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ABSTRACTS:  
1984 AFOSR/ONR  
CONTRACTORS MEETING  
ON AIRBREATHING  
COMBUSTION RESEARCH

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June 20-21, 1984  
Pittsburgh Hilton Hotel  
Pittsburgh, Pennsylvania

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**1984 AFOSR/ONR**  
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June 20-21, 1984  
Pittsburgh Hilton Hotel  
Pittsburgh, PA 15213

Day 2: Thursday, 21 June

Session Chairman: E.A. Lezberg, NASA Lewis Research Center

Topic: SOOT

8:30 - 9:00 am                   A. Stanton,  
Aerodyne Research, Inc.

9:00 - 9:30                       R.J. Santoro,  
National Bureau of Standards

9:30 - 10:00                   G.M. Dobbs and L. Boedecker,  
United Technologies Research Center

10:00 - 10:30                   BREAK

Session Chairman: H.L. Beach, NASA Langley Research Center

Topic: IGNITION/COMBUSTION ENHANCEMENT

10:30 - 11:00                   M. Lavid,  
ML Energia, Inc.

11:00 - 11:30                   W. Braun and M.D. Scheer,  
National Bureau of Standards

11:30 - 12:00pm               D.A. Santavicca,  
Princeton University

12:00 - 1:00                    LUNCH

Session Chairman: D. Mann, Army Research Office

Topic: SPRAYS

1:00 - 1:30                    J.E. Peters, H. Krier and K. Kim,  
University of Illinois

1:30 - 2:00                    W.A. Sirignano and H.T. Sommer,  
Carnegie-Mellon University

2:00 - 2:30                    A.H. Lefebvre, S.N.B. Murthy and J. G. Skifstad,  
Purdue University

2:30 - 3:00                    J.F. Verdieck,  
United Technologies Research Center

3:00 - 3:30                    BREAK

Session Chairman: M.K. Ellingsworth, Office of Naval Research

Topic: LIQUID AND SOLID PARTICULATES

3:30 - 4:00

F.L. Dryer,  
Princeton University

4:00 - 4:30

C.K. Law,  
Northwestern University

4:30 - 5:00

D.E. Rosner,  
Yale University

ADJOURN

**PROGRAM SCHEDULE FOR THE 1984 AFOSR/ONR  
CONTRACTORS MEETING IN COMBUSTION**

**Day 1: Wednesday, 20 June**

Morning Chairman: C.R. Martel, AF Wright Aeronautical Laboratories

Topic: SOOT

8:30 - 9:00 am	H. Calcote and D. Olson, AeroChem Research Laboratories
9:00 - 9:30	I. Glassman, F.A. Williams and F.L. Dryer, Princeton University
9:30 - 10:00	BREAK
10:00 - 10:30	P. Bonczyk, United Technologies Research Center
10:30 - 11:00	A.H. Lefebvre and P. Sojka, Purdue University
11:00 - 11:30 pm	C.A. Moses and L.G. Dodge, Southwest Research Institute
11:30 - 1:00	LUNCH

Topic: GOVERNMENT RESEARCH SUPPORT

1:00 - 1:20	A.D. Wood, Office of Naval Research
1:20 - 1:40	M.J. Salkind, Air Force Office of Scientific Research
1:40 - 2:00	J.M. Tishkoff, Air Force Office of Scientific Research
2:00 - 2:20	D. Mann, Army Research Office
2:20 - 2:40	E.A. Lezberg, NASA Lewis Research Center
2:40 - 3:00	BREAK

STATEMENT "A" per D. Tyrell  
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3:00 - 3:20	E.J. Mularz, NASA Lewis Research Center
3:20 - 3:40	A. Laufer, Department of Energy
3:40 - 4:00	R. Rostenbach, National Science Foundation
4:00 - 4:20	Mr. W. Oran, NASA Headquarters
4:20 - 5:00	AFOSR, ONR Business Meetings, Contractors Only
6:30	BANQUET

# IONIC MECHANISMS OF SOOT FORMATION IN FLAMES

(AFOSR Contract No. F49620-83-C-0150)

H.F. Calcote

AeroChem Research Laboratories, Inc.  
P.O. Box 12, Princeton, NJ 08542

## SUMMARY/OVERVIEW

The mechanism of soot formation in flames, especially the initial chemical steps (nucleation), is being developed on a quantitative basis by experimentally studying low pressure premixed flames and interpreting the observations in terms of elementary steps. Because of the fundamental nature of the data obtained using this approach, the soot formation mechanism should also be applicable to other more complex systems such as high pressure engines and diffusion flames. Of course, the relative importance of individual steps in the process will change with the environment, but a quantitative understanding of what controls the individual steps should permit one to simulate the effects of these changes and include them in the model. →

The soot formation mechanism involves rapid ion-molecule reactions to make the transition from small molecules to large multi-ring aromatic hydrocarbons, in contrast to the more commonly proposed free radical mechanism. In addition to elucidating details of the proposed ion-molecule mechanism, we are continually answering the criticism of others, which often takes the form of alternate explanations of the dramatic changes in flame ions associated with the appearance of soot. The experimental measurements employed in this work include: molecular beam ion sampling mass spectrometry, Langmuir probes, thermocouples, and two-wavelength optical emission pyrometry. We also make extensive use of data obtained by others.<sup>1-4</sup>

## TECHNICAL DISCUSSION

We summarize here progress on some of the specific tasks which have been pursued since the last meeting.

1. Construction of MIT Burner. Many people have studied soot formation in very nearly the same "basic flame" ( $C_2H_2/O_2$ ,  $\phi = 3.0$ ,  $P = 2.67$  kPa,  $u = 50$  cm  $s^{-1}$ ), but have used different burners. In order to make available the large amount of data measured at MIT by Howard and coworkers for comparison with our charged species data, we have duplicated the MIT burner and will use it in some future measurements. The all copper MIT burner has a 7.1 cm diam, 1.3 cm thick top with about 600 holes, 1.0 mm in diam. The burner is water cooled only at its base. The AeroChem burner which was previously used in this program is 8.6 cm in diam and has a top with about 900, 1.2 mm i.d. stainless steel tubes 2.9 cm long, microbrazed into two stainless steel perforated plates. Thus the burner top itself is cooled with water flowing around the tubes. Some differences in burner temperatures are thus expected.

2. Temperature Profiles. Temperature profiles on the basic  $C_2H_2/O_2$  flame have been determined using both the MIT and AeroChem burners and for equivalence ratios of 2.00, 2.25, 2.50, 2.75, 3.00, 3.25, and 3.50. Fine wire Pt/Pt-Rh thermocouples

were used with the radiative heat loss compensation method. The maximum temperatures are accurate to about  $\pm 60$  K, whereas lower temperatures downstream of the maximum are accurate to about  $\pm 30$  K. Some results are shown in Fig. 1. The temperature difference between the two burners at otherwise identical conditions is due to different thermal losses, mostly to the cooled burner surface.

3. Characteristic Time Analysis. The availability of good temperature measurements makes more extensive interpretation of these flame measurements possible. We report here the calculation of characteristic times,  $\tau$ , for some of the potentially important steps. This is shown in Figs. 2 and 3 for locations 1.5 and 2.5 cm above the burner at  $\phi = 3.0$  corresponding to where both neutrals and ions peak, and where the number density of soot has attained half its maximum value. For free radicals and other neutral species, peak concentrations were used; they occur before the "precursor" peak. The times are to be compared with the experimental flow time and it should be noted that some of the steps need only occur once, and are thus directly comparable, whereas other steps are typical of processes requiring many sequential steps which must occur about  $10^3$  times by 2.5 cm. These individual steps must therefore be very rapid, i.e.,  $\tau < 10^{-6}$  s. The rate coefficients used for this analysis are those quoted by the protagonist of the reaction.  $k_c$  is either the hard sphere collision cross-section for R assumed to be a six carbon ring compound, or the Langevin cross-section for an ion  $R^+$  (including  $C_3H_3^+$  and very large ions). P,  $P^+$ ,  $P^-$  represent soot particles of the size observed at 2.5 cm in this flame. One observation which emerges from the present exercise is that, for low molecular weights, ion-molecule reactions are distinctly faster than neutral-neutral reactions; however, an increase in molecular size (assuming  $C_2H_2$  as the building block), and an increase in temperature both favor neutral-neutral reactions. Also, as ions increase in size, their recombination coefficients increase, so that the larger ions are removed more rapidly than the smaller ions. Thus, as the incipient soot particles grow, the ionic nature of the process becomes less important. This explains one of the mysterious observations that neutral soot particles appear to grow more rapidly than do charged particles (see, e.g., Fig. 4, Ref. 5).

The techniques used for this analysis form the basis for developing computer codes to simulate soot formation processes.

4. Ion-Electron Recombination. In the basic flame the positive ion concentration reaches a maximum near the flame front and then decays with distance, correlating with a simultaneous increase in the concentration of neutral soot particles, and thus giving the impression that the ions are being replaced by neutral particles. This correlation is, of course, somewhat dependent on the sensitivity limit of the particle measurement technique. The decay of positive ions can be characterized by a bimolecular recombination rate coefficient,  $\alpha$ , (determined from the linear slope of a  $1/n_+$  vs. time plot) which decreases with increasing equivalence ratio up to the soot threshold, implying an increasing concentration of negative ions (since positive ion-negative ion recombination is much slower than ion- $e^-$  recombination). At the soot threshold,  $\alpha$  suddenly increases by more than an order of magnitude to a value consistent with the formation of larger ions. As the equivalence ratio is further increased beyond the threshold soot point to very sooty flames,  $\alpha$  continuously decreases by almost two orders of magnitude indicating the increasing importance of large negative ions in heavily sooting flames.

Quantitative data and analysis continue to support the chemi-ionization, ion-molecule reaction mechanism for soot nucleation.

#### Acknowledgment

The significant contributions of Drs. D.G. Keil and D.B. Olson are gratefully acknowledged.



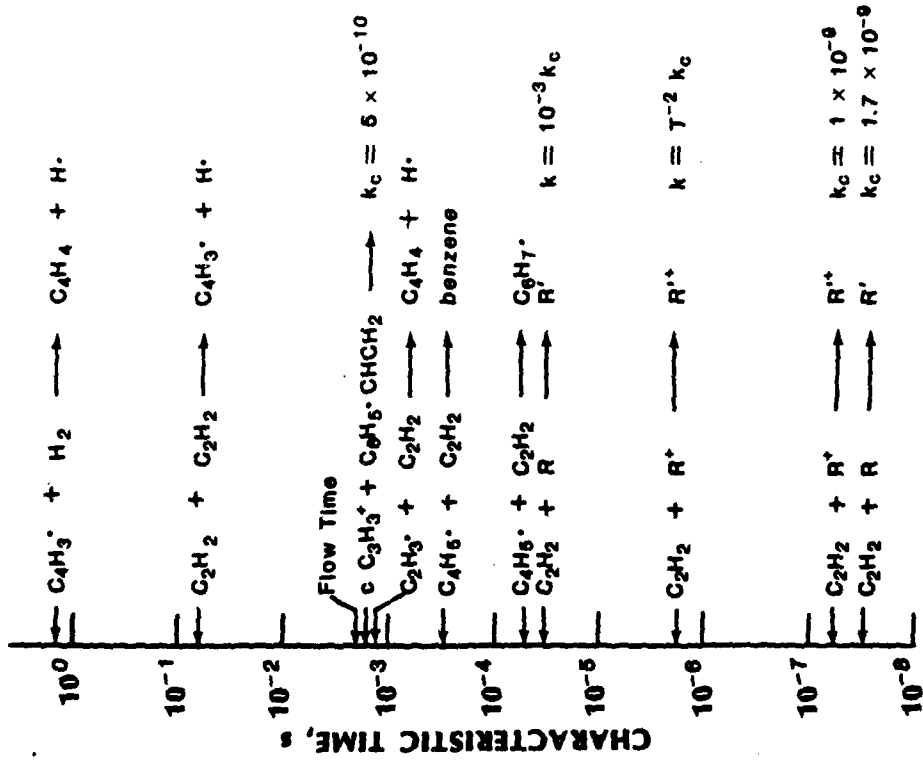


FIGURE 2 CHARACTERISTIC TIMES IN THE FLAME OF FIGURE 1 AT 1.5 CM ABOVE THE BURNER

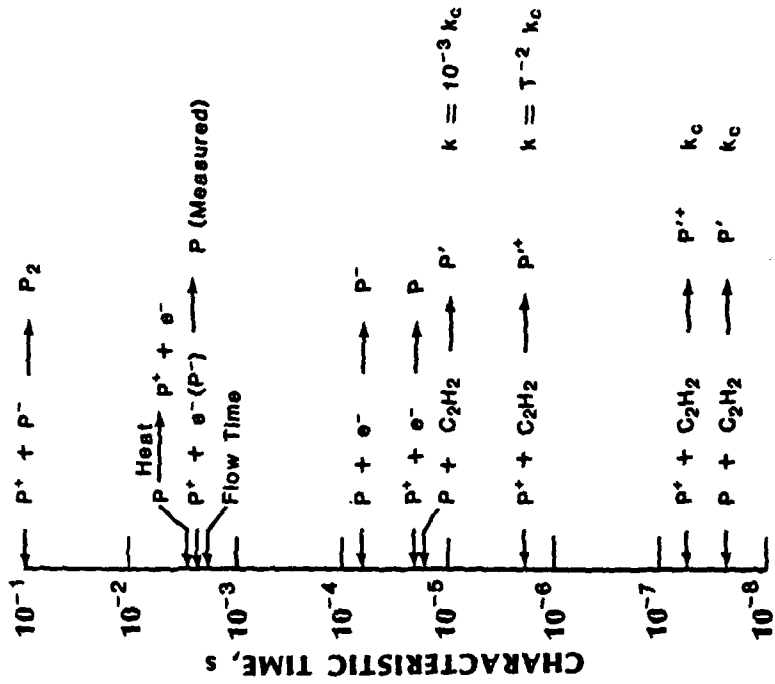


FIGURE 3 CHARACTERISTIC TIMES IN THE FLAME OF FIGURE 1 AT 2.5 CM ABOVE THE BURNER

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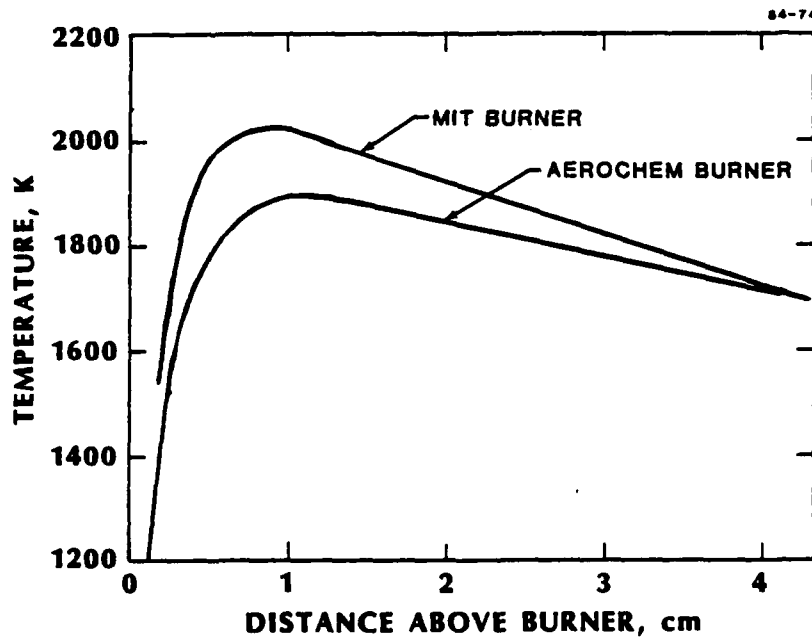


FIGURE 1 FLAME TEMPERATURES MEASURED BY FINE WIRE THERMOCOUPLES FOR A  $C_2H_2/O_2$  PREMIXED FLAME

$$P = 2.67 \text{ kPa}, \phi = 3.0, u = 50 \text{ cm s}^{-1}$$

# SOOT FORMATION PROCESSES AND OXIDATION OF AROMATIC HYDROCARBONS

Advanced Fuels Combustion Research

(AFOSR Contract No. F49620-82-K-0011)

Principal Investigators: Irvin Glassman, Frederick L. Dryer, Forman A. Williams

Department of Mechanical and Aerospace Engineering  
Princeton University  
Princeton, New Jersey 08544

## SUMMARY/OVERVIEW:

Little is known about the processes which control the formation of soot in combustion systems and the effect of fuel type, particularly aromatics. By use of pre-mixed and diffusion flame systems in which flame temperatures are controlled, it is possible to determine the relative effects of flame temperature, equivalence ratio, C/H ratio and fuel structure in a particular system. Corresponding studies of the high temperature oxidation and pyrolysis mechanisms of aromatic, naphthenic and paraffinic fuels using the Princeton turbulent flow reactor are not only providing important kinetic data but also the fundamental information necessary to understand the controlling processes in soot formation and the efficient combustion of heavy fuels. Thermochemical calculations demonstrate appreciable advantages associated with the addition of boron to fuels, particularly for airbreathing propulsion concepts. Droplet and slurry combustion studies have been initiated to develop fundamental understanding of the processes that could lead to boron becoming an effective fuel.

## TECHNICAL DISCUSSION:

During this period further measurements were made under pre-mixed flame conditions of the critical sooting equivalence ratio ( $\psi_c$ ) of pure fuels. To date practically all possible types of hydrocarbon fuel structures have been evaluated. More importantly it has been shown that when compared at the same temperature an excellent correlation could be obtained by plotting  $\psi_c$  (based on a stoichiometry to CO and H<sub>2</sub>O) as a function of the total number of carbon to carbon bonds. A simple model of the processes occurring in a pre-mixed flame predicts that the size of the fuel molecule and the C/H ratio are the fundamental parameters which govern the rate of soot formation. Recall it is the competitive reactions of fuel pyrolysis and hydroxyl attack on the precursors formed that govern soot formation under pre-mixed conditions (1). The size of the molecule determines the rate of pyrolysis of the fuel since size controls the radical pool. The C/H ratio essentially establishes the hydroxyl radical concentration. Since a double bond in the structure would be counted as two bonds and signifies less H, one can readily perceive why the parameter of number of C-C bond works so well. The model and all data have been reported in recent publications (2,3) and the data are shown in Figure 1. The importance of this correlation is that it implies that for pre-mixed conditions the original fuel structure plays no role in the soot formation process. To verify this implication mixtures of fuels were evaluated. Mixture A tested is 33% octene and 66% ethene, and has the same C/H ratio as butene and the same average number of C-C bonds. Mixture B tested is 66% octene and 33% ethene and has the same C/H ratio and average number of C-C bonds as hexene. One will notice in Figure 1 that the results with these mixtures fall exactly on the correlating curve.

Much new data have been obtained as well on sooting tendencies of fuel under diffusion flame conditions. All these data are shown in Figure 2 in which the log of one over

the mass flow rate of the fuel (FFM) is plotted as a function of  $(1/T)$ . The fact that straight line correlations were obtained for all fuels indicates that fuel pyrolysis is a controlling step on soot formation under diffusion flame conditions and fuel structure is important. In order to show the fuels trends without confusion all the data points have been omitted from Figure 2. The significance of these data is that if a fuel pyrolysis mechanism is known, its relative tendency to soot can be predicted. For example it is known that cyclopropane immediately pyrolyzes to propene; thus it is not surprising that the Princeton smoke height test results show that cyclopropane and propene have the same tendency to soot. All the data and their analysis from our study of pyrolysis kinetics have been reported in other recent publication (4,5). Perhaps more importantly, Frenklach and co-workers (6,7) by shock tube measurements have found the same order of sooting tendencies for acetylene, butene, butadiene, allene and the aromatics. This agreement is most significant in that it gives further validation to the well controlled, simple Princeton smoke height experiment. Application of all our soot results to power plants is discussed in a recent AFOSR Report (8).

With regard to that phase of our program directed at studies of hydrocarbon oxidation processes, our previous flow reactor research on toluene (9) and ethyl benzene (10) produced a basis for the oxidation of the n-alkylated aromatics. Assuming the high selectivity for benzylic hydrogen abstraction, the n-alkylated aromatics should yield styrene as the major stable product for fuel consumption, as the alkanes yield an olefin. This hypothesis was tested in experimentation with the oxidation of n-propylbenzene and the results (see Figure 3) confirmed that styrene was a major stable intermediate product. There is evidence however that abstraction from the terminal carbon atom may also play a role, consequently a study of isopropylbenzene has begun. The intermediate product distribution from this compound will more readily indicate the relative abstraction rates from the benzylic and terminal carbon atoms.

Previously (10,11) it was suggested that the subsequent reaction of styrene was by the hydrogen atom displacement of the vinyl group to form benzene and a vinyl radical. However further experimentation and analysis suggest that oxidative attack on the vinyl side chain might also be important. Observations of significant amounts of toluene in the products led to this conclusion. Due to the presence of other routes to toluene in the ethylbenzene system studied earlier, it was difficult to distinguish between the displacement and oxidative attack reactions on the styrene intermediate. Consequently experiments with styrene oxidation were performed and show significant amounts of toluene and benzene early in the reaction zone (Figure 4). These results indicate that oxidative attack is a significant route for styrene consumption and further extend our knowledge of the oxidation of the alkylated aromatics.

Our work on boron and slurry combustion has progressed in both theory and experiment. The principal findings of our theoretical studies on the mechanisms of ignition and combustion of boron particles, such as the importance of migration of boron through the oxide, have been summarized in earlier abstracts. A paper on the subject will be presented at the 20th International Combustion Symposium (12); this research has served to assess our current knowledge in the subject and to identify unknown aspects in need of further study. In addition, theoretical and experimental work on the combustion of slurry droplets has been completed.

In our theoretical studies of the burning of boron slurry droplets, transient processes that occur during the vaporization and combustion of the liquid component were analyzed. The model adopted for detailed investigation was designed to apply best for situations in which the solid particle fraction is large. The liquid was assumed to evaporate from the regressing surface of an inner slurry sphere concentric with an outer porous shell of solid particles, of fixed radius. A singular perturbation technique was used to obtain approximate solutions for the transient temperature profiles of the inner sphere and for the regression velocity of the interface. The parameter

of the expansion is the ratio of the sensible enthalpy increase caused by droplet heating to the enthalpy of vaporization. From the analysis it is found that the cube of the diameter of the inner sphere decreases linearly with time, while the burning time nevertheless is proportional to the square of the initial diameter of the slurry droplet and to the volume fraction of liquid in the droplet. Additional predictions are constancy of the flame radius during burning and internal temperature profiles, needed for addressing possibilities of disruption. Experiments currently are being performed to test the latter predictions.

