice, or by various electro-magnetic or diffusion schemes. The initial design chosen was a streamlined wedge shaped chamber with a sonic orifice (0.03" dia.). A vacuum pump evacuates the chamber so that sonic conditions are maintained at the sampling orifice. With sonic flow a maximum flow rate for the given orifice size is maintained. In addition, the streamlines are forced to curve, sucked inward toward the sampler orifice. As a result of their inertia, the larger particles tend to travel in a straight path in their initial direction. Most of them therefore bypass the sampling orifice. The small particles with much less inertia follow the curved streamlines into the sampler orifice. The collecting surface geometry inside the sampler should remove any large particles which may have entered, and it should further spread out the particles collected. The design employed provides for two kinds of collection surfaces. One is a thick flat plate with a rounded leading edge. The leading edge catches the large particles and the small ones are spread out over the flat surface. The other collection surface

that fits into the sampler is a hexagonal cylinder which permits collection of particles at different angles to the flow. The design has proven effective. Large particles by-pass the orifice, and the submicron particles are distributed over the collection surface.

Examinations of very small particles of the order of 100Å requires the use of the transmission electron microscope (TEM). It permits a magnification greater than any other kind of microscope so that very small particles can be photographed and their morphology determined. The resolution of most TEMs permit observation of particles down to 20Å . The substrate required, however, must be transparent to the electron beam of the microscope and must also be microscopically flat and clean. A technique which meets these requirements is a thin carbon film supported on a strip of mica. The mica is cleaved along its lattice surface so that it is microscopically smooth. A layer of carbon is deposited on it by surface condensation in an evaporator kept at very low pressure. After particles are collected on the coated mica, they are "shadowed" in the evaporator by depositing a thin film of chromium (or platinum-palladium) at an angle to the surface of the mica. The chromium layer is opaque to the electron beam so that shadows are created which give a three-dimensional character to the image. The higher the particle stands above the surface, the longer the shadow. If grain size of the opaque shadowing material is kept fine by proper use of the evaporator, good photographs are obtained at greater than 100,000 magnification.

Figure 1 shows an example of the photographs taken. The darkest parts of the photographs are particles. The grey background is the shadowing material. The light "tails" are the shadows where no shadowing material falls.

PLANNED ACTIVITIES FOR 1979

The preliminary work done has demonstrated in a general way the feasibility of the laboratory approach. Refinements of the equipment and the experimental techniques hold the promise of significant results. Modifications to the equipment should be made to insure substantial progress.

The changes presently considered are:

- a new coal hopper section for steadier flow of fine coal dust
- an improved mixing tube geometry to remove the boundary layer
- a cleaner sampler inlet with filtered bleed-in
- addition of a positioning device for locating the sampler
- a heated flame holder ring for wider flame stabilization conditions

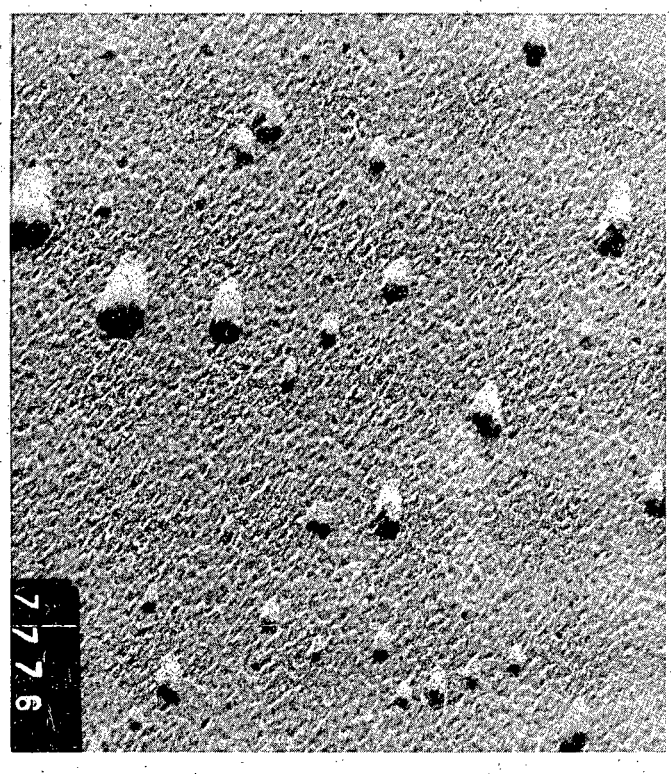

Fig. 1. Micrograph of shadowed particles

Flow rates: coal ~ 2.7 gms/min
methane ~ 2.7 liters/min
oxygen ~ 5.8 liters/min
air ~ 20.3 liters/min

Run time ~ 10 minutes
Sampler orifice ~ 21 1/2" from mixing tube exit.