Construction of the experimental apparatus for investigation the combustion of free slurry droplets has been completed, and the apparatus has been tested with slurry loadings up to five percent. Additional tests including work with slurries at higher loadings are in progress. The droplet generation device basically consists of a tube through which liquid flows, with its exit positioned along the axis of a high-velocity gas jet. A stream of droplets is produced by inducing detachment of droplets formed at the end of the inner tube. Varying the liquid and gas flow rates results in controllable droplet diameters between 200  $\mu$  and 500  $\mu$ , with spacings of 100 to 700 diameters and initial velocities of 2 to 3 m/s. Experiments are now beginning with this apparatus for studying the combustion of slurry droplets.

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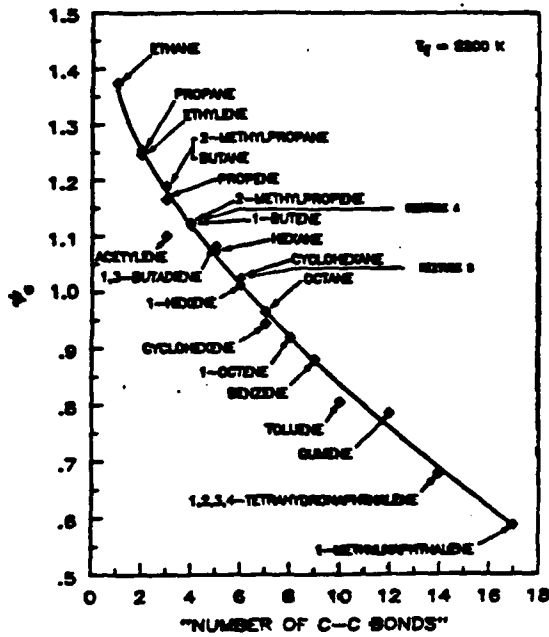


FIGURE 1 The pre-mixed flame correlation between the effective equivalence ratio to soot ( $\psi_c$ ) at 2200 K and the number of C-C bonds in various fuels and fuel mixtures.

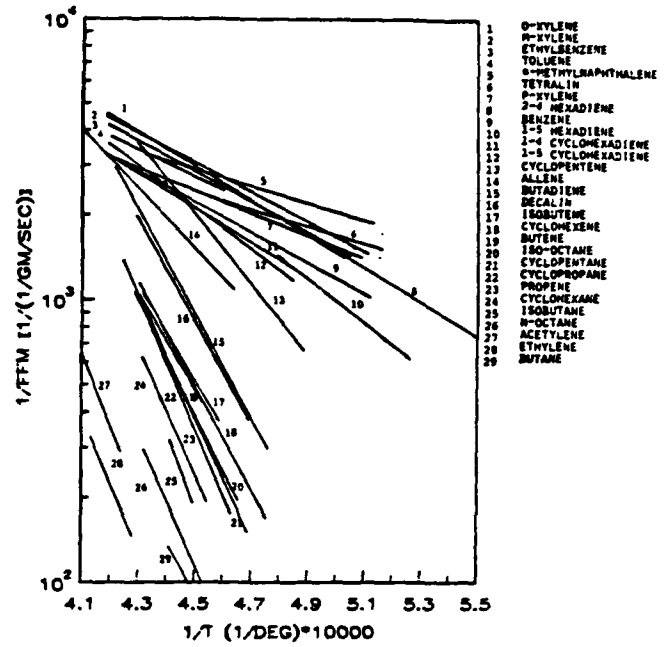


FIGURE 2 Fuel sooting tendencies under diffusion flame conditions. The log of the inverse of the fuel mass flow rate at the sooting height is plotted as a function of the inverse calculated stoichiometric flame temperature. The temperature variation is by nitrogen dilution.

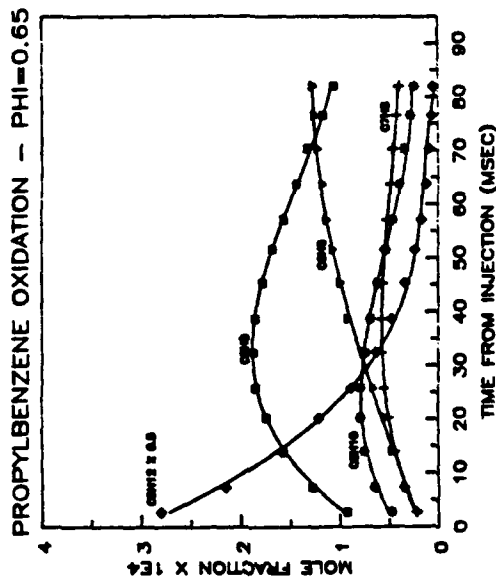


FIGURE 3 The intermediate oxidation products of propylbenzene oxidation at  $\phi = 0.65$  showing styrene ( $C_6H_8$ ) as the primary initial constituent.

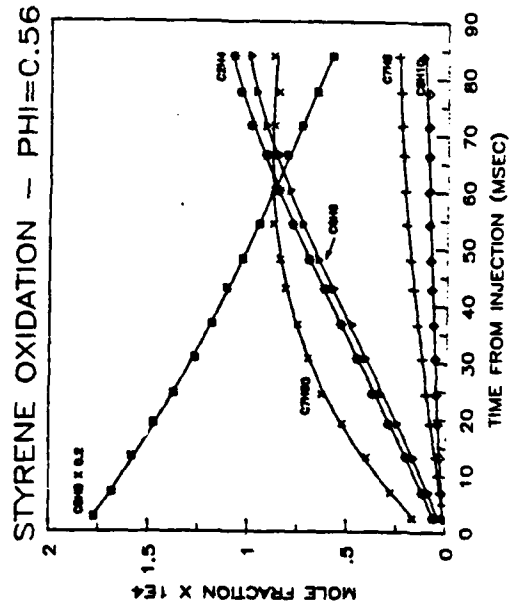


FIGURE 4 The intermediate oxidation products of styrene at  $\phi = 0.56$  showing toluene as an initial intermediate as well as benzene.

# FUEL ADDITIVE EFFECTS IN SOOTING FLAMES

(AFOSR Contract No. F49620-83-C-0113)\*

Principal Investigator: P. A. Bonczyk

United Technologies Research Center  
East Hartford, Conn. 06108

## SUMMARY/OVERVIEW

Soot is a combustion product which increases plume visibility and, hence, aircraft vulnerability, and may cause reduced engine durability. In the past, fuel additive use has been shown, qualitatively, to be effective in reducing soot. This approach is simple to execute and is a practical alternative to radical engine redesign. The present difficulty with additives is that the mechanisms responsible for their soot abating action are poorly understood, which hampers more effective additive selection and evaluation. The objective of this research is to initiate a comprehension of the latter mechanisms and, thereby, develop specific analytical criteria for future additive selection. To achieve this objective, an approach has been adopted which is a significant departure from that of earlier more qualitative and restrictive experiments, and offers more hope of clarifying the chemistry of additive soot suppression.

## TECHNICAL DISCUSSION

### Background/Approach

In large part, past additive experiments have been intrusive in nature and/or restricted to postflame soot analysis. Although useful for comparing and cataloguing the effectiveness of various additives, such experiments offer little hope of clarifying soot suppressing mechanisms. To this end, it is necessary, as a very minimum, to measure the concentrations of soot, additive and additive derived species throughout the flame zone with spatial precision. In addition to concentration measurement, it is essential to assess the potential importance of flame temperature and parameters such as fuel type and fuel/air ratio. In this program, techniques for concentration and temperature measurement either presently in use or projected for use in the near term are in-situ and spatially precise. Specifically, the techniques include Mie scattering, laser-induced fluorescence, and laser-excited coherent anti-Stokes Raman scattering. These are appropriate, in the preceding order given, to measure soot particulate size and concen-

\*Co-funded by AFOSR and AF Engineering and Services Center,  
Tyndall AFB, Fla.

Page 3

tration, additive and unseeded flame species concentrations, and temperature. It is anticipated that measurements of this type, coupled with a systematic variation of fuel/air parameters, will aid significantly in seeking to clarify additive mechanisms. Emphasis is being given to K, Ba, Mn, Fe and Ce additives since the latter metals are known, qualitatively, to be effective soot suppressants. Measurements are being carried out for gaseous and liquid fuels to which are added, respectively, inorganic and organic compounds of the above referenced metals.

#### Current Status

Gaseous Fuels: Scattering of visible laser radiation by soot particulates has been used to measure their size, concentration and volume fraction in a laboratory-scale laminar ethylene/air diffusion flame with and without additives present. The soot parameters have been determined throughout the flame zone for various salts of the previously referenced metals. Light scattering has been supplemented by optical/spectroscopic emission measurements to identify the chemical states of additive derived flame species. Preliminary results have demonstrated that dissimilar metals behave differently as soot suppressants; consequently, their discussion below is segregated.

In Figs. 1 and 2, results are given for soot size and volume fraction, at one position in the flame, for two different Ba compounds in varying concentration. The additive is introduced into the oxidant stream of the flame via an atomized spray of water containing the salt at the molar concentrations given. The soot diameter, which has a weak dependence on concentration, is determined from the angular dissymmetry of laser light scattered at  $20/160^\circ$  (Ref. 1). Knowing the diameter,  $D$ , the concentration,  $N$ , is evaluated from the absolute scattered intensity at either  $20$  or  $160^\circ$ . The volume fraction,  $f_v$ , in Fig. 2 is calculated from,  $f_v = (\pi D^3/6)N$ , and is normalized with respect to its value with water alone present,  $f_v^0$ . The sharp reduction in  $(f_v/f_v^0)$  at higher molarities results principally from a decrease in  $N$  since  $D$  remains relatively constant. As is evident in Figs. 1 and 2, the acetate and nitrite of Ba are equally effective as additives thereby establishing the metal atom as the critical species. In fact, a number of other Ba salts were evaluated with identical conclusions. In addition to particulate characterization at the measurement point appropriate to Figs. 1 and 2, the additive species Ba, BaO and BaOH have been identified as present there as well from their optical emission spectra. Such identifications are essential to isolating the one or more additive related species responsible for soot suppression. It is equally important to determine the effectiveness of an additive at various points in the flame. Figure 3 gives data which demonstrate unequivocally that Ba is most effective as a soot suppressant at points corresponding to relatively long residence times. Additional spatial data which have been obtained also indicate that at a median height in the flame maximum effectiveness occurs at or near the main reaction zone.



Measurements were made for K compounds as additives as well, where the approach and specific measurements were very similar to those for Ba above. Results for  $\text{KNO}_3$  are given in Figs. 4 and 5, and two aspects of the data are worthy of particular attention. First, K has a much more pronounced effect on size than does Ba. Second, at a measurement height of 18 mm, K is a strong soot suppressant whereas the Ba efficiency in Fig. 3 is clearly diminished from its peak value. Based on Figs. 4 and 5 and accumulated spatial data, the K mechanism of soot suppression appears to differ from that for Ba.

As mentioned, dissimilar metals may behave very differently as regards soot suppression. This is evident in Fig. 6 below where Fe is seen to be unlike both Ba and K as a fuel additive. Here, as was the case for Ba,  $D/D^0$  is nearly unity; but unlike Ba and K, Fe is seen to enhance soot concentration and volume fraction. The precision of the data at 13 mm in Fig. 6 is, for the present, relatively poor and, hence, inferences regarding soot suppression at 13 mm or lower are not possible. Data with consequences similar to those in Fig. 6 for  $\text{Fe}(\text{NO}_3)_3$  have been obtained for  $\text{FeSO}_4$ ,  $\text{Mn}(\text{NO}_3)_2$  and for 1,1'-ferrocene dicarboxylic acid in 14%  $\text{NH}_4\text{OH}$  (ferrocene = dicyclopentadienyl iron).

Liquid Fuels: Ferrocene has been tested as a fuel additive in both liquid fuel wick and counterflow diffusion flames. For the wick flame, 0.25% ferrocene by weight added to a 5/1 iso-octane/toluene fuel mixture resulted in the complete suppression of a heavy soot plume, as determined both visually and by laser/optical extinction measurement. Several compounds closely related to ferrocene, like hydroxymethyl ferrocene, for example, were decidedly less effective than ferrocene itself. In addition to ferrocene, methylcyclopentadienyl manganese tricarbonyl was found to be an effective soot suppressant for the wick flame. For the liquid counterflow flame, optical measurements were limited to the vicinity of the laminar forward stagnation zone where for the same fuel mixture as above ferrocene was ineffective as a soot suppressant.

#### Near Future Work

For gaseous fuels, the concentrations of additive derived species in the flame will be measured via laser-induced fluorescence. In addition, the importance of fuel type and flame temperature on additive effectiveness will be determined. In the liquid fuels area, spatial mapping of ferrocene effectiveness for the wick flame will be carried out, and Ce will be evaluated similarly in view of its recently demonstrated effectiveness in practical combustors.

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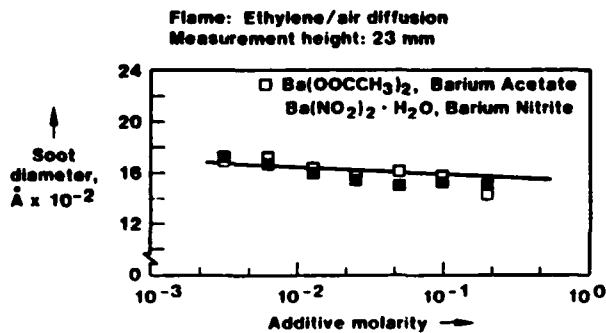


Fig. 1. Soot Size Dependence on Additive Concentration

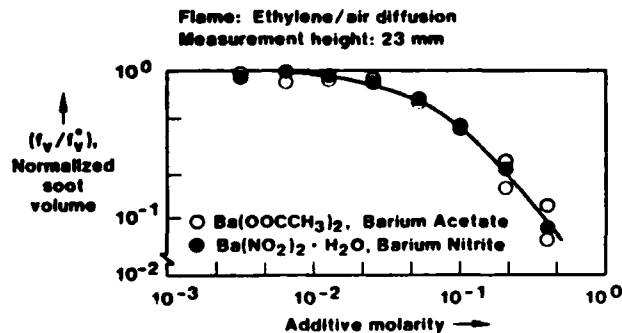


Fig. 2. Soot Volume Dependence on Additive Concentration

Flame: Ethylene/air diffusion  
Measurement direction: Vertical flame axis  
Additive: 0.2 M  $\text{BaCl}_2 \cdot 2\text{H}_2\text{O}$

z →	Measurement height, mm				
	13	18	23	28	38
$D, \text{Å}$	1321	1471	1428	1457	1536
$D/D^*$	0.96	0.98	0.96	0.92	0.94
$N/N^*$	1.01	0.88	0.69	0.34	0.29
$t_v/t_v^*$	0.90	0.82	0.61	0.26	0.23

Fig. 3. Spatial Dependence of Additive Effectiveness

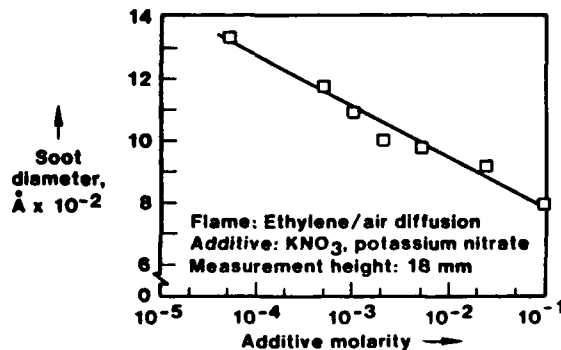


Fig. 4. Soot Size Dependence on Additive Concentration

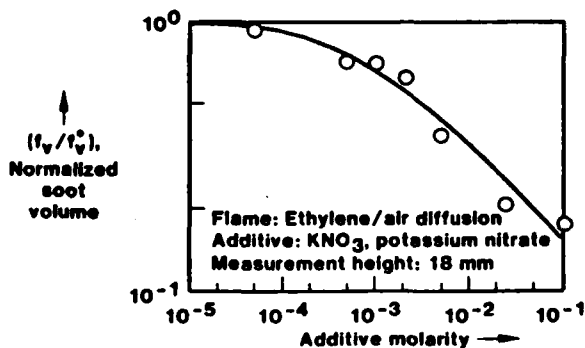


Fig. 5. Soot Volume Dependence on Additive Concentration

Flame: Ethylene/air diffusion  
Measurement direction: Vertical flame axis  
Additive: 0.2 M  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$

z →	Measurement height, mm				
	13	18	23	28	38
$D, \text{Å}$	1136	1141	1538	1655	1579
$D/D^*$	1.07	1.02	1.01	1.02	1.03
$N/N^*$	0.78	0.98	1.07	1.17	1.61
$t_v/t_v^*$	0.97	1.05	1.10	1.23	1.76

Fig. 6. Spatial Dependence of Additive Effectiveness

## FLAME RADIATION IN GAS TURBINE COMBUSTORS

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### SUMMARY

A major obstacle to the successful design of gas turbine combustors is that no reliable experimental data have yet been obtained on flame radiation and flame emissivity for these systems. This is due largely to the wide variations in temperature, fuel/air ratio, chemical composition and spray characteristics that exist throughout the combustion zone. The objective of this research program is to acquire experimental data on flame radiation and soot concentration obtained under sensibly uniform and controlled conditions of pressure, inlet air temperature, fuel composition and fuel mean drop size. These data will then be used to derive basic relationships between flame emissivity, flame temperature, soot concentration, optical soot properties, and fuel chemistry.

### TECHNICAL DISCUSSION

The working section of the proposed test rig, shown schematically in Fig. 1, comprises a tubular liner containing an array of narrow ( $\dagger$  3mm) annular vee-gutters, fitted with radial interconnectors to facilitate passage of flame from the centrally-located spark ignition source.

A primary advantage of the proposed fuel injection system is that it allows the mean drop size of the fuel spray to be varied in a controlled manner, while maintaining all other flow conditions constant. Thus the influence of fuel drop size on soot formation, soot physical properties, and flame radiation may be readily determined. Furthermore, when carrying out tests on the effects of fuel composition on flame radiation and soot formation, it is possible to adjust the atomizing air flow rate so as to achieve a constant drop size for all fuels. Alternatively, based on a knowledge of the density, viscosity, surface tension, and evaporation constant for each fuel, it is possible to select for each fuel a mean drop size that will ensure a constant rate of evaporation for all fuels. This means that all observed differences in flame radiation, soot properties and soot concentration can be attributed directly to variations in chemical properties, such as aromatics content or hydrogen content.

Pending the completion of the high pressure test rig some preliminary measurements have been conducted at normal atmospheric pressure. First, the integrated spectral intensity was measured with a broadband pyrometer. Second, the black body flame temperature was measured using a monochromatic optical thermometer.

The broadband pyrometer consists of a bank of copper tubes oriented parallel to the test section. A constant flow rate of water was maintained through the tubes. The integrated spectral intensity was determined by measuring the water

temperature at the pyrometer inlet and outlet. The temperature difference, coupled with the known flow rate of water, allowed calculation of the total power absorbed by the pyrometer. The integrated spectral intensity was determined from the measurement of total power.

The monochromatic optical thermometer is a commercially available unit manufactured by Leeds and Northrup (M/N 8632-F). This instrument determines flame temperature by comparing the flame emission intensity at a single wavelength (653 nm) to that of a standard lamp. A wavelength of 653 nm was chosen to be in a region of the spectrum where the molecular band structure contribution to the integrated spectral intensity is negligible. Thus, the flame is assumed to radiate as a black body at 653 nm.

The results of investigations of integrated spectral intensity versus equivalence ratio are presented in Fig. 2. It is evident that the integrated spectral intensity increases with equivalence ratio at constant Sauter mean diameter (SMD). This is to be expected as, in general, any decrease in fuel flow rate automatically lowers the fuel concentration in the reaction zone. The lowered fuel concentration reduces the soot formation, and hence the flame emissivity. This is illustrated by the results of soot probe measurements presented in Fig. 3. In addition, decreasing the fuel flow rate causes a simultaneous drop in flame temperature, as shown in Fig. 4. The combined effects of decreasing soot concentration and decreasing flame temperature are to decrease integrated spectral intensity with equivalence ratio.

The observed decreases in soot concentration, flame temperature and integrated spectral intensity with increased SMD are believed to be due to a change in the mechanism of flame propagation that occurs with variation in mean drop size for the range of drop sizes used in this study, namely from 10 to 30  $\mu\text{m}$ . A previous study by Burgoyne and Cohen [1] revealed that increases in mean drop size above 30  $\mu\text{m}$  always reduced flame speed, whereas increases in mean drop size in the range from 10 to 30  $\mu\text{m}$  gave the opposite result, namely an increase in flame speed. These investigators explained this phenomenon in terms of a change in the mechanism of flame propagation. In the case of fine atomization, flame was thought to exist in the interdroplet space, whereas for larger drops flame was relayed from one droplet encased in a diffusion flame envelope to the next, with little or no combustion occurring in the interdroplet region.

Thus the observed effects arising from variations in SMD may be due in large measure to the effects of changes in the basic mechanisms of combustion and flame propagation that accompany a change in SMD. Clearly more results are needed at higher levels of inlet air pressure and temperature, and over much wider ranges of mean drop size. Work is now in progress to obtain more data at pressures up to 1.5 MPa (15 atm.) and inlet air temperatures up to 800K.

#### REFERENCES

1. Burgoyne, J. H., and Cohen, L., "The Effect of Drop Size on Flame Propagation in Liquid Aerosols," Proc. Roy. Soc. London A. 225, p. 375, 1954.

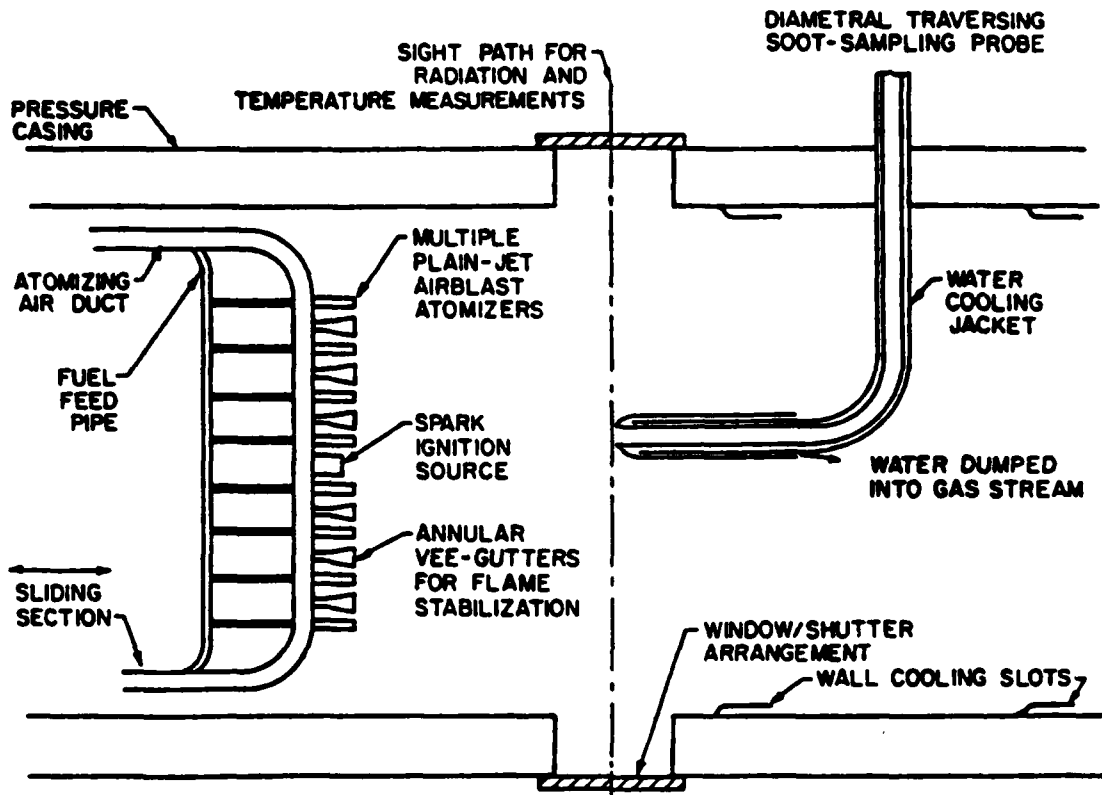


Fig. 1. Schematic diagram of test rig

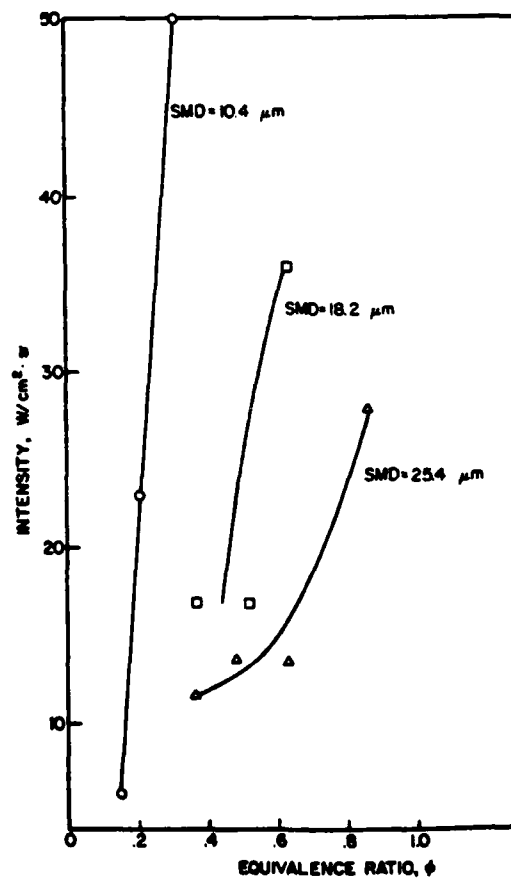


Fig. 2. Integrated spectral intensity versus equivalence ratio

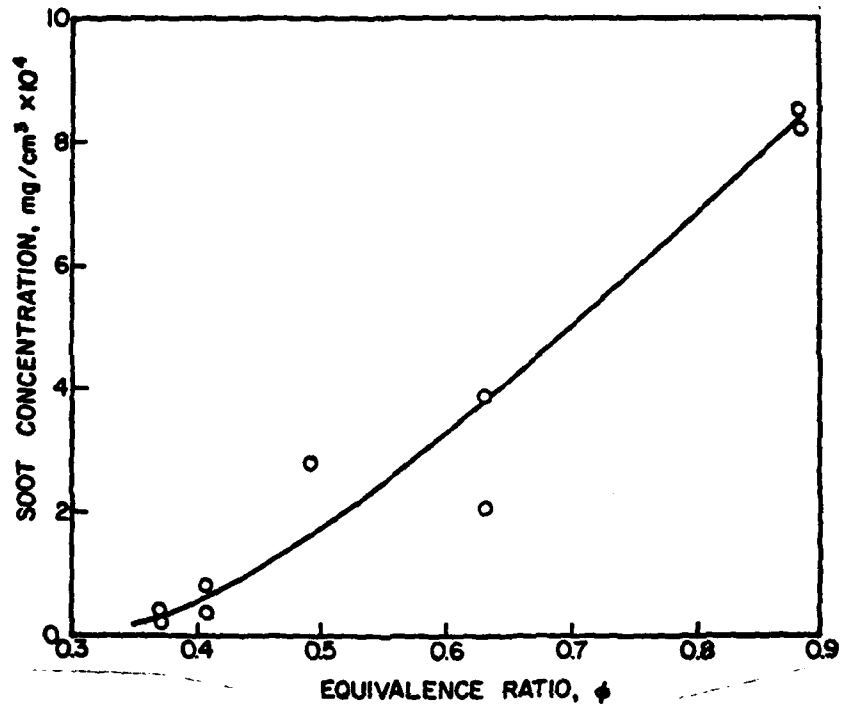


Fig. 3. Influence of equivalence ratio on soot concentration

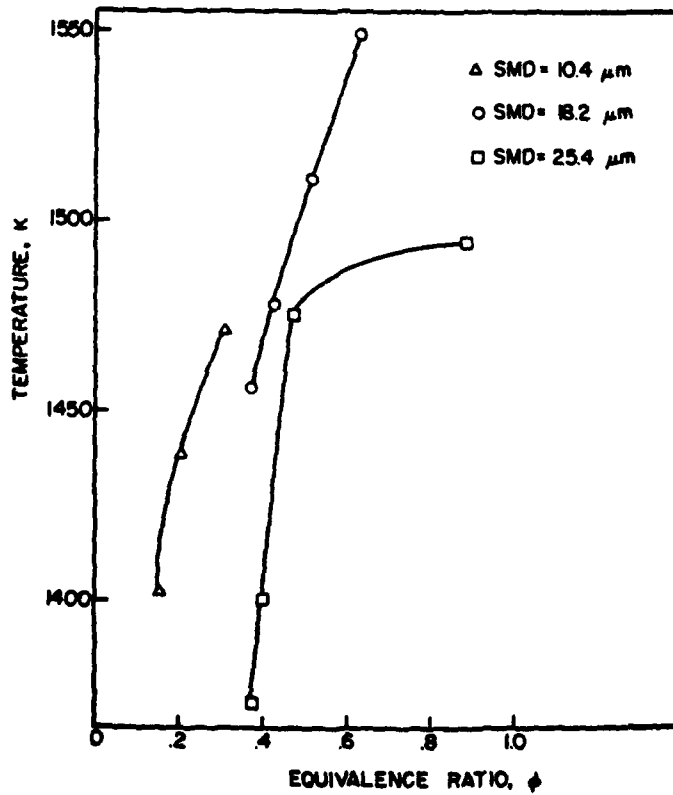


Fig. 4. Influence of equivalence ratio and mean drop size on flame temperature.

## EVAPORATION CHARACTERISTICS OF EMULSIFIED FUELS

ONR Contract No. N00014-80-K-0460

Principal Investigator: C.A. Moses

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### SUMMARY/OVERVIEW:

The spray formation and evaporation characteristics of emulsified and neat multi-component and single-component fuels in high-pressure, high-temperature turbulent air have been examined. Drop-size distributions have been determined with a laser-diffraction technique, and vaporized fuel concentration with a phase-discriminating probe. In order to help interpret these results, a spray model has been developed which predicts drop trajectories, heat-up rates, steady-state "wet-bulb" temperature, and evaporation rates. Several conclusions have been drawn from these experiments. First, even in sprays from real nozzles at high Reynolds numbers (which enhance internal drop circulation), microexplosions appear to occur for hexadecane/water emulsions at some air conditions. This conclusion was inferred from the smaller average drop sizes of the emulsified fuel, and its higher vaporization rate. Second, initial atomization depends on air conditions, with higher densities producing better atomization. Third, changes in drop-size distribution have been predicted fairly well by a computer model which includes detailed computations of heat and mass transfer rates.

### TECHNICAL DISCUSSION:

It has been shown by Moses<sup>(1)</sup>, Klarman et al.<sup>(2)</sup>, Spadaccini and Pelmas<sup>(3)</sup>, Kinney and Lombard<sup>(4)</sup>, and others that adding water to fuel in the form of emulsions can reduce soot in gas-turbine combustors. Several reasons have been suggested for the soot reduction including: (a) a reduction in gas-phase pyrolysis reactions due to the lowered combustion temperature resulting from the increased heat used to vaporize water or an increase in endothermic reactions, (b) a reduction in liquid-phase pyrolysis due to lowered drop temperatures, (c) an increase in soot precursor oxidation due to an increased OH concentration, or (d) an improvement in fuel/air mixing resulting from "microexplosions" caused by superheating of the water dispersed within the fuel drop.

Microexplosions can occur when water is contained in a fuel drop which has a higher boiling point than water. During the heatup of such a drop, the water may either be brought to the surface to evaporate, or, if that transport process is too slow and the drop exceeds the boiling point of water, the superheated water may violently boil and shatter the drop into many smaller drops. These smaller drops enhance mixing and reduce the probability of soot formation. Although soot reductions for emulsions observed in full-scale tests have often been attributed to microexplosions, it has never been possible to confirm them in these tests. Disruptive burning has been observed in single-drop laboratory experiments<sup>(5,6,7)</sup>, but the fuels and/or air conditions have been chosen to maximize the probability of microexplosions and are not representative of the environment in a gas-turbine combustor.

Comparative drop-size measurements in sprays of emulsions of 20-percent water, 2-percent surfactant, and 78-percent jet-A and non-emulsified (neat) jet-A were performed in a noncombustion turbulent coaxial (to the spray) airflow. A simplex pressure atomizer with a capacity of 3.8 liters/hour (at 862 kPa) and 45° spray cone was used. The initial atomization of the emulsified and neat jet-A was similar, and at lower temperatures and pressures, the drop-size distributions followed similar trends further downstream from the nozzle. However, at temperatures of about 600 K and higher, and pressures of 450 kPa (4.5 atm) and higher, the drop-size distributions diverged with the emulsified fuels producing smaller drops.

An emulsion with the same water and surfactant contents was prepared using hexadecane. Again, drop-size measurements were performed along the nozzle axis for a variety of air temperatures and pressures. Figure 1 presents typical distribution histories; note that SMD normally increases downstream because smaller drops are evaporating and disappearing. The size distributions diverged at higher temperatures ( $> 600$  K), with the emulsified fuels showing smaller drop sizes. At constant air temperature, but varying air pressure, a similar divergence was observed at elevated pressures, as shown in Figure 2. Raising air temperature or air pressure can result in a higher drop temperature. The size distributions diverge at a predicted drop temperature of about 515 K. This is reasonably close to the upper limit for the spontaneous nucleation temperature of water/hexadecane mixtures of 539 K<sup>0</sup>, which represents the maximum drop temperature before microexplosions would have to occur if water were still present in the drop. These trends suggest that microexplosions were reducing the average drop size of the emulsions relative to the neat fuel. However, it is conceivable that the high heat of vaporization of water could retard the evaporation of the emulsions so that smaller drops have longer lifetimes, thus resulting in smaller SMD's relative to the neat fuel.

Measurements with a phase-discriminating probe, shown in Figure 3, were used to resolve this question. Microexplosions should enhance the overall vaporization rate, while the heat-sink effect of water should retard it. The results shown in Figure 4 indicate a higher vaporization rate for the emulsions, indicating that the microexplosions dominate over any heat-sink effect.

#### REFERENCES

1. Moses, C.A., Presented at the Western States Section of the Combustion Institute, University of California, La Jolla, California (1976).
2. Klarman, A.F., Rollo, A.J., and Scott, H.C., Naval Air Propulsion Center, Trenton, New Jersey, Report No. NAPC-PE-7 (1978).
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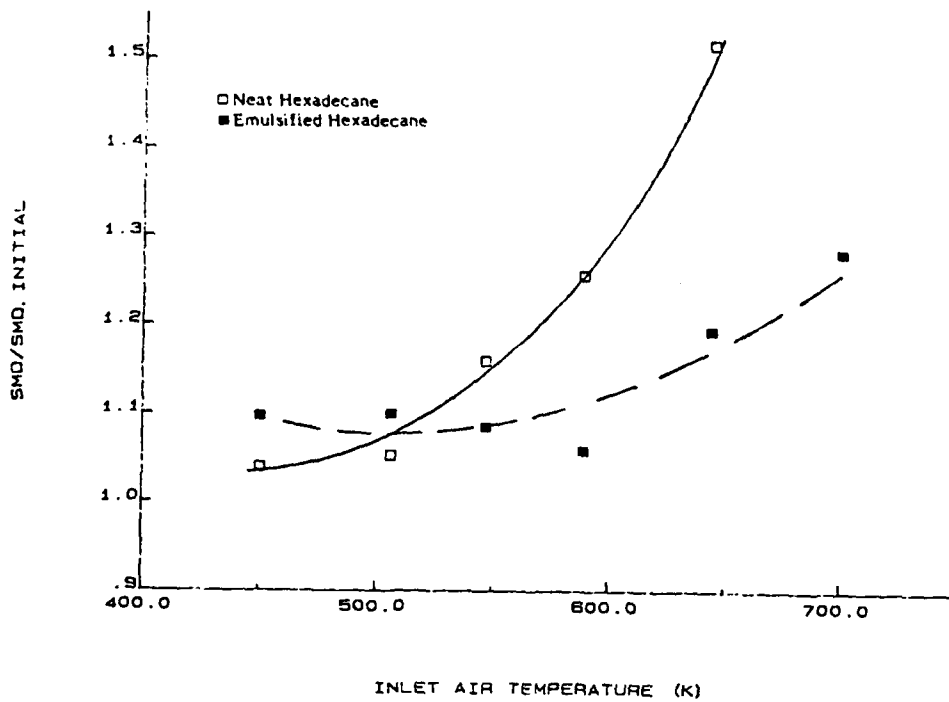


FIGURE 1. EFFECT OF AIR TEMPERATURE ON SMD OF EMULSIFIED AND NEAT HEXADECANE AT 26 mm FROM NOZZLE, AIR PRESSURE OF 448 kPa (6.42 ATM)

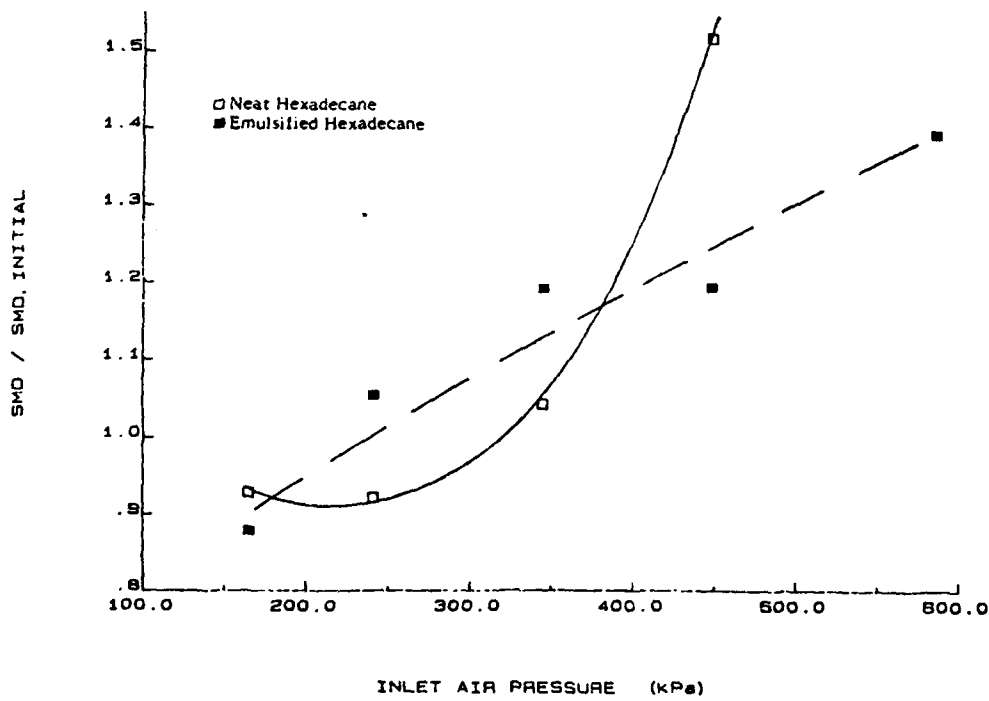


FIGURE 2. EFFECT OF AIR PRESSURE ON SMD OF EMULSIFIED AND NEAT HEXADECANE AT 26 mm FROM NOZZLE, AIR TEMPERATURE OF 644 K

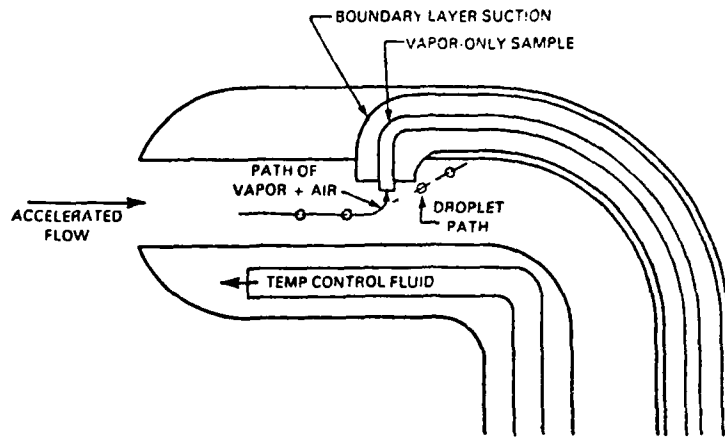


FIGURE 3. TEMPERATURE-CONTROLLED TWO-PHASE PROBE

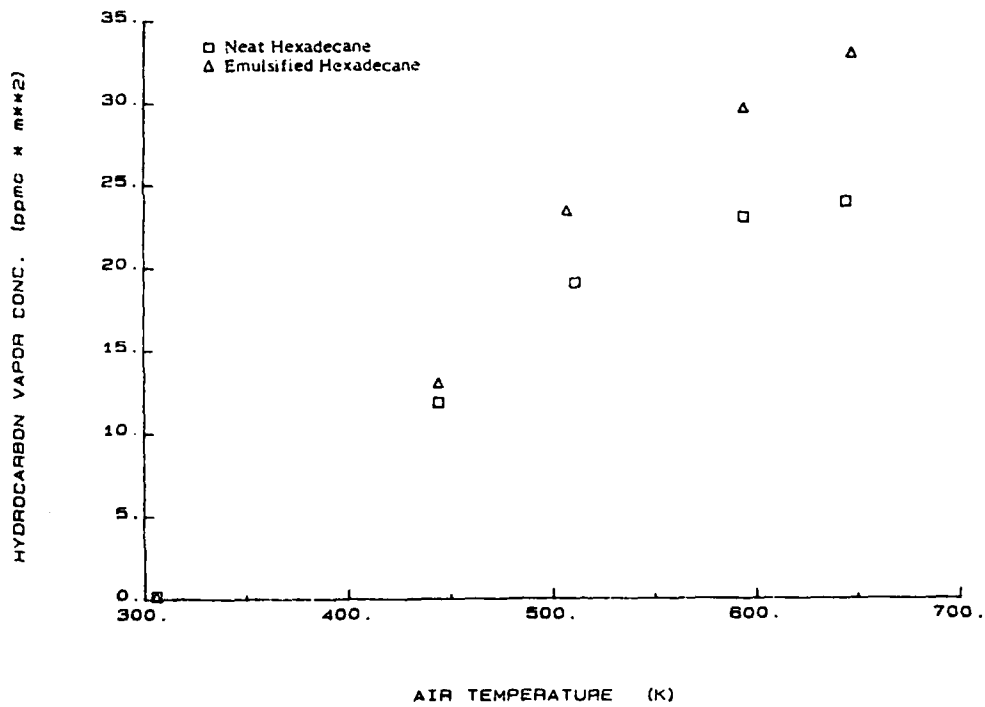


FIGURE 4. COMPARISON OF HYDROCARBON VAPOR CONCENTRATION FOR EMULSIFIED AND NEAT HEXADECANE AT 57 mm

## AFOSR SPONSORED RESEARCH IN AIRBREATHING COMBUSTION

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**SUMMARY/OVERVIEW:** The Air Force Office of Scientific Research (AFOSR) program in airbreathing combustion is currently focused on seven areas of study: turbulent mixing, turbulent combustion, soot, sprays and slurries, combustion instability, combustion enhancement and supersonic combustion. An assessment of major research needs in each of these areas and new interests in combustion chemistry, is presented.

### TECHNICAL DISCUSSION

AFOSR is the single manager for Air Force fundamental research, including programs based on unsolicited proposals and in-house work at Air Force Laboratories. Airbreathing combustion is assigned to the AFOSR Directorate of Aerospace Sciences along with programs in rocket propulsion, diagnostics in reacting flow, fluid and solid mechanics, and civil engineering.

Current interests of the AFOSR airbreathing combustion program are given in the SUMMARY section above. Many achievements can be cited for these interests, yet imposing fundamental research challenges remain. The objective of the program is publications in the refereed scientific literature describing significant new understanding of multiphase turbulent reacting flow. Incremental improvements to existing scientific approaches, hardware development and computer codes are not considered to be valid research goals.

Decisions on support for research proposals are based on scientific opportunities and technology needs. Current AFOSR perceptions of scientific opportunities appear in Figure 1. Highlights include model-free theoretical simulations of turbulent reacting multiphase flows as a full partner to experiments using advanced diagnostics; near-injector dense sprays; and turbulence interactions relevant to soot formation, interphase transport, chemical reactions and radiation. The addition of combustion chemistry to the seven current subject areas anticipates novel experimental and theoretical approaches for analyzing the chemistry of combustion. Since the relationship between the AFOSR Program Manager and the researcher should be an ongoing dialogue, the perceptions of Fig 1 are subject to continuous modification.

Technology needs include improvements to current propulsion systems and development of scientific understanding necessary to achieve new performance capability. Soot represents a scientific challenge underlying limitations of current propulsion systems. Excessive heat transfer from luminous soot particles to gas turbine hot section components as well as detectable exhaust signature motivate continued research in this area. Significant gains in propulsion capabilities could be realized through supersonic combustion and metallized propellants. Neither of these areas has been addressed by significant segments of the research community.