- added instrumentation:
  thermo-couples and pyrometers to obtain the temperature field; laser light absorption or scattering to measure the coal dust flow rate.

In addition, an alternate burner approach should be investigated. In the open flame arrangements now employed, the free jet mixing process and resultant temperature and concentration fields, although somewhat predictable, cannot be independently controlled. A flame enclosure with walls which can be heated or cooled would provide for better control of heat transfer and mixing with secondary air.

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Polymer Combustion and Flame Chemistry*

N. J. Brown, R. F. Sawyer, R. W. Schefer, and W. J. Pitz

INTRODUCTION

New energy technologies and conservation measures have resulted in an increased use of polymeric materials. Although they are advantageous from the perspective of energy considerations, polymeric materials sometimes create a fire hazard. In order to assess their potential risk, it is important to characterize the flammability of these materials. For this reason a combined experimental and theoretical program is underway to investigate steady state polymer combustion, gas phase flame inhibition, and flame chemistry. Fundamental combustion characteristics of polymeric materials, including burning rates, mass transfer numbers, extinction limits, and flame structure, are determined in a series of opposed-flow diffusion flame experiments with the objective of relating the basic physical and chemical properties of the polymer to flammability. A complementary study of flame inhibition is underway, and the results will be used to explain the chemical inhibition of polymer combustion.

Flame inhibitors are broadly classified as being either of the physical or chemical type. The former is believed to act simply as a physical diluent while the latter is thought to participate directly in the reaction mechanism important to flame propagation. Although no general consensus exists regarding the mechanism(s) of chemical inhibition, it is recognized that certain molecules have been observed to retard flame propagation out of proportion to their thermal influence which leads to the supposition that this type of inhibition is directly linked to chemical reactivity. Since effective, rapid suppression of unwanted fires is most desirable, theoretical and experimental studies of flame chemistry and flame inhibition have been undertaken to determine combustion characteristics and chemical kinetic mechanisms which are important in understanding inhibition.

ACCOMPLISHMENTS DURING 1978

Extinction measurements have been performed on uninhibited and inhibited polyethylene samples burning in the opposed flow diffusion flame apparatus.[1] The contrasting cases of oxidizer inhibitor addition and fuel inhibitor addition have been investigated, and in the former case various concentrations of the inhibitor HCl have been added to the (N_2/O_2) oxidizer stream. Since polyvinyl chloride differs chemically from polyethylene by the substitution of a chlorine atom for a hydrogen atom in the monomer, the polyvinyl chloride may be thought of as inhibited polyethylene and was used for the set of extinction measurements where the inhibitor was added to the fuel. In comparing the extinction data for the addition of chlorine to the oxidizer with its addition to the fuel, it is important to compare only cases with identical amounts of chlorine in the flame zone and suitable data for comparison are shown in Fig. 1. The results of such a comparison suggest that inhibition is more effective when the inhibitor is added to the fuel side; however, the differences in physical properties of polyethylene and polyvinyl chloride and presence of impurities in each polymer preclude a definite conclusion. Further studies are currently underway with pure samples.

A numerical boundary layer model was developed to aid in analyzing extinction data from opposed flow diffusion flame experiments. The model relates overall kinetic parameters to various extinction data and may indicate the influence of inhibitors on overall kinetics. In addition, an improved aerodynamically designed nozzle was built which yields a more uniform laminar velocity profile in the flame zone of the opposed flow burner and gives a closer match between experiment and numerical model. Preliminary gas composition measurements with a quartz microprobe have been performed to determine characteristics of the flame chemistry close to extinction.

Work has been completed on the construction and demonstration of a two zone flame model which is largely based on flame chemistry and is suitable for computing flame propagation velocity and average properties of the radical generation region and fuel attack region of a flame.[2] An experimental study of low pressure hydrogen/oxygen flames concerned with the flame structure analysis of lean, near stoichiometric and rich flames has also been completed.[3]

A computational study of flame inhibition has been made using the model of the perfectly stirred reactor. The flame system selected for study was hydrogen/oxygen/argon and the inhibitors studied were Ar, N_2, HCl and HBr. The variables considered in this study were 1) H_2/O_2 mechanism, 2) pressure, 3) equivalence