# Air Force Basic Research Aerospace Sciences

## Research Trends

Science Area	Trend	Decrease	Increase
● Turbulent Mixing	↗	Uniform Density	Simulations, Variable Density
● Turbulent Combustion	↗	Time-Averaged Models, Stable Flames	Simulations, Flame Limits, Ignition
● Soot	↗	Global Behavior, Laboratory Flames	Fluid Transport Effects, Turbulent Flames, Radiation, Pressure
● Sprays and Slurries	↗	Dilute Sprays, Time-Averaged Models	Dense Sprays, Drop Interactions, Simulations, Atomization
● Combustion Instability	↗	Combustor Experiments and Models	Flame/Flow Interactions, Active Control
● Combustion Enhancement	↗	Catalytic Combustion	UV and IR Techniques, Pulsed Combustion
● Supersonic Combustion	↗	Combustor Development	Flame Holding, Flame Structure
● Combustion Chemistry	↗		Sensitivity Theory, Metal Combustion

Figure 1

# Air Force Basic Research

## Aerospace Sciences

### Gas Turbine Hot Section FY 85 Initiative

<u>Current Investment</u>	<u>FY 85 Enhancement</u>
Turbulent Combustion	\$1.8 M
Soot and Sprays	\$1.3 M
Aerothermodynamics	\$0.6 M
Metals and Coatings	\$0.9 M
Ceramics	\$1.0 M
Carbon-Carbon	0
Other Areas	\$1.9 M
<b>Total</b>	<b>\$7.5 M</b>
	<b>\$2.8 M</b>

Figure 2

## ARO COMBUSTION SCIENCES PROGRAM

Dr. David M. Mann

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### SUMMARY/OVERVIEW:

The Army combustion dynamics research program is broadly scoped, covering the fundamentals of combustion in engine, rocket, and gun systems. The program is conducted as a partnership between the Army Research Office (ARO) and the Army Laboratories. The Army Laboratories are primarily concerned with in-house research and development while ARO contracts with universities, corporations and, occasionally, national laboratories to obtain needed research. This presentation will focus on details and plans for the ARO extramural Combustion Sciences program.

### TECHNICAL DISCUSSION

The Combustion Sciences program can be divided into three subsections:

a. Engines and Fuels. Apart from increasing fuel efficiency, the Army's primary interest in this field lies in the design of new combustion engines with increased multi-fuel capabilities. For both of these goals, the potential gains of novel combustor hardware design, as well as different fuel treatments, are being investigated. Ceramically coated engines presently being investigated may present a near-term solution to engine damage by knock, which is expected to increase with the predicted deterioration in the quality of fuel supply. Projects concerned with the mathematical modelling of heterogeneous flames, new diagnostic techniques, unsteady turbulent combustion processes, catalytic surface effects, atomization mechanics, and fuel stability are also important topics being addressed in this research area.

b. Propellants. The Army requires a broadly based knowledge in the combustion behavior of gun and rocket systems. In order to optimally design these systems, it is necessary to predict the propellant ignition and combustion behavior throughout the operating regime. This calls for basic understanding of the interrelated processes of heat and mass transport, reaction kinetics and multiphase, reacting flow dynamics. The current program includes studies of flame spreading and erosive burning phenomena and the multi-phase, transient combustion characteristics of regeneratively-driven, liquid propellant guns.

c. Explosives. This area of obvious interest to the Army, forms a small subsection of the Combustion Sciences program. All aspects of explosive efficiency, ignition and propagation mechanisms, stability and safe storage and handling are of great importance in this field. A more detailed understanding of the explosive reactions of energetic materials is clearly required. Work supported in this area currently is concerned with the propagation of detonations between layers of explosive media and with the shear-induced initiation of detonations in explosives.

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NASA COMBUSTION RELATED RESEARCH IN  
FUELS, KINETICS, AND THERMODYNAMICS

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NASA Lewis Research Center

The general objective of fuels research at NASA Lewis is to generate a technical data base to ensure that current and future aircraft can use future fuels with little or no loss in performance, service life, or safety. The Fuels Branch conducts both fundamental and applied research through three sections, a Fuels Research Section with major program elements in fuel thermal stability and fuel flow dynamics, and a Kinetics and Thermodynamics Section with major program elements in combustion kinetics and thermodynamics and transport properties of fuels and combustion products. The Chemical Analysis Section provides support for an extensive analytical effort in fuels.

Research and technology needs addressed by the program include:

1. Obtaining an improved understanding of the chemical stability of fuels exposed to severe operating conditions to suggest approaches toward increasing the operating life of fuel injectors, fuel controllers, and heat exchangers.
2. Obtaining a fundamental understanding of the effects of chemical additives on fuel flow characteristics in support of efforts to evolve acceptable approaches to their use in aircraft fuels systems.
3. Obtaining a more detailed knowledge of the chemical structure of fuels to help us understand and control deposit formation, soot formation, low temperature flow and elastomer wear, and hot section corrosion and oxidation.
4. Extending the data base for reaction mechanisms and rates and thermodynamic and transport properties to enhance the utility and accuracy of computer programs formulated to model combustors and fuel systems.

Research activities in fuel thermal stability include characterization of deposit precursors and reaction mechanisms as fundamentals; and applied fuel system simulation studies to determine effects of engine operating variables, and to develop concepts to control fuel deposition. Fuel flow dynamics research includes the characterization of molecular structure and fundamental fluid properties and applied research in heat transfer and fluid flow effects. Kinetics and thermodynamics research includes; the generation of a data base, multi-component hydrocarbon thermodynamic and transport property models, basic hydrocarbon oxidation rates, reaction mechanisms and rates for soot formation and oxidation, and the development of elementary reaction rate models for hydrocarbon combustion and soot formation.

The research activities are carried out by a combination of in-house studies, university grants and contracts, or cooperative efforts with other government research laboratories. Research reviews are held periodically in the fundamentals and applied areas and, to the extent possible, are coordinated with similar activities in other government agencies. During the past year, reviews or

symposia were held at Lewis in Fuels Fundamentals (ref. 1), Oxidation Kinetics and Soot Formation (ref. 2), and Alternative Aircraft Fuels (ref. 3). Copies of the abstracts and figures are available on request.

References

1. "Fuel Fundamentals Research Review," NASA Lewis Research Center, April 12-13, 1983.
2. "Oxidation Kinetics and Soot Formation Research Review, NASA Lewis Research Center, October 6, 1983.
3. "Assessment of Alternative Aircraft Fuels," Symposium, NASA Lewis Research Center, November 2-3, 1983.



FUTURE TRENDS IN NASA-SPONSORED  
COMBUSTION FUNDAMENTALS RESEARCH

by

Edward J. Mularz  
Propulsion Laboratory, USARTL and  
NASA Lewis Research Center

Research on combustion is being conducted at Lewis Research Center to provide improved analytical models of the complex flow and chemical reaction processes which occur in the combustor of gas turbine engines, in order to enable engine manufacturers to reduce the development time of new concepts and to increase the durability of these concepts. The current program is organized into two categories: combustion fundamentals research and applied combustion research. This presentation will restrict itself to the combustion fundamentals portion of the program. The objective is to obtain a better understanding of the various physical processes that occur in the gas turbine combustor and to develop analytical models which can accurately describe these processes. The thrusts under the combustion fundamentals area include: (1) combustion computational fluid mechanics - analytically characterize the physical phenomena associated with turbulent reactive flows; (2) model verification experiments - provide benchmark data with well-specified boundary conditions to assess the accuracy of the analytical models; (3) fundamental experiments - achieve a more complete understanding of the fundamental processes occurring in reacting flows; and (4) advanced numerics - develop improved numeric techniques which can be applied to highly turbulent, recirculating, reacting flowfields.

Research activities under the combustion fundamentals category are classified under the subject areas of model assessment, sprays, mixing, radiation - chemistry, and combustion dynamics. In each of these subject areas, there are in-house research projects, university grant activities, and contracts with industry; see Table. Each of these subject areas have research activities to develop and improve analytical models and to perform experiments to better understand the physical processes and provide data for the modelers.

The NASA Combustion Fundamentals Conference, reference 1, summarizes the current program. The emphasis over the next several years will focus on computational fluid mechanics of non-reacting highly turbulent flows. Support will also continue on the application of advanced numerics to these complex flows. Fuel spray benchmark experiments will also be emphasized. A moderate amount of work will continue in computations of combustion-flow interaction and soot formation and radiation heat transfer, and later years will see this area receive more emphasis. Work on non-steady combustion will continue at a very modest level for the next five years; at that time, it is anticipated that this area will then undergo substantial growth.

Continued balance between in-house and contract/grant activities will be sought with an enhancement of in-house fundamentals research being achieved through the creation of the Basic Combustion Laboratory (reference 2) and additional in-house researchers with Sverdrup Technology, Inc.

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## COMBUSTION FUNDAMENTALS

	ANALYTICAL MODELS	MODEL VERIFICATION EXPERIMENTS	FUNDAMENTAL COMBUSTION EXPERIMENTS	ADVANCED NUMERICS
MODEL ASSESSMENT	I-H C	I-H		
SPRAYS	I-H C	I-H GRANT C	I-H GRANT	
MIXING	GRANT	I-H GRANT C		I-H GRANT C
RADIATION, CHEMISTRY	I-H GRANT C	I-H GRANT	I-H GRANT	GRANT
COMBUSTION DYNAMICS	I-H GRANT		I-H GRANT	

CD-83-11712

DOE/BASIC ENERGY SCIENCES SUPPORTED RESEARCH ASSOCIATED WITH  
COMBUSTION SCIENCE

Allan H. Laufer  
Chemical Sciences Division/BES  
U. S. Department of Energy  
Washington, D. C. 20545

The DOE/BES program in combustion-related science is a rather broad effort whose goal is to add significantly to the knowledge base on which successful energy technologies can grow. For this reason scientific excellence is a major criteria applied in the selection of research supported by BES in general, and Chemical Sciences in particular. Indicative of the fundamental approach are the areas which are important in the program. The most well represented research efforts, with Chemical Sciences funding, includes those in combustion diagnostics, fundamental chemical kinetics, theoretical chemistry, spectroscopy and, with other BES division funding, fluid dynamics and applied mathematics. The overall funding level, within BES, is about \$14.5M. About \$9.2M is the level through the Chemical Physics program of the Chemical Sciences Division.

A major component of the combustion program is centered at the Combustion Research Facility (CRF)-Sandia National Laboratories in Livermore, California. Though the main emphasis of the research at the CRF is on laser diagnostics, both development for and application to combustion, there are important chemical kinetic and modelling efforts underway.

The combustion diagnostics aspects of the program extend to universities and include investigation of fluorescence techniques applied to flame radicals and fuel species, both of which are important for a complete chemical understanding of the combustion process. The diagnostic efforts are supported by fundamental spectroscopic investigations.

Aspects of the DOE program from our vantage point will be discussed as will several research projects in the area of diagnostics.

SUPPORT OF COMBUSTION RESEARCH BY THE ENGINEERING ENERGETICS PROGRAM

Program Director: Royal E. Rostenbach

Engineering Energetics Program  
Division of Chemical and Process Engineering  
National Science Foundation  
Washington, DC 20550

SUMMARY

The Engineering Energetics Program presently supports 31 basic research projects in combustion. The general areas include: chemical reactions, detonations/explosions, diagnostics, nature of flames, jet ignition, turbulence, and odor. The average grant for 12 months approximates \$57,000. Grants are also made to purchase research equipment and to support international conferences in combustion. The support by the program amounts to:

FY82	\$1,082,000
FY83	\$1,522,000
FY84	\$1 184,000 (est.)

# SINGLE PARTICLE SIZING BY MEASUREMENT OF BROWNIAN MOTION

(AFOSR Contract No. F49620-83-C-0154)

Principal Investigators: Alan C. Stanton and Wai K. Cheng<sup>+</sup>

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## SUMMARY

Few nonintrusive techniques are available for particle measurements in the submicron size range ( $< 0.1 \mu\text{m}$  diameter), yet measurement of these particles is basic to an understanding of important processes in combustion, such as soot formation and oxidation. The objective of the present research is the development and application of a technique for measurement of individual submicron particles in a gas stream. The approach is to measure the inertial relaxation time of individual particles in Brownian motion, by statistical analysis of the time-resolved (100 MHz) heterodyne signal obtained in a system resembling a more conventional laser Doppler velocimeter. When this approach has been demonstrated satisfactorily, the technique will be applied to studies of particle size evolution in combustion systems.

## TECHNICAL DISCUSSION

Existing optical techniques for measurement of submicron particles do not yield direct information on the particle size distribution. Our studies are aimed at development of a technique for measurement of individual submicron particles, based on the statistics of Brownian motion of the particles. The effort in the first year of the program has concentrated on the design and development of an experimental interferometric system to study this approach, combined with detailed numerical simulations (Monte Carlo modeling) of the time-dependent heterodyne signal. The simulations have been used to guide the experimental design and to devise an approach for signal analysis.

The optical and data acquisition instrumentation developed for this study are shown in Figure 1. The output from an argon ion laser is expanded and split into two collimated beams, which are focused to a spot size (beam waist) of approximately  $50 \mu\text{m}$ . Light scattered from the two beams by a (single) particle in the probe volume is collected and mixed at a photomultiplier, as in the usual fringe-Doppler laser velocimeter. In order to resolve statistical behavior arising from Brownian motion, fast (10 ns) time resolution of the signal is required. Time-domain pulse-height analysis of the signal is performed, and the data are transferred to a microcomputer for final processing and data storage. Preliminary particle measurements using this system will be described.

It is important to realize that the mean particle excursion due to Brownian motion is much smaller than the wavelength of visible light and is therefore smaller than a fringe spacing for the system shown in Figure 1. The Brownian modulation amplitude of the signal is thus dependent on the spatial location of the particle within the probe volume, and only time (not Brownian velocity) information may be derived from analysis of signal fluctuations. It is also important to realize that signal fluctuations, which are resolved in 10-ns time increments, represent the statistics of Brownian motion (the superposition of many random velocity changes), but do not represent individual collision events between the particle and gas molecules. These observations suggest a strategy in which the time-statistics of the "velocimeter" signal are analyzed to determine a characteristic time for the Brownian motion. This characteristic time is the relaxation time, or the time scale for the particle velocity distribution to approach a Maxwellian distribution at the temperature of the surrounding gas.

We have simulated the signal for the Brownian motion sensor described above using a Monte Carlo technique. In this approach, the velocity history of a particle is generated at time sampling intervals  $\Delta t$ . The correct statistical properties of the velocity history are maintained by imposing the requirement that the velocity distribution is Maxwellian in the limit  $t \rightarrow \infty$ . With the velocity history simulated in this fashion, the particle trajectory through the probe volume and the scattered intensity from the two beams can be calculated in straightforward fashion. Thus, the simulated time history of the interference signal at the detector may be obtained. Two such simulated signals are shown in Figure 2, for particles of 0.1  $\mu\text{m}$  and 0.01  $\mu\text{m}$  diameter. The signal for the smaller particle exhibits larger modulation and higher frequency fluctuations than the signal for the larger particle.

An appropriate statistical analysis of the signal time histories appears to be an analysis of the mean time between local extrema in the signal. This time can be thought of as a measure of the inertia of the particle and is longer for larger, more massive particles. A plot of this characteristic time as a function of particle size is given in Figure 3, based on the Monte Carlo simulation. Our present efforts are directed toward an examination of the experimentally measured signals from submicron particles in order to validate the application of this statistical approach.

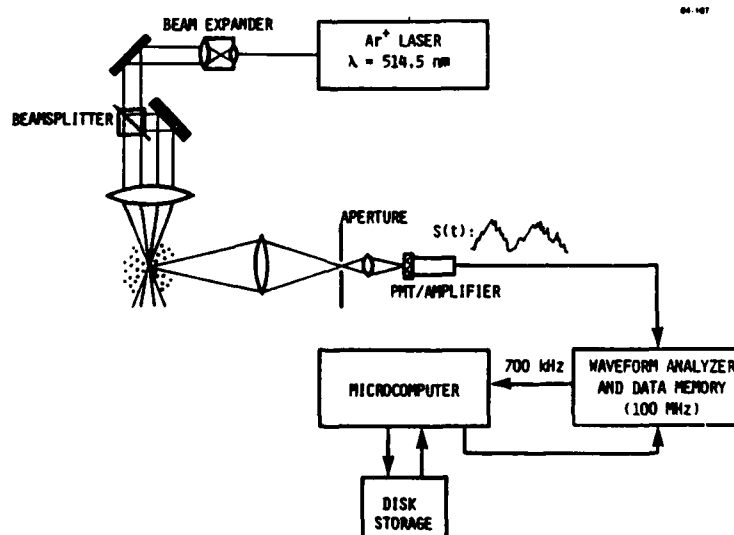
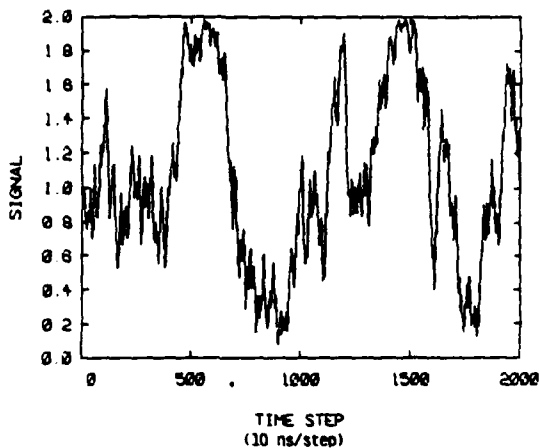
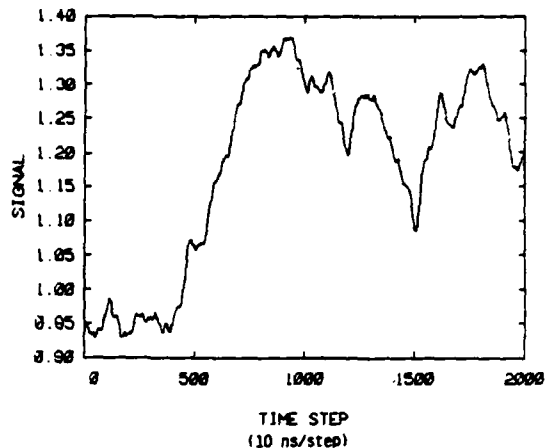


Figure 1. Schematic of optical instrumentation for the Brownian motion sensor.



(a) Particle diameter = 0.01  $\mu\text{m}$



(b) Particle diameter = 0.1  $\mu\text{m}$

Figure 2. Simulated interference signal for two particle sizes ( $T = 300 \text{ K}$ ,  $p = 1 \text{ atm.}$ , particle density =  $2 \text{ g cm}^{-3}$ ).

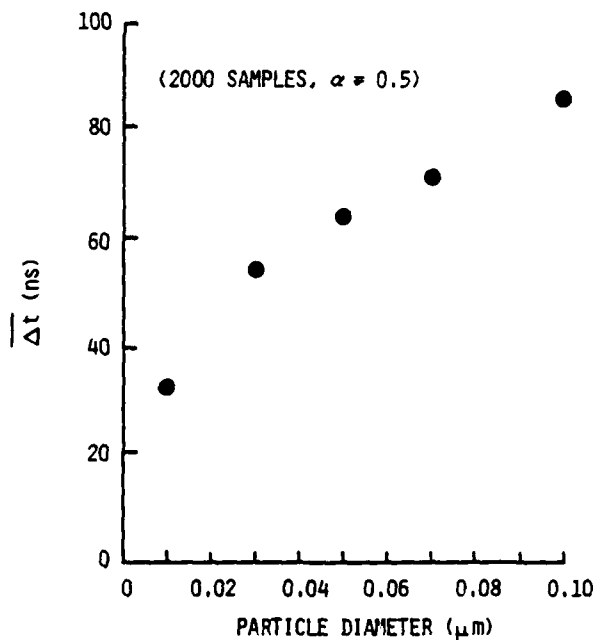


Figure 3. Mean time between local extrema in the interference signal.



SOOT FORMATION: EFFECTS OF FUEL STRUCTURE,  
TEMPERATURE AND PRESSURE

Principal Investigators: R.J. Santoro and H.G. Semerjian

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SUMMARY/OVERVIEW:

Soot formation is now well recognized to be a major challenge for the next generation of gas turbine engines which will operate with broader specification fuels at higher operating pressures and under stricter emission standards. However, the present understanding of the fundamental processes leading to soot particle formation, growth and subsequent oxidation is insufficient to allow a reliable evaluation of the impact that soot formation is likely to have on future engine technology. In order to gain a better understanding of these processes, it is proposed that a study of soot formation in laminar diffusion flames be undertaken. In these studies, specific attention will be given to the effects of fuel structure, temperature and pressure on soot formation processes. Detailed measurements of the particle, velocity and temperature fields in the flame will allow an investigation of the dependencies of the underlying rate processes. These results are expected to provide an understanding of the fundamental processes involved in soot formation under conditions which are characteristic of practical combustion systems.

TECHNICAL DISCUSSION

Recent interest in the formation of soot in combustion processes has been motivated by several related developments. It is now well recognized that future combustion systems will be operated with broader specification fuels under conditions of higher operating pressures and stricter emissions standards. Each of these developments require appropriate optimization of combustion processes and system performance capabilities; increased soot formation represents a major challenge in this process. Since soot production has been shown to have strong sensitivity to fuel properties and operating conditions (temperature and pressure) [1, 2], it would be desirable to have an understanding of the fundamental processes governing formation and subsequent oxidation. However, such understanding must also be developed under conditions which can be directly extended to processes occurring in practical combustion systems.

The objective of the proposed work is to investigate the effects of fuel composition, temperature and pressure on the rates of soot formation, particle growth and burnout in a well characterized flow field. A coannular diffusion flame apparatus will be used to study the soot formation processes in gaseous hydrocarbon fuels. The program will stress the use of non-intrusive optical diagnostic instrumentation for in-situ measurements. Laser-based techniques

such as laser scattering/extinction for particle measurements and laser velocimetry for flow field characterization will be utilized. Initially, fine wire thermocouple measurements will be used to characterize the temperature field. Later, non-intrusive techniques presently under development will be employed.

Initial efforts will be aimed at establishing the importance of chemical structure on soot formation for a variety of fuels. These studies will involve adding selected fuel constituents to previously well characterized ethene diffusion flames [3, 4]. Chemical structures typical of important fuel constituents will be considered: alkanes (e.g. propane), alkenes (e.g. propene), alkynes (e.g. acetylene) and aromatics (e.g. toluene). The combined particle, velocity and temperature field measurements will allow investigation of the particle nucleation, surface growth and oxidation stages. Recent work in similar ethene diffusion flames [3] has shown the capability of laser based particle measurement techniques to resolve these growth and burnout processes.

The effects of temperature on the rates of soot particle formation and oxidation will be investigated through addition of inert species. Studies in which such species (e.g. nitrogen or argon) are added to either the fuel or oxidizer flow allows the effective flame temperature to be varied. Soot particle size, number density, and volume fraction measurements can then be used to examine the temperature dependence of the rates of formation, growth and subsequent oxidation of the soot particles. Recently, a similar approach has been used to investigate soot particle formation in single fuel component diffusion flames [4]. These studies established the strong temperature dependence of the soot production processes. In those studies, the early formation processes were observed to be similar for similar flame temperature conditions for a simple series of fuels (methane, ethane and ethene). Extension of these studies to a wider range of fuel structures should provide further valuable insights into the soot formation and growth processes.