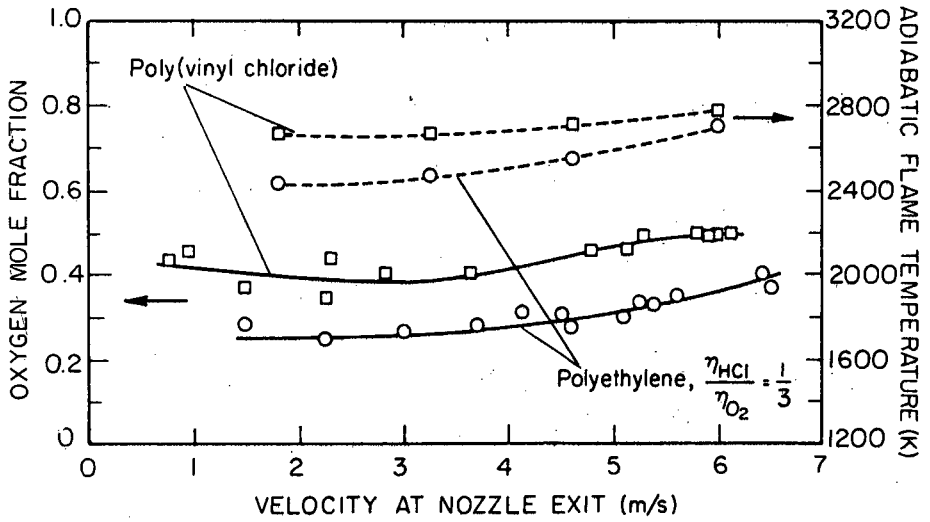

Fig. 1. Comparison of extinction curves and adiabatic flame temperatures of PVC with N_2/O_2 mixtures and PE with N_2/O_2/HCl mixtures where η_{HCl}/η_{O_2} = 1/3. (XBL 784-4832)

ratio and 4) inhibitor type and concentration. The perfectly stirred reactor equations were solved for a series of residence times, and the corresponding compositions and temperatures between the blowout condition and thermodynamic equilibrium were obtained. An inhibition parameter was defined to characterize inhibition in a perfectly stirred reactor.

The blowout parameters: residence time, temperature, composition, reaction rate and heat release rate were especially sensitive to inhibitor type and concentration in the perfectly stirred reactor calculations. Radical concentrations were also found to be sensitive to the variables considered. Figure 2 illustrates the effect of HBr on the radical pool fraction for a lean H_2/O_2 mixture. A paper[4] describing the cases of HBr, N_2 and Ar inhibition has been written and another contrasting the inhibitors HCl and HBr is in preparation.[5] Computational studies of HBr inhibition in plug flow and HBr inhibition of wet CO/O_2 mixtures in the perfectly stirred reactor are in progress.

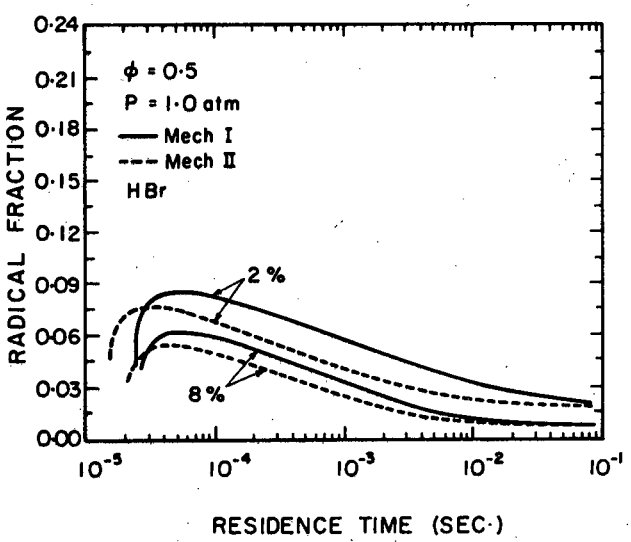

Fig. 2 Radical pool fraction as a function of residence time for 2 and 8 mole percent HBr for lean H_2/O_2/Ar mixtures reacting via mechanisms I and III at one atmosphere. (XBL 784-7962)

PLANNED ACTIVITIES FOR 1979

This project is to be completed during 1979 and planned activities are:

1) Completion of the experimental studies of polymer inhibition in the opposed flow diffusion apparatus.

2) Determination of the composition and temperature profiles of polyethlene/oxygen/nitrogen opposed flow diffusion flames for various oxidizer velocities and compositions.

3) Completion of the computational studies of HBr inhibition of hydrogen/oxygen/argon mixtures in plug flow and of wet carbon monoxide mixtures in the perfectly stirred reactor.

Papers describing this work will be submitted for publication.

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Soot Radiation in Foam Polystyrene Flames*

C. L. Tien,† S. C. Lee,† and T. W. Tong†

INTRODUCTION

The flaming properties of plastics have become an increasingly important concern in fire safety considerations. Several recent studies have been devoted to the radiative properties of plastic flames.[1-3] Of particular interest is the soot contribution to thermal radiation from these flames, which is quite significant but little understood. A good understanding requires detailed information on soot characteristics, such as optical properties, size, shape and number density, as well as how they vary with fuels and flaming conditions.[4-7] Soot optical properties have been studied for different soots in combustion systems,[8-9] but information on soot size, shape and number density in different flames is comparatively scarce.

Assuming that the characteristic size of soot particles is small compared to the characteristic wavelength of thermal radiation, soot radiation can be analytically described by Rayleigh absorption, the limit for small, absorbing particles in the general Mie theory.[10] In this limit, the analytical description is greatly simplified in that detailed information on soot size, shape and number density becomes unnecessary, and soot radiation depends only on the soot volume fraction and the optical properties of soot.[4,5] Indeed, it is found experimentally that the soot size in solid-plastic flames is much smaller than the characteristic radiation wavelength,[3] and the soot extinction coefficient follows closely that due to Rayleigh absorption.[11] It is on this simple model that most calculation methods for luminous flame radiation have been developed,[4-6] and a useful tabulation of soot volume fractions for different diffusion flames is presented.[6]

The present work reports experimental results of soot radiation in foam polystyrene flames, which exhibit radiation characteristics distinctively different from Rayleigh absorption as previously observed in solid polystyrene flames.[1] This interesting, but surprising, finding not only provides valuable information in the fire-safety analysis of widely-used foam plastic materials, but also suggests the general use of the full Mie theory in analysing soot radiation.

EXPERIMENT

The experimental system for infrared transmission and emission measurements is essentially the same as that used by Buckius and Tien.[1] Foam polystyrene samples (National Bureau of Standards Special Reference Materials GM 48) of size 20(H) x 8 x 5 cm were each placed in aluminum foil trays of size 0.7(H) x 8 x 5 cm with the short side along the path of the light beam emitted from the source unit. The light path was 2 cm above the burning surface. The present measurements show that the radiative properties of foam polystyrene plastic during solid-foam and liquid-pool burnings display essentially the same characteristics, but for convenience, most data were taken during the pool burning period. Each test was run at a fixed wavelength from 1.6 to 5.0 μm, and the pathlength was determined photographically.

DATA ANALYSIS

Away from the absorbing bands of gases, a beam of monochromatic radiation is attenuated along a homogeneous polydisperse aerosol according to

$$I_\lambda(L) = I_\lambda^o e^{-\kappa_\lambda L} \tag{1}$$

where I_λ^o and I_λ are the initial and transmitted intensities respectively, L the optical pathlength, and κ_λ the spectral aerosol extinction coefficient. In terms of particle parameters, κ_λ can be expressed as[11,12]

$$\kappa_\lambda = \int_o^\infty \pi r^2 N(r) Q_e(r) dr \tag{2}$$

where r is the particle radius, N(r) the particle size distribution, and Q_e the single-particle extinction efficiency. For spherical particles, Q_e has been analytically expressed and numerically tabulated in terms of the particle size parameter, $\alpha = 2\pi r/\lambda$, and particle optical properties.[10]

The particle size distribution N(r) is often represented by the following three-parameter distribution[3,11]

$$N(r) = ar^{b-3}e^{-cr} \qquad (b \geq 3,\ c > 0) \qquad (3)$$

and the constants a, b and c are related to the basic distribution parameters as

$$a = \frac{N_o c^{b-2}}{(b-2)}, \quad b = 2 + c^2\sigma^2, \quad c = \frac{b-3}{r_m} \qquad (4)$$

where N_o is the toal number of particles, σ the standard deviation, and r_m the most probable radius. The soot volume fraction is thus

$$fv \equiv \int_o^\infty \frac{4}{3}\pi r^3 N(r)dr = \frac{4}{3}\pi a \frac{\Gamma(b+1)}{c^{b+1}} \qquad (5)$$

Based on the experimental values of K_λ, an iterative least-squares fit to equation (2), with N(r) given by equation (3), and the appropriate optical constants[8] and Q_e[10] were employed to determine a, b, and c, and thus the basic distribution parameters.

RESULTS AND DISCUSSION

The spectral variation of the soot extinction coefficient for foam polystyrene flames is shown in Fig. 1, along with those for solid polystyrene flames. The bars represent the upper and lower bounds of the experimental data. The solid polystyrene data of Buckius and Tien[1] clearly show an inverse wavelength dependence, denoting that scattering is negligile, soot particles are small, and the Rayleigh absorption limit can be applied. The distinctively different spectral variation for foam polystyrene implies that scattering is appreciable, particles are large, and the full Mie theory must be employed. The results in Fig. 1 show that the spectral soot extinction coefficients are generally higher for foam than solid polystyrene due to the larger size of soot in foam polystyrene flames. This means, of course, that the total emissivity or radiance of foam polystyrene flames is accordingly higher than that of solid polystyrene flames.