Studies of the pressure dependency of soot formation processes will be investigated subsequent to the initial fuel structure and temperature studies. These studies will be conducted in a separate high pressure burner similar to the coannular burner used in the above experiments. Soot production will be examined over the pressure range of 1 to 10 atm; detailed particle, temperature and velocity data will also be obtained in these flames. This extensive characterization of the particle/flame environment will allow separation of the effect of residence time variation from particle nucleation, surface growth and coagulation effects.

The essential thrust of this research is to provide a fundamental understanding of the processes underlying soot particle formation and oxidation. Through detailed particle, temperature and velocity measurements, particle nucleation, surface growth and oxidation can be investigated for a variety of fuel structures, as well as over a range of temperature and pressure conditions. The measurement approaches involve the application of well characterized techniques [5] which have been successfully applied to similar problems [3].

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LASER DIAGNOSTIC ANALYSES OF SOOTING FLAMES

ONR Contract No. N00014-81-C-0046

Principal Investigators:

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United Technologies Research Center  
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and

Irwin Glassman

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SUMMARY/OVERVIEW:

The objective of this program is to understand how temperature and fuel structure influence soot formation by making temperature, major species concentration, soot particle size, and soot number density measurements, at high spatial resolution, in a variety of flames. Understanding the chemical nature of the precursors to soot may lead to the choice of proper strategies for soot control in practical devices such as gas turbine and diesel engines. The investigations to date have yielded significant improvements in the methodology of CARS thermometry, have created a data base which suggests that radiation is an important effect in these systems, and have uncovered questions on the fundamental structure of diffusion flames.

TECHNICAL DISCUSSION:

Temperature is an important parameter for soot formation in diffusion flames. Most prior studies have been qualitative ones using thermocouples. Coherent anti-Stokes Raman spectroscopy (CARS) was shown<sup>1</sup> some time ago to be feasible and attractive for temperature measurements in a sooting environment. Recently, as part of a more general investigation of soot formation and diffusion flame structure, and using refined experimental and analytical CARS capabilities, an extensive set of high-spatial-resolution N<sub>2</sub> CARS measurements have been obtained in a 1 cm dia, axisymmetric, ethylene/air diffusion flame.

Temperature distributions are determined for various amounts of fuel and diluent  $N_2$ . In general, these show that peak temperatures are 200-400K lower than the adiabatic flame temperature (AFT), whereas the prior results showed peak values much closer to the AFT. Previously reported temperatures with propane were high in fuel-rich regions due to nonresonant susceptibility effects. We have shown recently that these effects can be accounted for by introduction of a two parameter algorithm.<sup>2</sup>

Temperature is shown to increase rapidly in the lower part of a flame. In the lower half of undiluted ethylene flames (AFT=2380K) the maximum temperature increases from about 2000 to 2100K as the fuel flow increases from 35 to 86% of the smoke point value. In the upper half, however, the maximum temperature drops from about 1950 to 1750K, indicating that a sharper drop off in temperature occurs at about the midpoint of the taller flame. For the 86% fuel-flow case, dilution with  $N_2$  was found to decrease temperatures in the lower part of the flame as expected. Somewhat surprisingly, however, the maximum upper-half temperature increases from 1750 to 1900K when  $N_2$ /fuel molar flow ratio increases from 0 to 3.0, an increase from about 74 to 87 % of respective AFT values.

Flames with  $N_2$  dilution are known to be less sooting. A typical series of diluted flames is given in Figure 1. Each flame has the same amount of fuel flow, and therefore total chemical heat release. The shroud air is adjusted to keep the overventilation constant, with a concomitant increase in velocity. The most diluted flame is an exception. In order to stabilize this flame which is on the verge of liftoff, the shroud air flow is reduced. Figure 2 is the axial temperature profile for these flames in reduced variables. While the luminous height may not be coincident with the chemical reaction zone, the former was used as the abscissa normalization factor. The lower part of these flames displays the expected ordering, where the heat capacity of the diluent causes the more diluted flames to be relatively cooler. However, the ordering is reversed in the upper part where the diluted flames are relatively hotter than the undiluted flame. These measurements suggest in conjunction with some recent findings of other workers<sup>3</sup> that radiation loss from soot may be affecting the temperature in upper portions.

Some calculations for the flames studied have also been performed using a generalized Burke-Schumann<sup>4</sup> model, which does not, however, consider radiation losses, fuel pyrolysis and finite reaction rate kinetics. The differences between calculated peak temperature and measurements are much greater at low  $N_2$  dilution--suggesting further that an additional loss mechanism such as radiation may be present. Efforts are underway to determine from measured particle size and number distributions throughout the flame an approximate upper bound for radiation heat loss.

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# EFFECT OF DILUENT N<sub>2</sub> ON LAMINAR ETHYLENE/AIR DIFFUSION FLAME

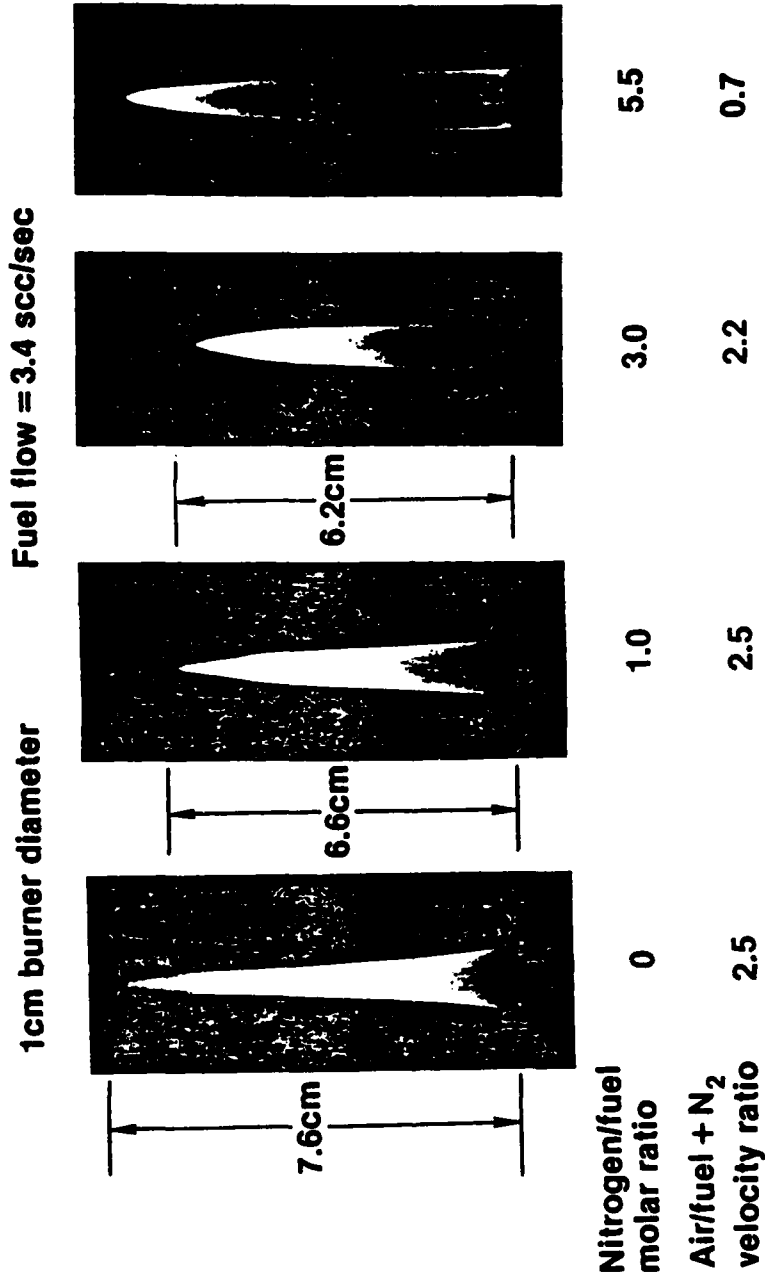


Figure 1

# EFFECT OF NITROGEN DILUENT ON ETHYLENE DIFFUSION FLAMES

## Axial Temperature Profiles at Constant Fuel Flow

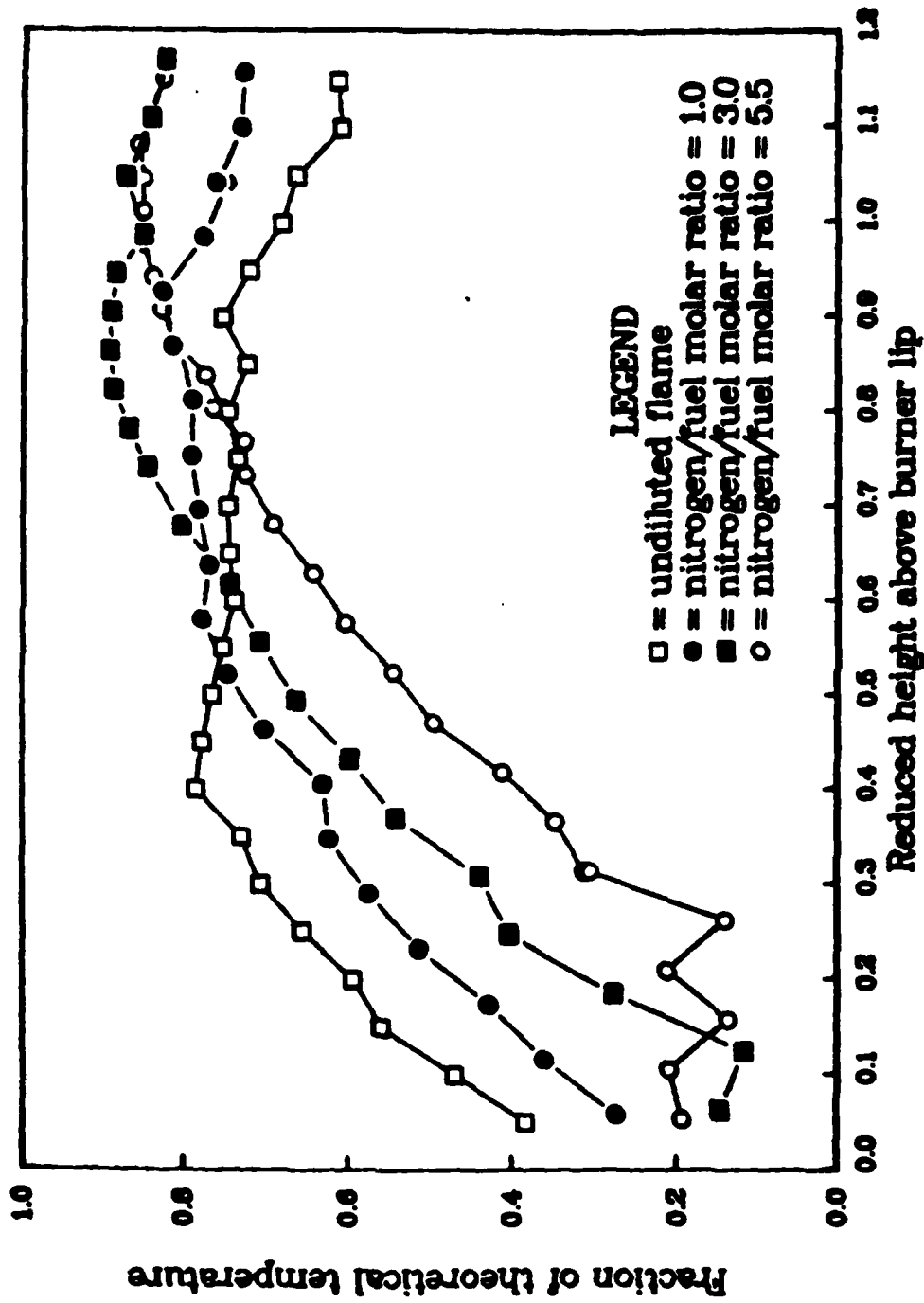


Figure 2

## RADIATIVE AUGMENTED COMBUSTION

(AFOSR Contract No. F49620-83-C-0133)

Principal Investigator: Moshe Lavid

ML ENERGIA, Inc.  
P.O. Box 1468  
Princeton, NJ 08542

### SUMMARY/OVERVIEW:

The radiative concept to enhance ignition and combustion is being researched. Advanced vacuum ultraviolet light sources are used to photodissociate molecular oxygen and other inhibiting species in the flame zone into reactive radicals. It is expected that the research will demonstrate proof of concept by igniting combustible mixtures at conditions where thermal ignition is unreliable, and by increasing the flame speed. Since the role of photochemical reactions within the whole kinetic scheme is currently not completely understood, it is further expected that this work will identify the most effective photodissociative paths. This, in turn, will assist in determining the feasibility of the concept based on the availability of newly developed light sources and their compatibility with the harsh combustion environment.

### TECHNICAL DISCUSSION

Radiative augmented combustion has been identified as a potential technique for extending current aircraft operating limits associated with combustion processes. This technique is based on the fact that radiation of selected wavelengths is capable of photodissociating stable molecules and combustion intermediates into more reactive radicals. Subsequent reactions involving these reactive radicals lead to radiative ignition and combustion enhancement. The potential of this radiative technique has been already demonstrated under laboratory static conditions. It has successfully ignited fuel-air mixtures, and has enhanced combustion processes utilizing vacuum ultraviolet (VUV) and ultraviolet (UV) radiations, emitted by high pressure xenon lamps and newly developed excimer lasers.

This program has been developed based on the guidance provided by the above encouraging results. It offers a logical continuation to the early work by emphasizing research under flow conditions. It is divided into two main subjects: ignition and enhancement. Each subject consists of an experimental effort supplemented by an analytical effort.

### EXPERIMENTAL EFFORT

The primary objective of this effort is to demonstrate radiative ignition and combustion enhancement under flow conditions. For this purpose, two specially tailored apparatus were designed: a plug flow combustor to conduct radiative ignition tests and a "pancake" burner to measure combustion enhancement in terms of increase in burning velocity.

The main concerns in the design were:

- \* Delivering maximum VUV flux, capable of producing detectable effects, to the reaction zone.
- \* Providing capabilities to measure these detectable effects.



\* Protecting the light sources from the high flame temperature. These were challenging concerns and after considerable technical discussions satisfactory solutions were found. The solutions offer very short optical pathlengths (minimizing light attenuation), and installation of the light sources on the reactants cold side.

These apparatus provide experimental conditions necessary to study the interaction between radiation and combustion during ignition or enhancement events in reactive flow systems. They can operate with various premixed combustible gases at pre-determined equivalence ratios and velocities. Tests are planned to begin with laminar hydrogen flames (where combustion theory is best understood). Provisions have been made to use Schlieren images to measure changes in flame speed. Three light sources are currently available: ILC, EIMAC and Excimer lasers.

#### ANALYTICAL EFFORT

Consistent with the experimental efforts, research in the area of analytical modeling has also proceeded on two fronts: ignition and enhancement.

Ignition: In previous work, the ignition model was used to determine the threshold concentration of atomic oxygen required to achieve radiative ignitions. Recently [1], the calculations were extended to include concentration profiles of other important species in the system. For a case simulating stoichiometric premixed  $H_2/O_2$  at atmospheric pressure, we obtained profiles for O, H, OH,  $HO_2$ , and  $H_2O_2$ . It was found that profiles of  $HO_2$  and  $H_2O_2$  are quite different from those of O, H, and OH. More importantly,  $H_2O_2$  concentration profiles exhibit an opposite trend to those of the other major radicals. Low concentrations of  $H_2O_2$  correspond to successful radiative ignition while high concentrations correspond to unsuccessful ignition. These analytical findings suggest that  $HO_2$  and  $H_2O_2$  might inhibit the radiative process. This insight was later corroborated by analytical results obtained for radiative combustion enhancement.

Enhancement: Promising results have recently been obtained from HCT modeling [2] of premixed  $H_2$  - air systems. The principle conclusion is that substantial enhancement of burning velocity (28%) appears if an additional photochemical reaction is included in the kinetic scheme. This is photodissociation of the metastable  $HO_2$  radical into OH and O. This is the most significant outcome of a series of analytical studies summarized below:

Case 1: Simulation of a "normal" (non-radiative) flame under stoichiometric conditions, without any photochemistry, resulted in a calculated flame speed of 260 cm/sec.

Case 2: Simulation of a "radiative" flame by adding only  $O_2$  photodissociation into the kinetics, under conditions identical to the first case, yielded a velocity of 250 cm/sec. This represents a slight decrease rather than the anticipated increase in flame speed. Several explanations for failure to obtain enhancement have been advanced [1] including the argument that enhancement would more likely occur under fuel-lean conditions, where free radicals ought to be in short supply.

Case 3: Simulation of same  $H_2$  - air system under fuel-lean conditions (equivalence ratio of 0.4) did not change the previous disappointing findings. It provided a flame speed of 47 cm/sec with no radiation and 43 cm/sec when  $O_2$  photodissociation reaction was included.

Significant differences in the concentration profiles of certain important species in these two fuel-lean cases provided explanation to the lack of enhancement. Fig. 1 shows that radiation produces an increase in O concentration outside the flame zone (1a), and a dramatic increase in  $H_2O_2$  concentration mainly in the unburned gas (1b). A reasonable explanation to the increase in  $H_2O_2$  concentration is higher rate of

bimolecular recombination of the metastable radical  $\text{HO}_2$ . This, in turn, suggests higher concentrations of  $\text{HO}_2$ , which is indicative of the increased importance of the chain terminating rather than the desired chain branching reactions under simulated  $\text{O}_2$  photodissociation. This led us to the idea that if  $\text{HO}_2$  were removed from the reaction zone by photochemical means, an enhancement of flame velocity may result.

Case 4: Simulation of case 3, with the inclusion of  $\text{HO}_2$  photodissociation yielded indeed flame speed of 60 cm/sec. This is an increase of 28% over the speed of 47 cm/sec with no radiation. The effect on radical concentrations is best shown in the figures.  $\text{HO}_2$  is dramatically reduced everywhere (Fig. 1c).  $\text{H}_2\text{O}_2$  is reduced in the unburned gas region (Fig. 1b), as anticipated from the drop in  $\text{HO}_2$  concentration. Conversely, O and H concentrations increase in the flame zone (Figs. 1a and 1d).

These analytical results suggest that previous experimental observations on combustion enhancement by radiation were probably due to the combined photodissociation of O, and  $\text{HO}_2$ .

A mechanism by which this occurs can be inferred from the absorption spectrum of  $\text{HO}_2$  and spectral band assignments. Strong  $\text{HO}_2$  absorption has been observed between 190 nm and 260 nm [3], and weaker absorptions up to 600 nm have also been reported [4]. Lack of vibrational fine structure in the absorption spectrum indicates that ultraviolet excitation will promote  $\text{HO}_2$  to a repulsive potential energy curve, causing dissociation.

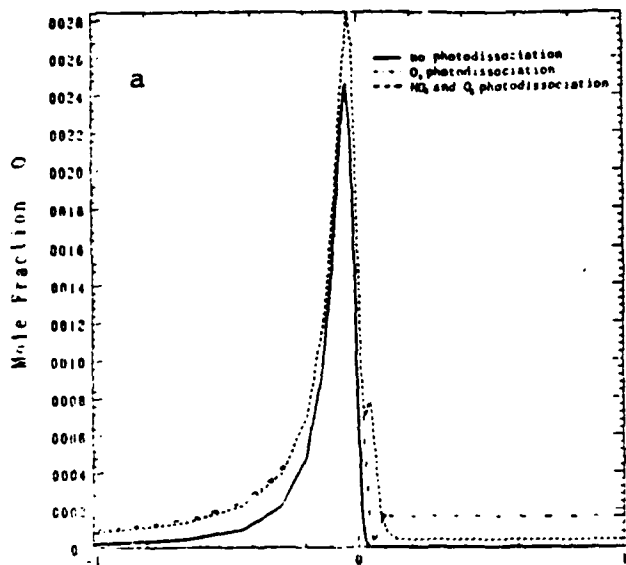
#### SUMMARY

Previous experimental findings and recent analytical modeling of the  $\text{H}_2$  - air system suggest that ignition can be achieved by photodissociating  $\text{O}_2$  with VUV radiation. On the other hand, preliminary analytical modeling of flame propagation suggests that combustion enhancement can be achieved by promoting  $\text{HO}_2$  dissociation at higher wavelengths. Due to the special absorption and photochemical characteristics of  $\text{HO}_2$ , this latter finding opens up new practical opportunities for combustion enhancement.

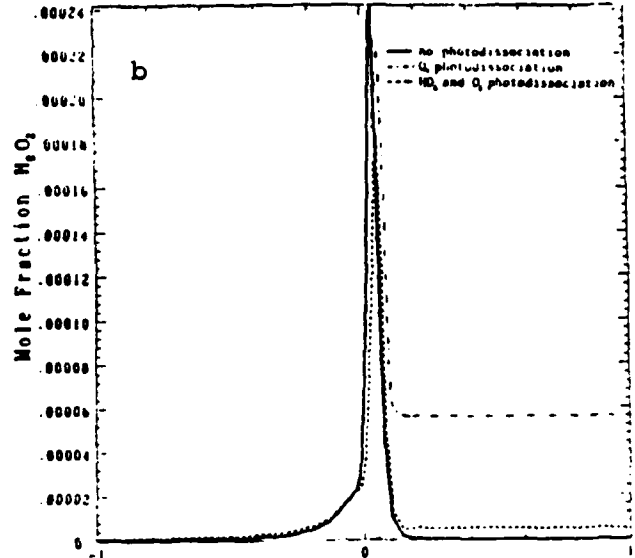
- \* CW Lasers can be used as radiation sources. For example, the frequency-quadrupled Nd-Yag laser (265 nm) or the Argon Ion laser (335 nm, 351 nm) emit in the spectral region for dissociation of  $\text{HO}_2$  to  $\text{O} + \text{OH}$ .
- \* Practical difficulties associated with VUV light sources (low power, special optics requirements, cost) are easier to deal with at longer wavelengths.
- \* Longer wavelengths more effectively penetrate to the flame zone. For example, above 200 nm, many combustion reactants ( $\text{O}_2$ ,  $\text{H}_2$ , aliphatic hydrocarbons) and products ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ) are virtually transparent. Thus, radiation can be delivered at high intensity to the flame zone where it will be most effective.