Analysis of the present soot-radiation data yields $a = 6.224 \times 10^{-4}$, μm^{-5}, $b = 4$, and $c = 7.5\ \mu m^{-1}$, which correspond to $r_m = 0.133\ \mu m$ and $f_v = 2.64 \times 10^{-6}$. In comparison, the solid polystyrene results indicate a comparable value of f_v (4.6×10^{-6} (ref. 3) and 4.2×10^{-6} (ref. 1)) and a much smaller r_m (0.021 μm (Ref. 3)). The basic cause for this interesting, but surprising, disparity in soot size is subject to anyone's conjecture, since there exists so little information on the basic mechanisms of soot formation and conglomeration. It appears, however, that one plausible cause is the differing interweaving arrangement of long-chain polymer molecules resulting from different manufacturing processes.

The soot size distribution obtained in this study is much broader than that measured by Pagni and Bard[3] using a laser-optical method. Their distribution with $a = 1.073 \times 10^3\ \mu m^{-7}$, $b = 6$, and $c = 49.2\ \mu m^{-1}$, which gives a smaller r_m (0.061 μm) and a slightly higher f_v (4.7×10^{-6}), does not yield the soot extinction coefficient in agreement with the present experimental results. The difference in the soot sizes is probably due to the larger ventilation rate used in their experiment which induces more complete combustion.

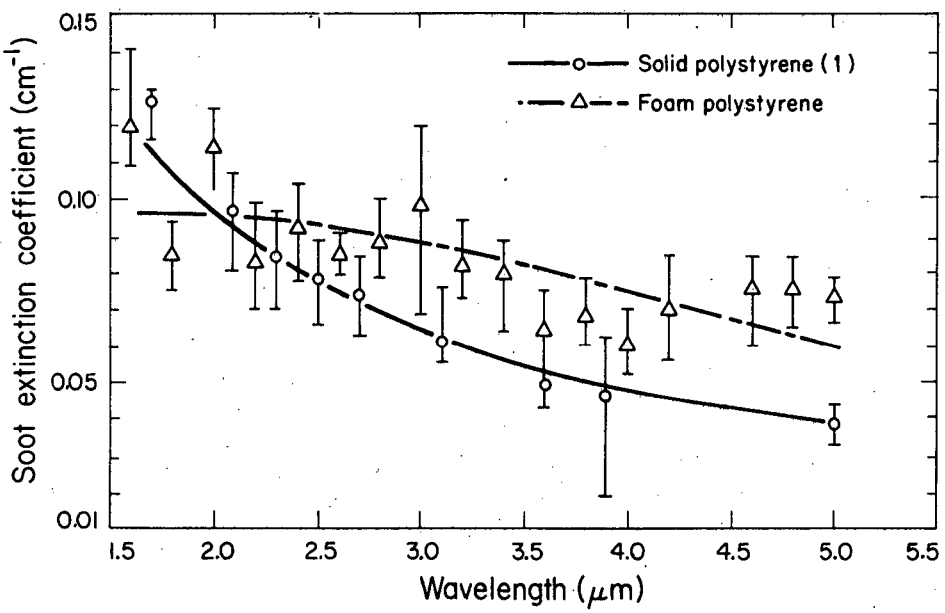

Fig. 1. Spectral variation of soot extinction coefficient for foam and solid polystyrene flames. (XBL 794-1094)

The different sample sizes (7.5 cm vs. 5 cm in the present study) might have some effect on the value of f_v. For solid polystyrene flames, Markstein[2] obtained for larger samples a higher f_v than that obtained by Pgani and Bard[3] and Buckius and Tien[1] for smaller samples.

CONCLUSION

The soot extinction coefficient determined from the measured infrared transmittance of foam polystyrene flames shows a wavelength dependence distinctively different from the inverse wavelength dependence of Rayleigh absorption as reported for solid polystyrene flames. The data analysis based on the full Mie theory yields the soot size distribution which indicates larger soot sizes in foam polystyrene flames. Consequently, soot and flame radiation of foam polystyrene flames is larger than that of solid polystyrene flames.

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* This work was supported by the National Bureau of Standards Fire Research Center and by the Product Research Committee. The conclusions are those of the authors and not of the Products Research Committee. The authors are also grateful for the assistance of G.L. Hubbard.

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Fire Modeling*

P. J. Pagni, T. M. Shih, R. Toossi, C. M. Kinoshita, S. Bard, R. A. Beier, A. Ortega, D. Wang, and K. Kayayan

INTRODUCTION

The overall goal of this project is to develop physical and mathematical models of the detailed combustion phenomena which control a fire's growth within a compartment of origin and its subsequent propagation through a structure. These experimental studies and theoretical analyses attempt to provide bases for eventual development of test methods and predictive capabilities for evaluation of the real fire hazard of specific materials and configurations. This work is divided into three broad categories: (1) extensions and applications of excess pyrolyzate concepts, (2) soot volume fractions in diffusion flames, (3) flat flame burner designs and experiments.

ACCOMPLISHMENTS DURING 1978

Excess Pyrolyzate

Several papers have been published describing the effects of fuel which is not consumed locally in the flame that produced it.[1,2,3,4,5] In preparation for applying this concept to compartment fires, the well-defined, steady, two-dimensional, laminar, opposed flow, diffusion flame was considered.[6] Predictions of flame heights and excess pyrolyzate have been obtained for axisymmetric and two dimensional geometries. Agreement within ten percent with preliminary flame height experiments using PMMA in an OFDF apparatus previously described by Sawyer and co-workers has been

obtained. The problem of a fuel jet impinging on a noncombustible plate with an oxidizing ambience has also been considered. Order of magnitude extension of laminar flame heights due to this impingement is predicted. In addition, experimental flame heights for PMMA were measured over a wide range of ambient oxygen concentrations in a forced flow apparatus. Agreement with predictions within twenty percent is obtained.

Soot Volume Fractions

Experimental values of the volume fraction of small turbulent diffusion flames occupied by combustion generated carbon particulate are listed in Table 1 for some of the common fuels tested.

Table 1. Sample soot volume fractions.

Fuel	Polystyrene (Foam)	Polystyrene (Solid)	Polyurethane (Foam)	PMMA (Solid)	Acetone (Liquid)
$f_v \times 10^6$	4.7	4.6	0.80	0.31	0.18

Since scattering appears to be important for flames with volume fractions greater than 3×10^{-7}, a multi-wavelength technique was required to determine accurate soot volume fractions. Measurement of the attenuation at several wavelengths of monochromatic laser beams passing through a flame determines, in addition to f_v, approximate detailed size distributions of the carbon particles within the flame.[7] Calculations of flame radiation back to polyurethane fuel in a pool fire geometry yields good agreement with experimental mass burning rates.[8]

Flat Flame Burner

The detailed temperature and velocity field around a cooling coil embedded in a porous plug burner have been predicted assuming a low Reynolds number media. The results indicate that the maximum extension of the coil wake beyond the front stagnation point is 5 coil diameters and that as the distance between the coils decreases, the length of the coil wake also decreases to a limit of approximately two diameters. The governing nondimensional groups have been identified and the character of the solution over their full range has been examined. Flat flame burners have been designed and built based on these results.[9]

Additional Accomplishments

Other studies of flame spread in opposed flow, excess pyrolyzate in compartments and heat and mass transfer in wet concrete are in preparation.[10]

Successful comparison between excess pyrolyzate and flame height predictions and laboratory data have been obtained in a wide variety of systems. The effects of physical and chemical parameters on flame height have been clearly delineated. A technique for measuring the volume fraction of soot in flames in situ has been developed, and data on f_v and detailed size distributions of combustion generated carbon particles have been obtained for several common solid, foam and liquid fuels. Temperature and velocity fields within water cooled flat flame burners have been predicted and apparata are available designed according to these analyses.

Flame radiation is now well accepted as the dominant heat transfer mode in full scale fires. This radiation is in turn controlled by the amount of soot in the flame which now can be measured in both laboratory and full scale flames by the techniques developed here. Criteria to be included in ranking material hazard may develop from our studies of excess pyrolyzate. In addition, similar analyses may have utility as sub-program components in compartment fire prediction models under development elsewhere. The flat flame burner described here is now in use in several laboratories and will permit useful comparisons of detailed flame structure experiments.

PLANNED ACTIVITIES FOR 1979

In the second year of this grant the present program will be continued with more emphasis on modeling compartment fires.

Further applications of excess pyrolyzate calculations in systems with both external and flame generated radiation, vitiated ambience and feedback from compartment configurations are under development. Experiments are continuing to obtain data on flame lengths for comparison with predictions. The multi-wavelength laser technique for in situ measurements carbon particulates in flames will be refined to give more accurate particle size distributions for a wide variety of fuels. The effects of flame scale and the variation of the size distribution in space and time will be explored.