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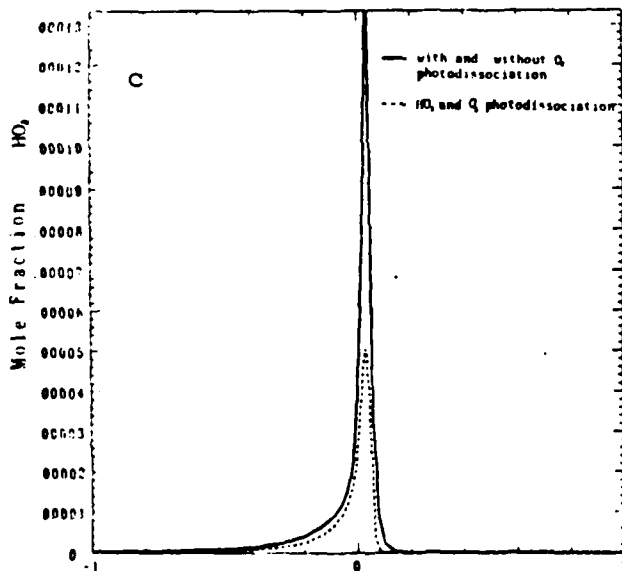
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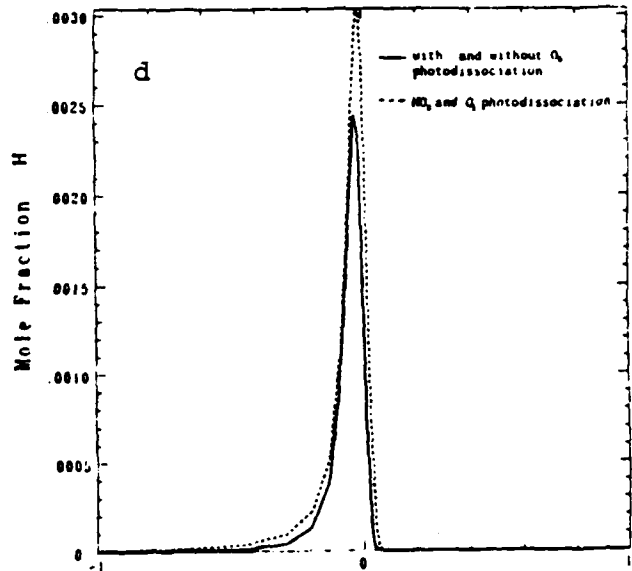
Relative flame position (cm)



Relative flame position (cm)



Relative flame position (cm)



Relative flame position (cm)

**FIGURE 1**

Calculated concentration profiles of important species in premixed  $H_2$  - air flame at equivalence ratio of 0.4, under radiative and non-radiative conditions.

(AFOSR Contract No. ISSA-84-00004)

Principal Investigators: W. Braun and M. D. Scheer

Chemical Kinetics Division  
National Bureau of Standards  
Washington D. C. 20234

#### Summary/Overview:

The influence of intense infrared laser radiation on the rate of decomposition of hydrocarbon (or hydrocarbon-like) molecules is not completely understood at the present time. There exists the strong possibility that the rates of unimolecular processes will be enhanced by the absorption of infrared photons when they are carried out at very high temperatures and are driven out of thermal equilibrium. Under such circumstances the laser photons supplement the collisions with the heat bath molecules in repopulating the high energy tail of the vibrational energy distribution. Such experiments have now been performed using ethyl iodide as a prototype molecule and will be discussed in some detail.

#### Technical Discussions:

##### Background:

The departure of systems undergoing chemical change from an equilibrium distribution of energies among their molecular degrees of freedom occurs only when rates of reactions are very large. Ignition and diffusion flame phenomena, occurring in heterogeneous and unmixed fuel-oxidant systems, as well as flame propagation through thoroughly mixed gaseous combustibles, are examples of such rapid high temperature chemical processes. One important property of these rapidly reacting systems is competition between the rate of collisional activation and the rate of surmounting the activation barrier leading to successful reaction. At low temperatures and high pressures, collisional activation maintains an equilibrium Boltzmann distribution of the energy required to overcome the activation barrier so that the process is activation limited. Since the collision rate varies as  $T^{1/2}$ , while the rate of overcoming the barrier varies as  $\exp(-E/RT)$ , it is readily seen that for any given pressure there exists a temperature beyond which the latter rate will surpass the former. Under these circumstances the high-energy 'tail' of the Boltzmann distribution becomes depleted with a consequent lowering of the overall reaction rate. Unimolecular

decompositions are the simplest examples exhibiting such fall-off behavior and are characterized by a depletion of those molecules with vibrational energies near that required to surmount the activation barrier. The pumping of infrared laser energy into the high end of the vibrational energy distribution of the decomposing molecules provides a means of enhancing their rates of decomposition. A quantitative comparison of these rates with and without measured doses of laser radiation will yield relative efficiencies for the transfer of vibrational energy at levels near the activation energy barrier by IR photons compared to heat-bath collisions. Recombination processes on the other hand demonstrate the inverse effect where the reaction exothermicity must be removed by collision with a heat-bath molecule in order to stabilize the adduct. Thus, only collisions which are efficient in removing energy rather than supplying it will enhance the recombination reaction rate and the absorption of IR photons will decrease the recombination rate.

Intense infrared radiation is therefore capable, in principle, of pumping the vibrational-rotational manifolds of a reactive molecule and thereby provide a means for decreasing the depletion factor in the Boltzmann distribution at high energies. It has been experimentally demonstrated that pumping the lowest vibrational energy levels of a reactive molecule with an appropriate resonant wavelength can, under favorable circumstances, enhance the rate of reaction. The very high vibrational-rotational energy levels near the top of the activation barrier on the other hand, are very closely spaced in a quasi-continuum so that pumping the high energy part of the Boltzmann distribution should be virtually wavelength independent.

#### Experimental Results:

During the past year a very rapid, high temperature heating method has been developed. Small volumes of fused silica can be heated to incandescence and beyond by the absorption of 10 micron infrared radiation at power density levels in the neighborhood of 1 kW/cm<sup>2</sup>. By using the focused beam of a cw CO<sub>2</sub> laser (P20 line of the 001-100 band) to heat only the orifice end of a fused silica reactor tube, one can achieve very short heating times for gases that flow through the tube and expand adiabatically out of the orifice into an evacuated region. Modulation of the orifice surface temperature is readily achieved by chopping the laser beam. It was found that when a 50% duty cycle was employed at frequencies between 10 and 1000 Hz, a 20:1 mixture of He and ethyl iodide flowing at a pressure of 5 torr produced I atoms that were in phase with the temperature modulation. The temperature modulation was detected by measuring the spectral radiance of the quartz orifice at 660 nm and the I atoms were detected by resonance fluorescence at 162 nm using an iodine resonance lamp and a solar-blind photomultiplier.

Under these circumstances the temperature modulation can be calculated from a measurement of the 660 nm spectral radiancy during the 'laser on' and 'laser off' times of the modulation cycle using the Wien (short wavelength) approximation to the Planck radiation law. When subscripts 1 and 2 identify the 'off' and 'on' times respectively, such a relation is given by

$$(T_2 - T_1)/T_2 = (k \cdot T_1 / (h \cdot \nu)) \cdot \ln(R_2/R_1) \quad (I)$$

where  $k$  is Boltzmann's constant,  $\nu$  is the center frequency of a narrow band of the radiation viewed and  $h$  is Planck's constant. Similarly if the I atom production follows the temperature modulation and is entirely thermal so that an Arrhenius relation is obeyed, the temperature modulation can also be written in terms of a measured ratio of the I atom flux during the 'on' and 'off' times of the modulation cycle and the Arrhenius activation energy  $E$ , namely

$$(T_2 - T_1)/T_2 = (E / (k \cdot T_1)) \cdot \ln(I_2/I_1) \quad (II)$$

The ratio of the two sets of measured quantities is therefore given by

$$\frac{\ln(I_2/I_1)}{\ln(R_2/R_1)} = \frac{E}{(h \cdot \nu \cdot N)} \quad (III)$$

where  $N$  is Avogadro's number. When the flow pressure is sufficiently small and the  $C_2H_5I$  decomposition is well into the fall-off, the value of  $E$  will be smaller than its high pressure limiting value and the high energy tail of the vibrational energy distribution will be significantly depleted. Nevertheless for strictly thermal behavior, the quantity  $(E / (h \cdot \nu \cdot N))$  will remain constant as the chopping frequency is varied. If there is significant absorption from the intense 10 micron laser field by the heated  $C_2H_5I$ , the reaction will tend towards the high pressure limit and the effective activation energy ( $E$ ) will increase. Such an effect becomes more pronounced as the chopping frequency increases, the temperature modulation  $(T_2 - T_1)/T_2$  decreases, and the modulation waveshape changes from an asymmetric on-off square wave to a symmetric saw-tooth wave. Thus an observed increase in the measured ratio given by the left side of equation (III) will be a strong indication that a successful photon induced manipulation of the vibrational energy distribution has occurred. Results of such experiments which compares the thermal modulation of a chemical reaction rate with that of a radiation field will be described in detail.

# THE EFFECT OF SURFACE REACTIONS IN CATALYTIC COMBUSTION\*

(AFOSR-83-0326)

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## SUMMARY/OVERVIEW:

An important, and yet unresolved, question regarding the interaction of the fundamental physical and chemical processes which control catalytic combustion is the effect of surface generated radicals on the gas phase chemistry under catalytic combustion conditions. Such an effect has been observed to be important in other catalytic processes and there is evidence that it may play a role in catalytic combustion, however this has not been studied. The objective of the proposed research is to evaluate the role of surface generated OH radicals in catalytic combustion. In particular, the effect of surface generated OH radicals on the ignition and extinction characteristics of propane in air over a platinum catalyst is under study. Temperature and OH concentration profiles between and downstream of two catalytic flat plates in a stacked-plate catalyst bed will be measured using laser induced fluorescence. The proposed study will attempt to determine whether or not, during catalytic combustion, there is significant OH radical production by catalytic surface reactions and the effect of such radicals on the ignition, flame stabilization and flammability limit characteristics of practical catalytic combustors.

## TECHNICAL DISCUSSION

A stacked-plate catalytic combustor configuration is being used which allows for the required optical access into the combustor. The catalyst plates are 50 mm wide, 100 mm long and 1 mm thick. There are a total of nine plates in the catalyst bed with an inter-plate spacing of 6 mm. The catalyst plates are made from a steel alloy substrate, coated with aluminum oxide and then platinum. Six 0.50 mm diameter holes have been drilled into the side of the center plate at six axial locations. Thermocouples have been inserted into these holes for measurement of the plate's axial temperature profile. A water cooled gas sampling probe and a thermocouple are used to obtain gas composition and temperature measurements at the exit of the catalyst bed. Optical access is available through windows in the sides of the test section located at several axial positions. The window aperture is 10 mm, therefore the entire distance between two plates can be probed.

\* Sponsored by AFOSR and NASA-Lewis.

Based on a similar experiment by Cattolica and Schefer [1,2], it was anticipated that the OH concentrations would be large enough for detection by resonance absorption spectroscopy. Under the conditions of this experiment the OH detection limit using the absorption technique is about  $10^{16}/\text{cc}$ , as compared to equilibrium OH concentrations of about  $10^{14}/\text{cc}$  (based on the overall equivalence ratio and the catalyst temperature). Measurements were attempted in the stacked-plate combustor using resonance absorption and were unsuccessful, implying that the OH concentration is less than  $10^{16}/\text{cc}$  but still possibly greater than the overall equilibrium concentration. In order to extend the OH detection limits it was decided to use laser induced fluorescence (LIF). Because of the limited optical access with the stacked-plate configuration, it is necessary to use "forward scatter" collection. The spatial resolution with "forward scatter" collection is comparable to that of the absorption measurements, which is adequate for the 2-D flow field between the catalyst plates. The main difficulty with this approach is in separating the fluorescence from the laser light. The optical configuration which has been successfully tested in a methane-air flat flame burner is shown in Figure 1. The absorption transition is  $v = 0$  to  $v = 1$  (2820Å) and the fluorescence from  $v = 1$  to  $v = 1$  (3090Å) is observed. The use of polarization rejection and a double monochromator effectively blocks the laser light. Tests using this "forward scatter" LIF system in the stacked-plate catalytic combustor are currently underway.

The objective of this research is to evaluate the effect of surface generated radicals on the ignition and blow-out characteristics of catalytic combustors. To date, however, there have been no experimental studies of transient catalytic combustion, although there have been several theoretical studies [3-5]. In order to better understand the basic characteristics of transient catalytic combustion, especially for the purpose of providing insights to guide the OH experiments, it was decided to investigate the transient behavior of the stacked-plate catalytic combustor in terms of the response of the substrate temperature and the exhaust gas temperature and composition. To date, ignition experiments have been conducted where the inlet temperature and velocity are fixed and the fuel is suddenly turned on. The fuel transient is less than one second. The transient response of the substrate temperature profile and the exhaust gas temperature are measured with thermocouples and recorded by a mini-computer data acquisition system. The transient response of the CO and CO<sub>2</sub> exhaust concentration is measured with NDIR gas analyzers, which have a characteristic response time of less than 5 seconds, and are also recorded by the minicomputer system. The transient response of the hydrocarbon exhaust concentrations are measured by a multi-loop gas sample storage system with subsequent analysis by gas chromatography. The characteristic response time of the gas sample system is less than 10 seconds.

A typical result for the transient response of the axial substrate temperature profile at two different inlet velocities is shown in Figure 2. These results show that the front of the catalyst heats up first and that as the inlet velocity increases the back of the catalyst heats up more quickly due to increased convective heat transfer from the front to the back of the catalyst. The characteristic time for the substrate temperature to reach steady state is of the order of 10 minutes.

The transient response of the exhaust gas composition, measured 25 mm downstream of the catalyst bed exit, is shown in Figures 3 and 4. The CO<sub>2</sub> concentration is found to increase immediately after the fuel is turned on, due to oxidation of the propane on the catalyst surface. Shortly after the fuel is



turned on the surface reactions become diffusion controlled and the rate of increase in the CO<sub>2</sub> concentration decreases. At approximately 400 seconds after the fuel is turned on there is evidence of the onset of gas phase reactions in terms of the production of CO and intermediate hydrocarbons. At 600 seconds the CO and HC concentrations peak and then begin to decrease due to increased gas phase reaction.

Additional experiments will be conducted for the case of a step change in the equivalence ratio over a range of inlet temperatures, velocities and equivalence ratios, as well as selectively repeating some of these tests with helium/oxygen/propane mixtures to test the effect of mass and thermal diffusivity. The results of these transient experiments will be compared to the theoretical results reported in the literature and will provide valuable insights for the transient OH measurements.

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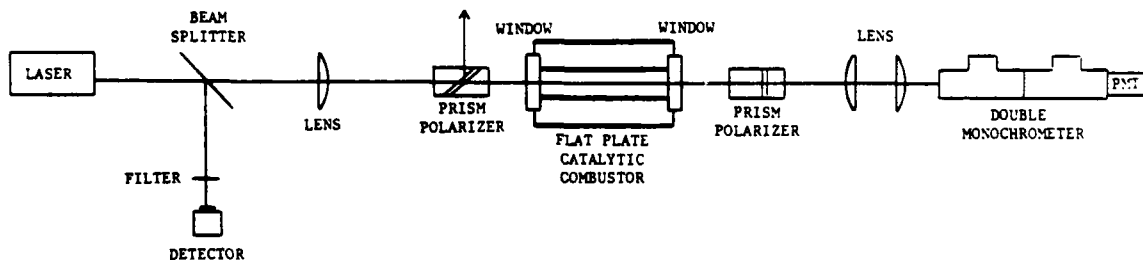


Figure 1 - Laser induced fluorescence optical configuration with "forward scatter" collection.

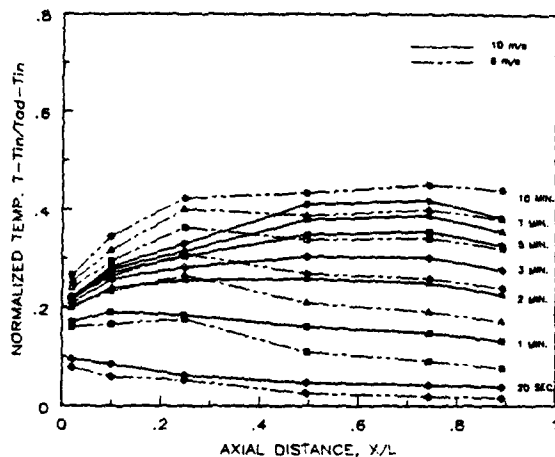


Figure 2 - Normalized catalyst temperature versus axial position at different times after fuel is turned on until steady state, for 700° K inlet temperature, 0.25 propane in air equivalence ratio and inlet velocities of 6 m/sec and 10 m/sec.

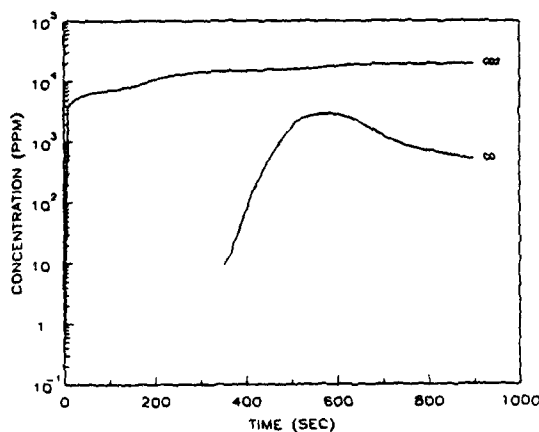


Figure 3 - CO and CO<sub>2</sub> exhaust concentrations versus time, after fuel is turned on until steady state, for 700° K inlet temperature, 0.35 propane in air equivalence ratio and 3 m/sec inlet velocity.

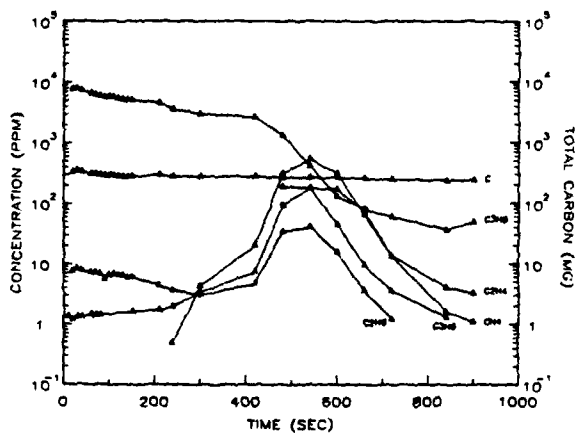


Figure 4 - Hydrocarbon exhaust concentrations versus time after fuel is turned on until steady state, for 700° K inlet temperature, 0.35 propane in air equivalence ratio and 3 m/sec inlet velocity.

## FUEL SPRAY EVAPORATION AND COMBUSTION

AFOSR Contract No. F49620-83-K-0027

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### SUMMARY:

The goal of this program is to provide detailed information on the evaporation and combustion characteristics of fuel sprays at thermodynamic conditions as seen in gas turbine combustors. Evaporation rates and flame speeds in liquid fuel sprays are being studied with the emphasis placed on the effects of inlet conditions and fuel properties. An acoustic excitation fuel injector was developed to produce monodisperse drops which are injected into a simulated gas turbine environment. Typical drop sizes are 70  $\mu\text{m}$  in diameter with an anticipated range of 20-200  $\mu\text{m}$ . Combustor conditions include flowrates of 1 kg/sec, pressures ranging from 100 to 900 kPa and air temperatures ranging from 300 to 900 K.

### TECHNICAL DISCUSSION:

Construction of the test facility is now complete. The system features a non-vitiated, high pressure air supply and a test combustor designed for evaporation and burning rate measurements of a liquid fuel spray. The components of the test facility are shown in Fig. 1 and include a flow straightening section, fuel injector, test section, proposed second test section, water cooling and exhaust. Experimental measurement capabilities include 1-D Laser Doppler Velocimeter (LDV), forward scattering drop sizing, high speed photomicrography and gas sampling with a phase discriminating probe. These systems will provide independent determination of the fuel spray evaporation rates in the test section through the measurement of drop size variations as a function of time (and position) and vapor phase fuel to air ratios. Upon complete characterization of the flowfield (velocity, drop size, equivalence ratio, etc.) the spray will be ignited and the rate of flame spread across the test section will be used to determine flame speeds.

A primary achievement in the first eighteen months of this work was the demonstration of our fuel injection technique for the generation of monodisperse sprays with controllable drop size and spacing. Our previous work on the generation of monodisperse drops had been performed with the formation of a

single jet and one dimensional array of jets which were broken into uniform drops by acoustic excitation. This technique has now been extended to a two dimensional array consisting of 1500 individual droplet streams in our test combustor. The droplet sizes generated were approximately 70  $\mu\text{m}$  in diameter with a droplet to droplet spacing of approximately 1-2 drop diameters. The drop sizes and spacing are independently variable through control of the acoustic wave amplitude and frequency, the fuel flowrate, and the physical dimensions of the injector face (hole size and spacing).

The fuel injector assembly developed for this work is shown in Fig. 2. The assembly includes electrical access for operation of the exciter and cooling water for temperature control of the fuel and exciter. A photograph of a typical spray generated by the injector is given in Fig. 3. The drops are again  $\approx 70 \mu\text{m}$  in diameter, and only the ones traveling along the focal plane of the viewing microscope objective have clear images in the picture. The upstream drops do not appear perfectly spherical due to the fact that they are still going through the mechanical vibrations (which are, in the first place, responsible for the breakup of the smooth jets into uniform drops). As expected, the downstream drops are seen to be more spherical. The velocity and production rate of the drops are, respectively,  $\sim 10\text{m/s}$  and 36.4 kHz. The total flowrate is approximately 0.7 liters/minute for this particular run, which of course, can be varied during the experiment by choosing a different set of operational parameters.

Now that the experimental facility has been completely built, preliminary measurements have concentrated on characterizing the gas phase flowfield. Prior to LDV measurements simple Pitot-static velocity profiles were obtained downstream of the fuel injector. As shown in Figure 4, these measurements indicate an axisymmetric flow and are in reasonable agreement with mean axial velocities computed using our version of the steady, incompressible but turbulent flow model, HELIOS (essentially a version of TEACH) code [1]. Experiments and further calculations are underway to examine the effect of the fuel spray on the gas phase flow field. Preliminary results indicate that due to the large momentum of the spray, the fuel jet dominates the flow and substantially alters the gas phase velocity field. In addition, the recirculation zone behind the injector does not appear to adversely affect the fuel droplet formation.

Experiments during the next year will allow us to determine the spray evaporation rates of liquid fuels as a function of the gas (air) temperatures (ranging from  $300 < T_g < 900 \text{ K}$ ), pressures (ranging from  $100 \text{ kPa} < P_g < 900 \text{ kPa}$ ) and the gas velocity which will vary linearly with air mass flowrates (ranging from  $0.2 < \dot{m}_a < 1 \text{ kg/sec}$ ).

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<sup>1</sup> N. S. Vlachos and J. H. Whitelaw, "Low Reynolds Number Flow in the Vicinity of Axisymmetric Constrictions," Journal Mechanical Engineering Science, Vol. 21, No. 2, pp. 73-84, 1979.