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Event Logic Models and Fault Tree Analysis of Fires

R. B. Williamson

INTRODUCTION

There has been a continuing interdisciplinary research project since 1971 at the University of California, Berkeley on "Fire Safety in Urban Housing". The original project was initiated through the College of Engineering on the campus, and the continuing research program was shifted to the Energy and Environment Division of Lawrence Berkeley Laboratory during 1978. The original sponsor was the National Science Foundation--Research Applied to National Needs (NSF-RANN) with additional support from the Department of Housing and Urban Development. In 1976 the fire research mission was shifted from the National Science Foundation (NSF) to the U.S. Fire Administration and the Center for Fire Research (CFR) at the National Bureau of Standards (NBS), and the sponsorship of the Berkeley projects was also shifted to those agencies. A variety of topics have been studied in the overall project and the specific subjects discussed here started several years ago before they were shifted to LBL.

The object of this portion of the fire research project has been to develop event logic models for fire and then incorporate fault tree methodology in their analysis. This has led to the development of a state transition model (STM) of fire growth and spread, as well as the identification of four submodels which make up the total fire event model.

The submodels are constructed to answer the following questions:

1. What is the extent of fire growth with time?
2. What is the extent of spread of combustion products (smoke) from the fire as a function of time?
3. What are the roles of people with the fire in causing its ignition, in fighting it and possibly in becoming its victims?
4. What fire protection techniques can be expected to prevent the fire spread of fire and smoke?

The first question is answered by the Fire Growth Model (FGM), the second by the Smoke Spread Model (SSM), the third by a Human Response Model (HRM), and the fourth by a Fire Protection Model (FPM). As mentioned above, the emphasis has been placed on developing the FGM with particular attention to the utilization of both deterministic calculation and experimental data to quantitatively validate the modeling techniques.

The potential impact of fire can be characterized by (1) the probability of ignition, (2) the probability distribution of fire growth as a function of time and (3) the conditional probability distribution of losses given that a fire has broken out. The total fire model should have the capacity to allow quantitative assessment of the potential temperature of a fire, and there should be sufficient generality to make it applicable to new types of fire situations. For instance, there are fire situations in new occupancies, such as nuclear reactors or wide-bodied airplanes, which have not yet generated a sufficient number of case histories to identify the many possible fire scenarios. Yet a fire situation in these cases could be disastrous. It would therefore seem important for such cases to take data from other occupancies where people are performing similar tasks, and the same behavior pattern of both people and equipment could be reasonably expected. For instance, the data from restaurants and theaters might be analyzed to see what might be expected in wide-bodied aircraft which has many of the same activities and equipment as restaurants and theaters. Similarly nuclear power plants might be compared with conventional power plants for fire that started with a common activity. These data and subsequent fault tree analyses would help to predict and hopefully prevent potentially dangerous fires.

ACCOMPLISHMENTS DURING 1978

The FGM for the room of origin is shown in Fig. 1. It follows the state transition format introduced by Williamson.[6] The events shown are not necessarily the only events which could be chosen, but they represent observable phenomena that are useful in quantifying full-scale fire tests. The histograms and cumulative distribution

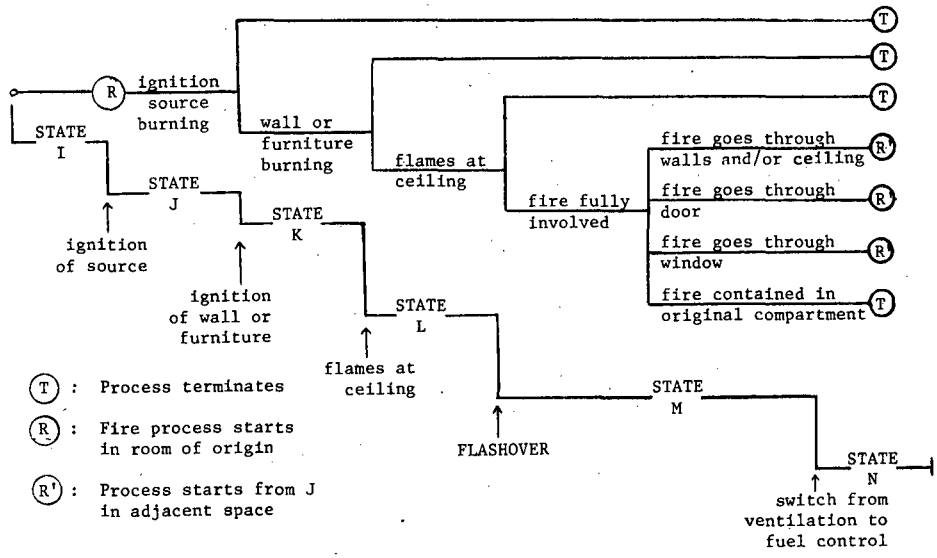

Fig. 1. Fire growth model for fire in a room. (XBL 794-9177)