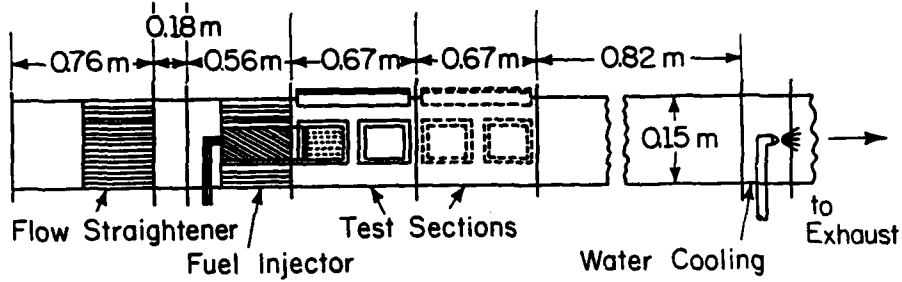


Figure 1. Combustion Tunnel Schematic.

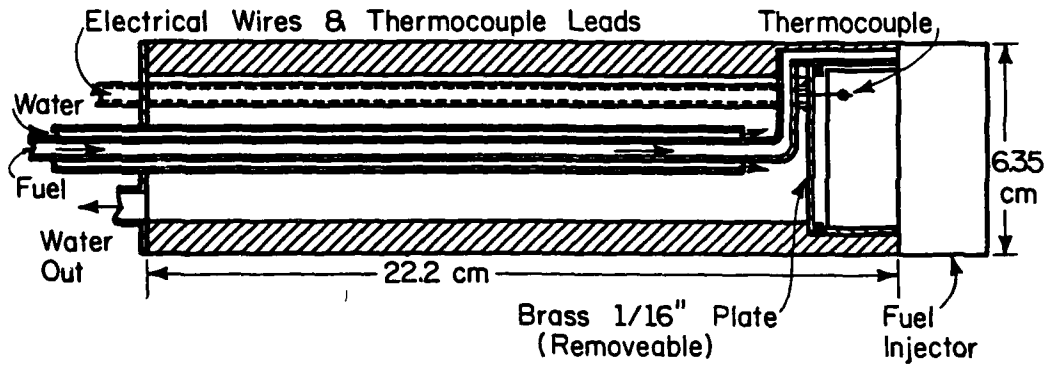


Figure 2. Fuel injector system.

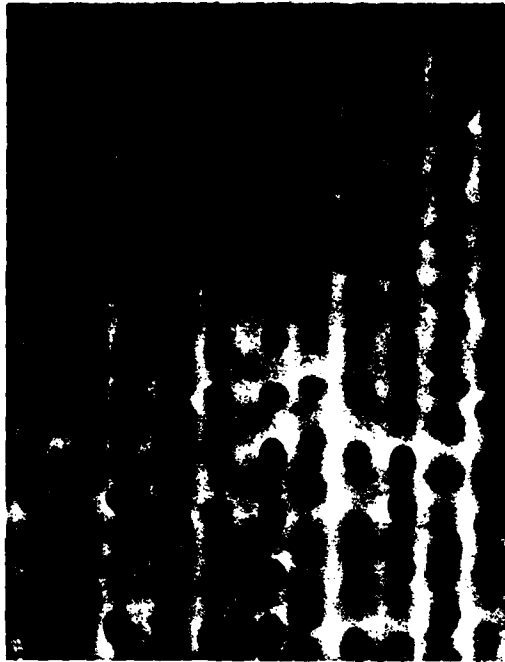


Figure 3. Two dimensional array of monodisperse drops.

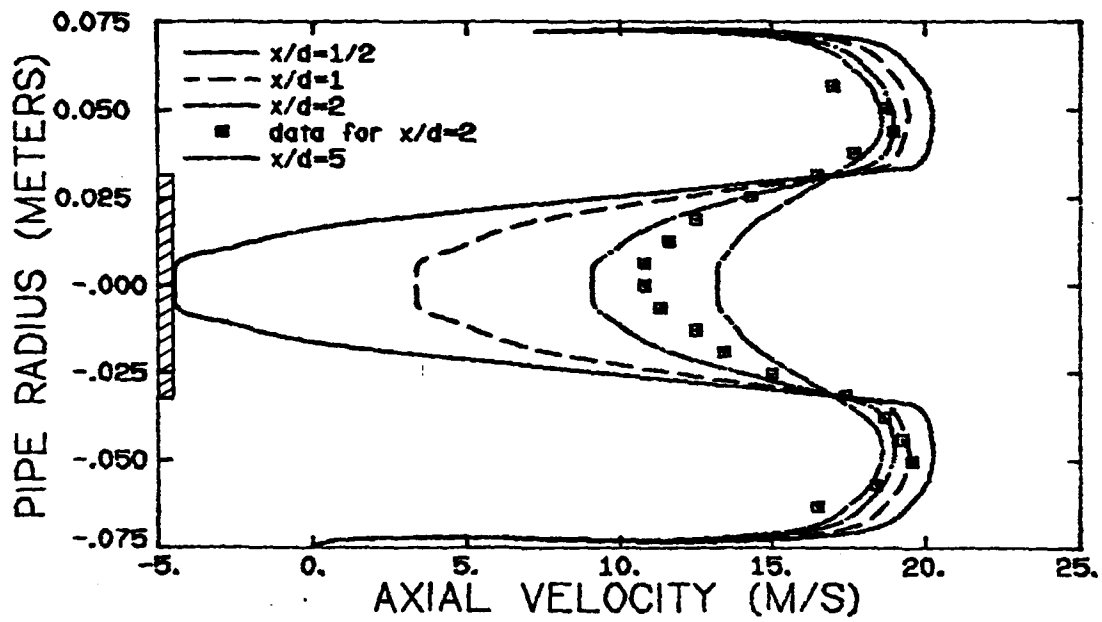


Figure 4. Computed and measured gas phase velocity profiles downstream of the fuel injector.

# IGNITION STUDIES OF LIQUID AND GASEOUS HYDROCARBON FUELS

AFOSR Grant/Contract No. 80-0203

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## SUMMARY/OVERVIEW:

Numerical results are presented on the prediction of the ignition of monodisperse sprays. The results indicate the existence of an optimum droplet size for the minimum ignition delay time. This optimum droplet size increases with increasing fuel volatility and overall equivalence ratio. An experiment has been designed and constructed to investigate spray ignition. The experiment consists of a monodisperse spray surrounded by an air flow of controlled fuel-vapor concentration. The performance of each component of the experiment and the reproducibility has been tested and experiments of the whole system show that the experimental apparatus performs as expected.

## THEORETICAL MODELING OF SPRAY IGNITION:

Preliminary results on the ignition of a monodisperse fuel-air spray in contact with a planar hot wall were reported in the last AFOSR Contractors' Meeting. The theoretical model was 1-dimensional unsteady. The numerical computations employed a hybrid Eulerian-Lagrangian scheme. During the last year, a detailed parametric study has been conducted. Effects of droplet size distribution, chemical kinetics, and overall fuel-air ratio have been examined. Some of the results are discussed in the paper to be presented in the 20th Symp. on Combustion, August 1984. Additional results would be presented at the AIAA 23rd Aerospace Sciences Meeting, January 1985.

The results for a monodispersed spray indicate the existence of an optimum droplet size for the minimum ignition delay. The optimum droplet size increases as fuel volatility increases or as overall equivalence ratio increases. The behavior can be explained by the total droplet surface area effect. Similarly, there exists an optimum equivalence ratio which depends on fuel volatility and initial droplet size. This is clearly demonstrated in Fig. 1, which gives the ignition delay versus equivalence ratio for different droplet radii. The results also indicate that the parameters used in representing the reaction scheme have a strong influence on the ignition delays. The present results advocate the use of non-unity exponents for fuel and oxidizer concentrations. The influence of initial size distribution is examined by using a bimodal size distribution. The results indicate (see Fig. 2) that for predicting the ignition delays, the use of Sauter means diameter does not accurately represent the polydisperse case. Another interesting result is illustrated in Fig. 3. A strong dependence of the ignition delays on the exact location of droplets nearest to the ignition source means that the spray ignition process has a statistical character. Thus for a given set of parameters, only a range of

ignition delays would be predicted.

Presently, the formulation for studying the ignition of flowing sprays over a hot plate is well underway. A two-dimensional flow of air-fuel spray mixture over a hot wall is considered. The theoretical model is based on an unsteady lagrangian formulation of liquid-phase properties and an Eulerian representation of gas-phase properties. Preliminary results will be based on the assumption that self-similar solutions exist for the gas-phase velocity and temperature fields. The ignition delays (in terms of the length of the hot surface up to the point of ignition) and the ignition energy will be obtained as a function of various parameters such as the temperature of the hot surface, fuel type, initial droplet size, initial size distribution, initial fuel vapor concentration, overall equivalence ration, and mixture velocity. The theoretical results will be compared with the experimental data which will be available from the parallel experimental effort.

#### SPRAY IGNITION EXPERIMENT:

The spray ignition experiment is operational, and first experiments to test the apparatus performance have been conducted. Accurate determination of the local vapor pressure or fuel-vapor concentration and droplet size is necessary since the ignition history depends on properties and conditions of the spray and the gas phase, such as droplet size and vapor pressure. Measurements of the gas phase stoichiometry have been conducted by means of a gas chromatographic sample analysis. These tests are necessary to determine the dynamics of the experimental apparatus and the reproducibility of experimental conditions. The calibration of the air-fuel vapor flow system which is an essential part of the experiment is currently being performed. The fuel vapor content of the co-flowing air entering the test section is intended to control the evaporation of the droplets during which the droplet size decreases and the fuel vapor concentration in the air increases. Before performing meaningful spray ignition experiments, the relationship between local fuel-vapor concentration and droplet size for several droplet sizes produced by the spray generator and varying vapor concentrations entering the test section has to be determined. This information establishes the initial conditions for the spray-vapor-air system at the location of the ignition source. The ignition test can then be conducted. The fuel vapor concentration of the co-flowing air entering the test section is varied by controlling the temperature of the cleaned and dehumidified air at the preheater outlet, the air residence time in the evaporation columns, and the water bath temperature. The strong dependency of the initial vapor concentration on the air temperature was observed during the first system performance test. The system provides the necessary control over the fuel-vapor concentration.

The low concentration range is covered by supplying the system with air colder than the water bath temperature, and the high concentration range up to saturation is reached by increasing the air temperature up to or above the water bath temperature.

Parallel to the test, characterizing the co-flowing air properties experiments using the droplet generator (TSI model 3450 vibrating orifice aerosol generator) with Toluene and with Benzene have been conducted to verify the instrument performance. These tests proved that the generator will cover the droplet diameter range up to 200  $\mu\text{m}$  (depending on the installed orifice and the orifice frequency). The test of the individual apparatus components has been successfully conducted. When integrating the two components spraying fuel into air of controlled fuel vapor concentrations, an asymmetric irregular flow pattern was observed in the test section. Measures are currently identified and tested to eliminate this problem which occurs in the lower part of the test section. The experiment needs to be equipped with



diagnostic tools to measure ignition quantities of interest. As mentioned earlier, light emitted during the ignition process and recorded by a photomultiplier tube, together with simultaneous high speed schlieren photography, will provide the means to determine ignition delay time and visualize the ignition process. Color schlieren cinematography has been demonstrated earlier.

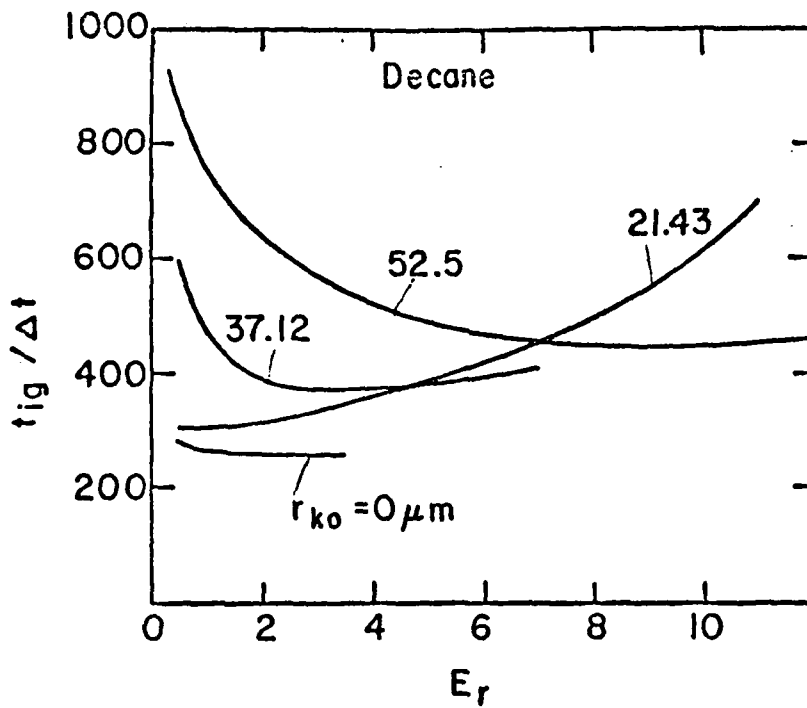


Fig. 1: Ignition time delay versus overall equivalence ratio for different drop sizes.  $\Delta t$  = time step size.

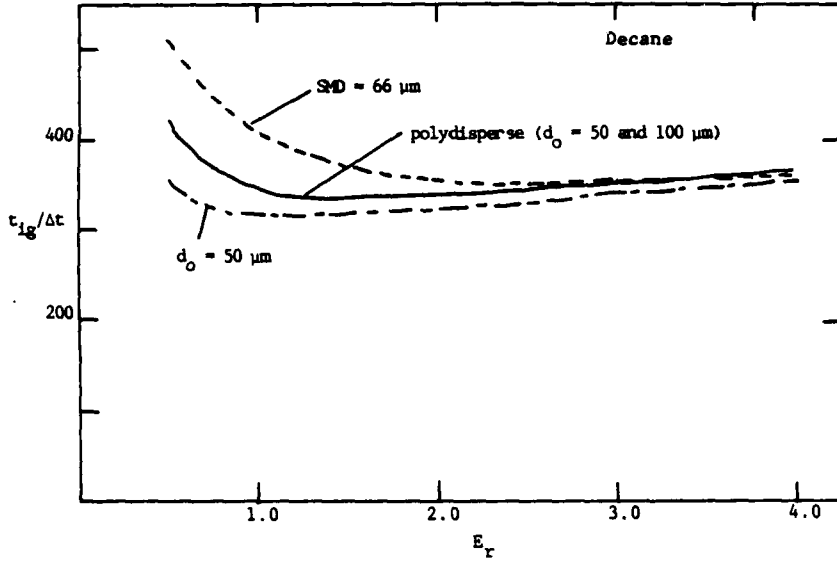


Fig. 2: Ignition time delays versus overall equivalence ratios for a polydisperse case with initial drop diameters of 50 and 100  $\mu m$ , for an equivalent monodisperse case and for a monodisperse case.

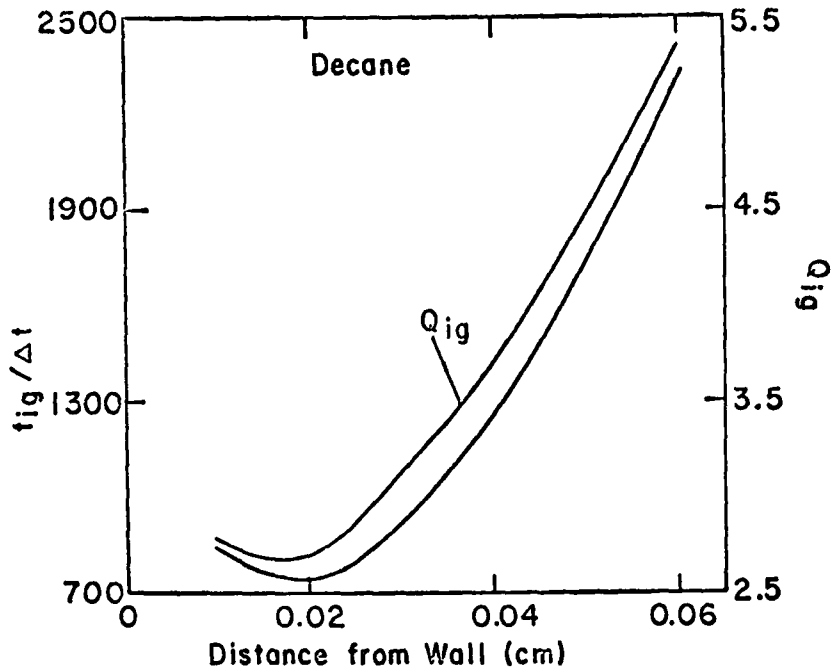


Fig. 3: Variation of ignition time delay and ignition energy with the location of droplets nearest to the wall.

# STABILIZATION OF FIRES BY LARGE-SCALE FLAMEHOLDERS

AFOSR Contract/Grant No. AF820107B

Principal Investigator: A. H. Lefebvre

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## SUMMARY

The objectives of the research are to extend the range of experimental data on the stabilization properties of bluff-body flameholders to include irregularly shaped flameholders, such as might arise on the external surface of an aircraft due to structural damage, and to derive suitable theoretical relationships to describe stabilization performance for the extended range of flameholder shapes.

## TECHNICAL DISCUSSION

Stability loops are obtained by the water injection technique. The main advantage of this injection technique is that it allows the combustion performance of large-scale combustion systems to be fully evaluated while operating within their normal range of velocities and fuel/air ratios. The test procedure is quite simple. The velocity and temperature of the gas flowing over the stabilizer are adjusted to the desired values; the fuel is turned on and a flame established in the recirculation zone downstream of the stabilizer. Water is then gradually admixed with the kerosine in increasing amounts until extinction occurs. This process is repeated at a sufficient number of fuel flow rates for a complete stability loop to be drawn.

The flameholders selected for this study included six Vee-shaped gutters manufactured to the same length (14 cm) and the same trailing edge width of 7.6 cm. They ranged in included angle from 30° to 180° in steps to 30°. After measuring the pressure loss and stability characteristics of all six gutters, four rectangular strips of material were removed from both sides of each gutter. These strips were 0.64 cm wide and they extended from the trailing edge to halfway back toward the nose. Subsequent cuts were then made, in steps of 0.64 cm, until finally the flameholder was restored to its original plain-vee shape, but having half its original width (see Fig. 1). For each configuration measurements were made of pressure loss, aerodynamic blockage, and stability performance, the latter using the water injection technique.

According to Rao and Lefebvre [1] the blowoff velocity of a bluff-body flameholder is given by the relationship

$$U_{BO} = C_s (1 - B_a) (D_c S_L^2 / \alpha_0) \quad (1)$$

where  $B_a$  is the aerodynamic blockage, which is related to  $B_g$ , the geometric blockage, by the expression

$$[1/(1 - B_a)^2 - 1] = 3.7 C_D [B_g/(1 - B_g)^2] \quad (2)$$

Values of  $B_a$ , and hence  $C_s$ , are determined using smoke tracers and photographic techniques.

For conventional Vee gutter flameholders the characteristic dimension for flame stability and blowoff velocity is the gutter width at its trailing edge. For slotted gutters the effective characteristic dimension can be derived by inserting appropriate values of  $C_s$ ,  $B_a$ , and  $S_L$  into Eq. (1), along with the measured values of  $U_{B0}$  and  $\alpha_0$ . It should be noted that although the gas properties  $c_p$  and  $k$  embodied in  $\alpha_0$  are calculated for the mixed gas temperature as measured just upstream of the gutter, the density term in  $\alpha_0$  is based not on the true gas pressure in the duct, which is always close to normal atmospheric, but on the "effective" pressure, which is much lower due to addition of water.

The characteristic dimension of each gutter configuration is shown non-dimensionally in Fig. 2 as the ratio of  $D_c$ , as calculated above, to the width of a plain Vee gutter of the same pressure loss. From inspection of this figure it is clear that the introduction of slots has a deleterious influence on flame stability. This is because the slots increase the surface area to volume ratio of the recirculation zone. As the amount of fresh material entrained into the wake region is proportional to surface area, whereas the ability of the combustion zone to consume fresh mixture is proportional to its volume, then clearly any increase in surface area/volume ratio must increase the chemical loading on the flameholder and thereby adversely effect flame stability. However, this does not fully explain why the gutter described as "2nd cut" in Fig. 1 should be inferior to the 1st and 3rd cuts shown in this figure. This is probably due to the fact that for the "1st cut" gutter the flow recirculation pattern remains basically the same as for the 1st baseline, and the effect of the slots is merely to allow the injection of more material into the recirculation zone. The same is true for the 3rd cut where flame stability is controlled essentially by the 2nd baseline gutter width and the "teeth" produced by the slots have little or no effect on flame stability. However, the effect of the 2nd cut is to create a gutter for which the size of the recirculation zone generated by the teeth is comparable in magnitude to the size of the recirculation zone produced behind the main Vee. Unfortunately these two separate flow recirculations do not compliment each other because their main axes lie at right angles to each other. Rather, the mutual interference induced by these two flow regions tends to impair stability, and this is reflected in a low value of effective characteristic dimension, as shown in Fig. 2. Work is continuing to examine the aerodynamic flow patterns generated behind flameholders of irregular shape in more detail. In the meantime it may be concluded that, for any given values of available flameholder blockage and available pressure loss, the most effective flameholder is one that produces a wake region having the minimum surface area to volume ratio.