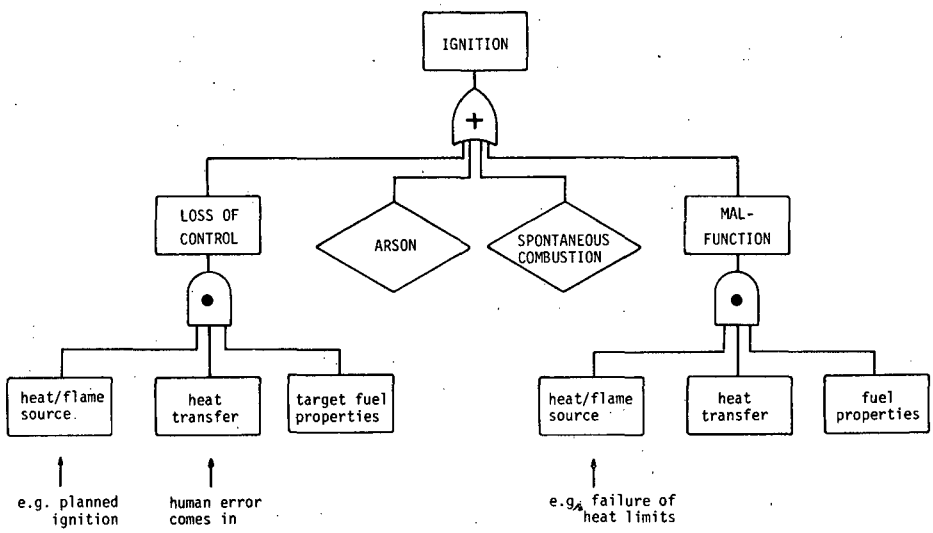

Fig. 2. A simple form of the fault tree for the original ignition process. (XBL 794-9178)

functions (CDF's) for the observed state durations can be directly utilized as probabilities of the end event for tested materials.[1]

One of the special features of the state transition model in Fig. 1 is that it spans the entire duration of fire in the room of origin, and subsequently, in adjacent spaces, the fire growth process starts from a new state J where the flames emerging from the room of origin can be considered the ignition source. This is schematically represented by the symbol (R') in Fig. 1.

The events which mark the beginning and end of the states shown in Fig. 1 can be considered as the top event in a fault tree. The goal of fault tree construction is to model the system conditions that can cause the undesired event at the top of the tree. When fault trees are constructed for the fire protection system of a whole building, they are quite large and complex; when they are applied to the limited number of state transition events, they can be relatively simple and the very important time factor is automatically taken into account. An example of a fault tree is shown in Fig. 2 where the ignition event is the top event and the four principal sources of actual fire ignitions are connected to ignition through an "or" gate.

An analysis has been performed on the origin of fires in kitchens and was published for the Fall 1978 meeting of the Western States Section of the Combustion Institute.[2] As shown in Fig. 2, the original ignition of unwanted fires has four principal causes: loss of control of wanted fire, arson, spontaneous combustion

and malfunction of equipment. Loss of control refers to ignitions which start with a planned or wanted ignition, but which, due to human error causing a sufficient heat transfer to the target fuel, results in unwanted spread. Malfunction refers to equipment failures such as overloaded electrical circuits or exploding heaters. A more detailed fault tree than Fig. 2 was constructed to reflect the findings of the National Household Fire Survey (NHFS) which found kitchens to be the origin of 65% of the 2,017 residential fires reported by the respondents.[3] There was sufficient quantitative information in the NHFS to estimate that the probability of human error in causing the heat transfer for loss of control to be 0.1. This would indicate that in nine out of ten incidences the heat source and the fuel were right for a fire, but the heat transfer did not occur to cause fire.

The fault tree on ignition of fire gives not only a graphical representation of the top event, but also a ranking of the scenarios according to their probabilities of occurring since the minimum cut sets of the fault tree are a listing of the possible fire scenarios to which probability of occurrence can be quantitatively assigned by using fire statistics from the field.

PLANNED ACTIVITIES FOR 1979

The NBS-CFR sponsors have shifted their emphasis for 1979 to the fire growth experiments leading toward a standard room fire test (see below), and thus major activities on this project will require new sponsorship. There are a number of potential avenues of research that should prove interesting and important. The Fire Growth Model (FGM) can be further developed to specifically treat the spread beyond the room of origin and the Fire Protection Model (FPM) can be constructed to control that spread. The concept of "defense in depth" can be quantitatively evaluated from the imposition of the FPM and the effects on the FGM beyond the room of origin. Standard fire test data on suppression systems, fire walls, fire doors and other fire protective devices and/or assemblies can serve as the pool of quantitative information to make the FPM meaningful.

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