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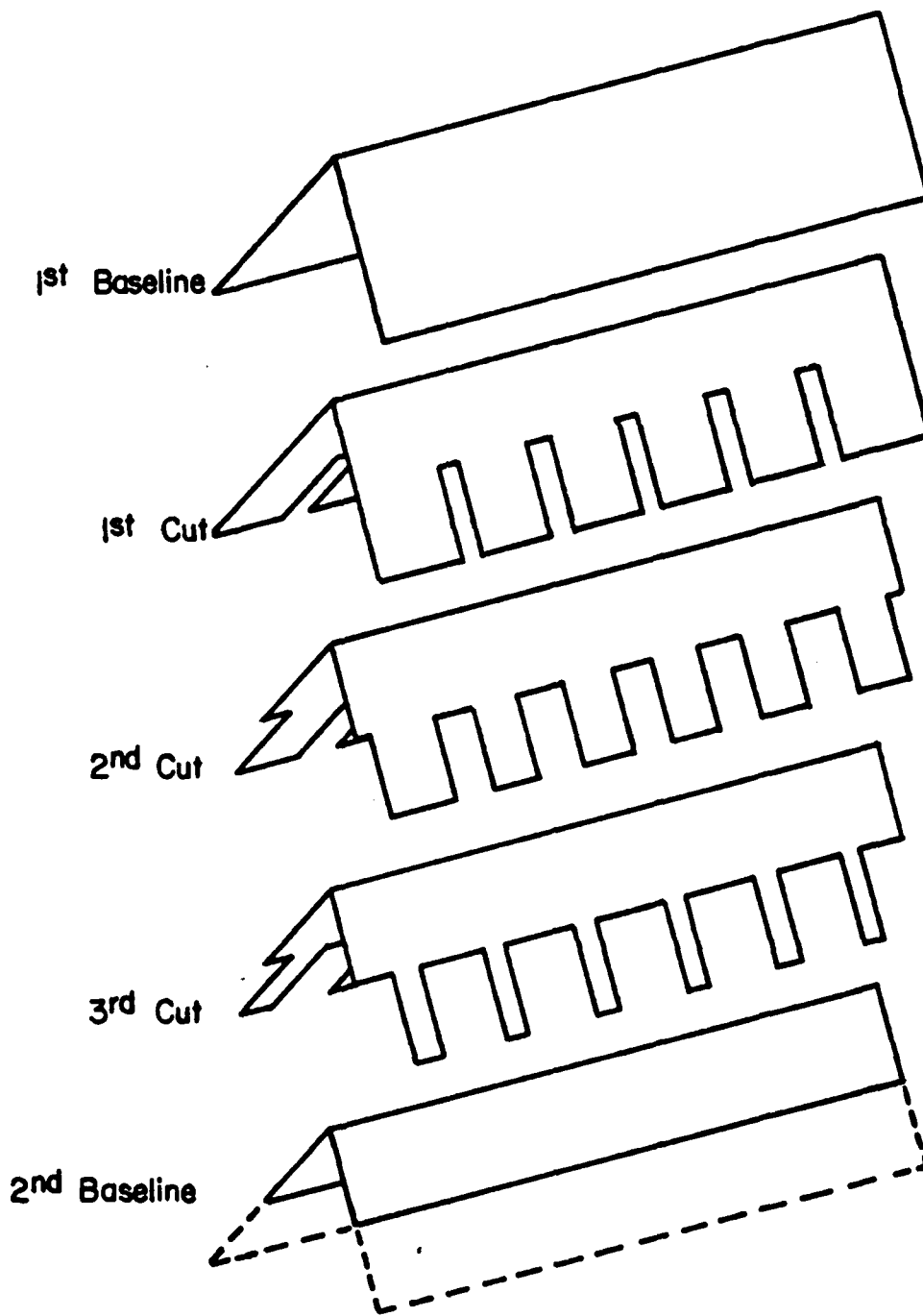


Fig. 1. Various types of Vee-gutter flameholders.



# MIXING AND COMBUSTION OF JET THROUGH PROTRUSION IN CROSS-FLOW

AFOSR Grant 82-0107 (Part III)

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**SUMMARY:** Experimental and analytical-numerical investigations are being conducted on the mixing and combustion characteristics of methane gas jet through wall protrusions in cross-flow of air, both streams at low speeds, in order to establish the influence of geometrical and flow parameters on flame stability and propagation.

## TECHNICAL DISCUSSION

(1) Application: The subject of combustion of fuel jets through protrusions in walls with cross-flow of air is of interest in the design of combustors for gas turbines and ramjets and in fire-related studies associated with fuel tank fires. The principal problem is the determination of the influence of mixing of the fuel jet in the three-dimensional, nonsteady flow field arising in the vicinity of the protrusion and the combustion-flow field interactions.

(2) Current Status:

(A) Experimental Investigations: The test configuration consists of a cavity of dimensions 10x15x60 cm. with the wall protrusion located in the 10x60 cm. wall, as shown in Fig. 1. The cavity is supplied with air flow, velocity ranging over 15-30 m/sec. The Reynolds numbers based on cavity dimensions, protrusion height and jet are of the order of  $1 \times 10^5$ ,  $1 \times 10^4$ , and  $1 \times 10^3$  respectively. The wall with the protrusion has provision for an ignition source that can be moved relative to the protrusion in all three coordinate directions. Transparent walls and (a) a photo-voltaic cell and (b) a thermal sensor are incorporated for observation of flow and combustion fields. The wall with the protrusion has also been instrumented to obtain static pressure distribution over an area of 7x5 cm. with 125 taps.

Several observations may be made from experimental studies.

(i) The flowfield in a rectangular region of dimensions 8x4x4 units of protrusion cross-sectional size is fully three-dimensional with several singularities, recirculation zones and concentrated regions of vorticity. It appears that no closed streamlines exist, although this observation is based on "integrated" planar viewing and recording of flow.

(ii) Considering the top surface of the protrusion, it appears that there is a critical range of the ratio of jet diameter to protrusion cross-sectional size within which the surface includes upstream low pressure regions with strong vorticity concentration. In photographs of smoke trace through a jet of, for example, 6.0 mm. issuing out of a cylindrical or cubic protrusion of cross-section equal to 1.2 mm., it is found that the jet spreads upstream over the surface and there is some entrainment of the jet upstream of the protrusion. When the jet size is about 3.0 mm., no such upstream effects arise.

(iii) The observations from photographs with smoke injection (through a hole of 0.01 cm. located at about mid-height of a 12.0 cm. protrusion) into the upstream

region of the protrusion show the formation of vortices related to the stagnation of the flow, at least one of them clockwise towards the wall and a second counter-clockwise away from the wall. No further discrimination has become feasible and one can only conclude that strong interactions are likely to occur between such vortices, flow pattern generated over the protrusion top surface and the jet.

The flow pattern over the protrusion surface (the two side walls in the case of a cuboid and the cylindrical surface in the case of a circular cylinder) is a function of (a) the local wall boundary layer thickness in relation to the height of the protrusion and (b) the orientation of the protrusion with respect to the streamwise direction in the case of bodies with corners. The influence of secondary flow generated by a corner on the main stream is very significant in the entrainment (of all but small jets) around the protrusion.

(iv) Finally, an attempt was made utilizing a stroboscope to establish a relation between the observed periodicity in vortex structures and the geometrical and flow parameters. The results are given in terms of the frequency of vortex shedding ( $\omega$ ) in the following table.

Protrusion Geometry	$D_j/D_p$	h	$\omega$
circular cylinder	0.250	(a) 0.125; (b) 0.500	(a) 30; (b) 20
	0.750	(a) 0.125; (b) 0.500	(a) 40; (b) 20
cuboid	0.250	(a) 0.125; (b) 0.500	(a) 25; (b) 20
	0.750	(a) 0.125; (b) 0.500	(a) 45; (b) 20

It may be pointed out that the frequency obtained with a protrusion of large height corresponds more nearly to that of a simple jet in cross-flow. The effect of jet diameter on frequency is not clear.

(B) Predictions of Flow Field Interactions: The flowfield in a cavity with a jet through a protrusion in a cross-flow has been analyzed on the basis of three-dimensional viscous flow equations with appropriate boundary conditions. A form of the so-called PHOENICS code has been employed with some modifications to solve the system of equations on a semi-parabolic approach. Details of solution procedure will become available elsewhere.

The coordinate system, the calculation domain and the grid size employed in the numerical solution utilizing a CDC 6600 machine are presented in Fig. 2. It will be observed that a total of 6,888 nodes has been employed in the cavity. The air flow velocity at inlet to the cavity is taken as 30 m/sec. and uniform across the transverse section. The jet is assumed to consist of methane gas issuing into the cross-stream at a velocity of 10 m/sec. The ratio ( $D_j/D_p$ ) and h have been varied in various calculations.

Figure 3 is an example of predictions of iso-concentration regions of methane in five planes surrounding a protrusion of height 0.5 cm.

The broad features of the flow, pressure and concentration fields are clearly obtained. The flowfield features relating to separation and formation of regions of vorticity have not been predicted. The nature of the recirculation zone downstream of the protrusion is reasonably clear. However, the complex flowfield upstream of separate calculation scheme (but again based on 3-d fully viscous flow equations utilizing finite difference procedure) with nearly 200,000 nodes also proved inadequate in this respect. The concentration and pressure distributions are particularly noteworthy from the point of view of ignition and flame stability.

(C) Immediate Plans: (i) Surveys of pressure field in the vicinity of the protrusion will be obtained. (ii) Combustion stability investigations will be completed with the following variables:  $D_j/D_p$ , protrusion shape, and  $V_j/V_c$ , utilizing



the moveable ignitor. (iii) Predictions will be extended to incorporate chemical reaction.

(3) Future Plans

(A) Discussions are being held on the use of quantitative flow visualization technique with laser-induced fluorescence for establishing the three-dimensional concentration field around protrusion. The levels of discrimination and sensitivity required are the central uncertainties.

(B) Several extensions to the predictive scheme are being considered to establish further details of combustion-flow field interactions, especially the vorticity-concentrated regions.

(4) Publications:

S.K. Hong, S.N.B. Murthy and C.F. Warner, "Jet through a wall protrusion in cross-flow," AIAA Paper No. 84-1167, to be presented at the AIAA Propulsion Conference, June, 1984.

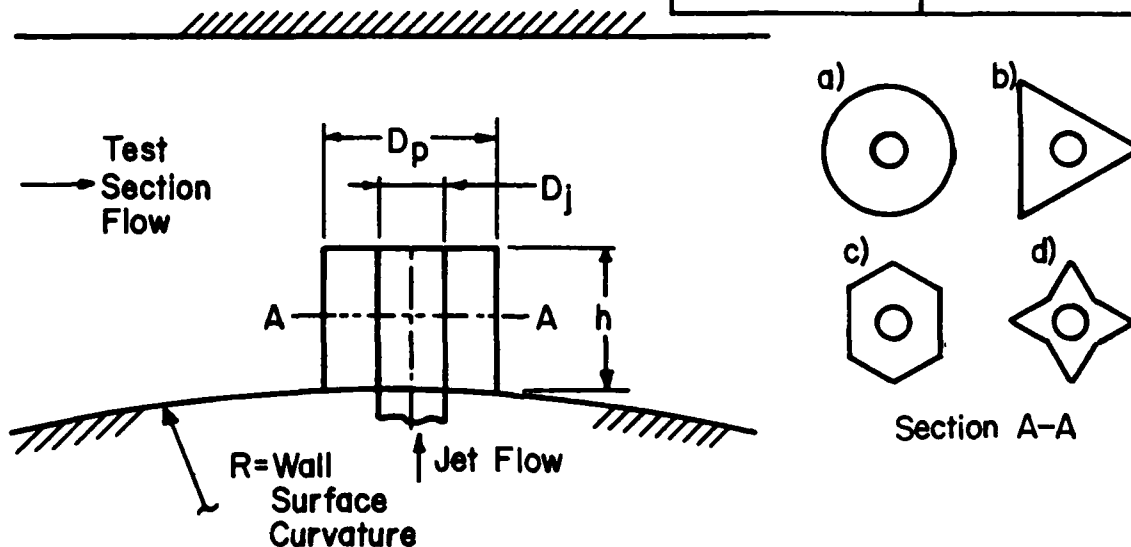
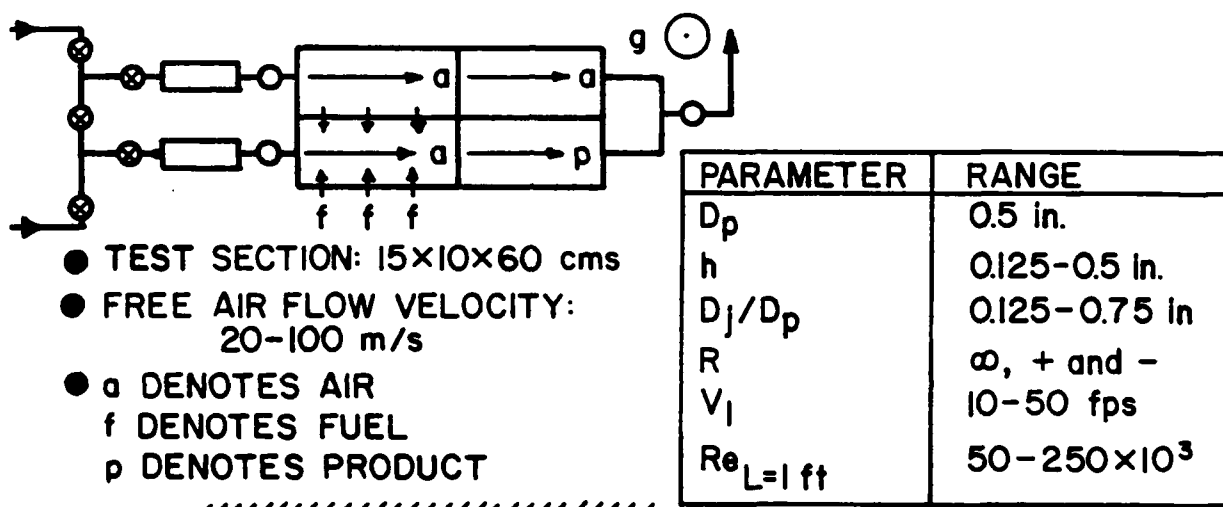


Figure 1.

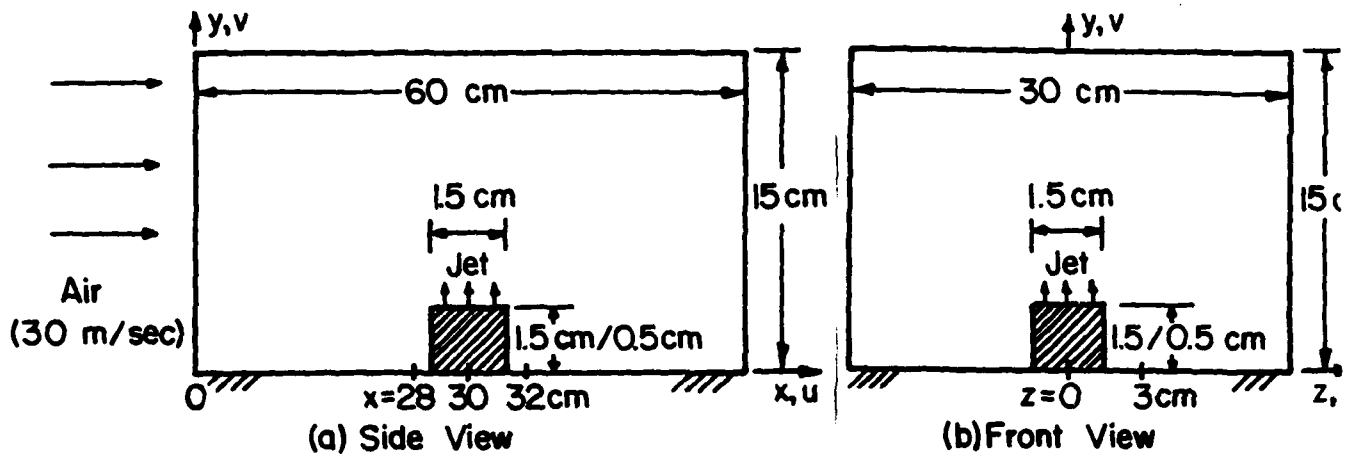


Figure 2.

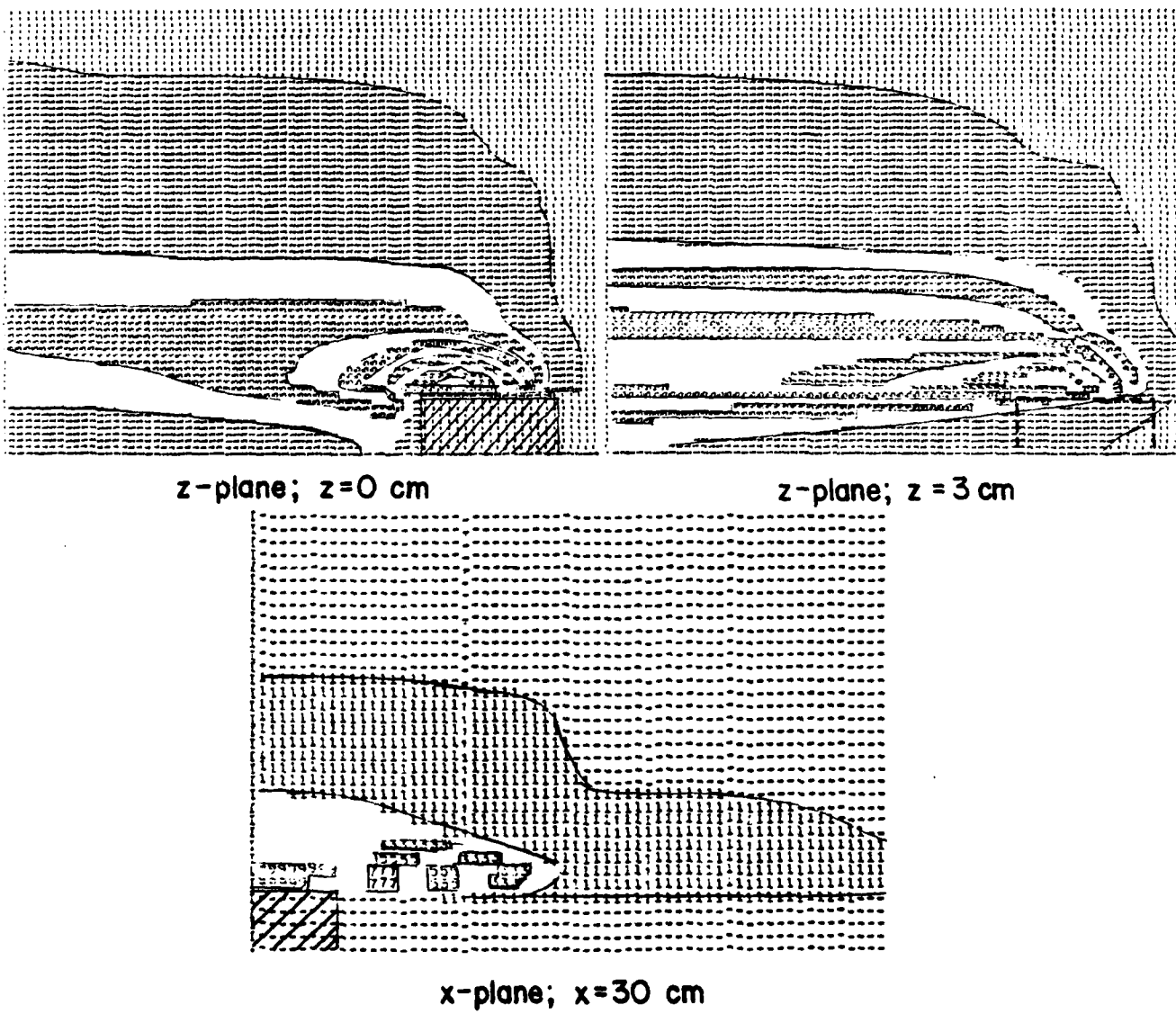


Figure 3.

## EXCIPLEX SYSTEMS FOR REAL TIME VISUALIZATION OF FUEL SPRAYS

AFOSR Grant No. 83-0307

Principal Investigators: Lynn A. Melton and James F. Verdick

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### SUMMARY/OVERVIEW:

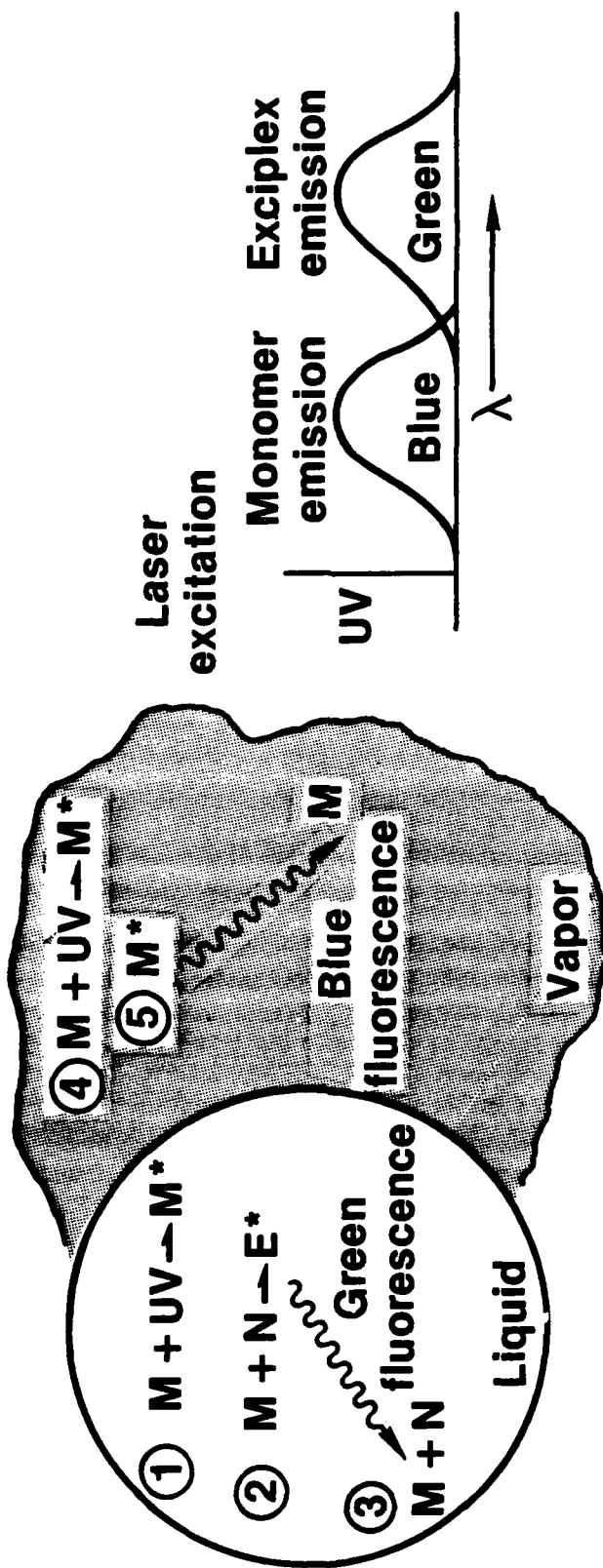
Through the use of laser-induced fluorescence from an organic exciplex doped into a fuel, the vapor and liquid distributions in a hollow-cone fuel spray have been separately photographed and analyzed. The fluorescence signals from the different phases were sufficiently intense to permit color photography, and with the use of high-speed black and white film, ten nanosecond "stopped action" photographs were obtained. This visualization technique can greatly aid our basic understanding of the spray evaporation process, which is fundamental to all liquid-fuelled combustion devices.

### TECHNICAL DISCUSSION

This presentation describes the results of an experimental demonstration which establishes that the spatial distributions of both liquid and vapor phases of the fuel may be visualized simultaneously by means of single-frequency, laser-induced fluorescence which occurs at two widely separated wavelengths from the two respective phases. The fundamental concept, which is the essential feature of this promising technique, is to dope (in low concentration) the fuel with a non-corrosive, organic additive which can form an exciplex in the liquid phase, but not in the vapor phase. Figure 1 schematically illustrates this concept, where the monomer dopant fluoresces in the blue, and the exciplex in the green.

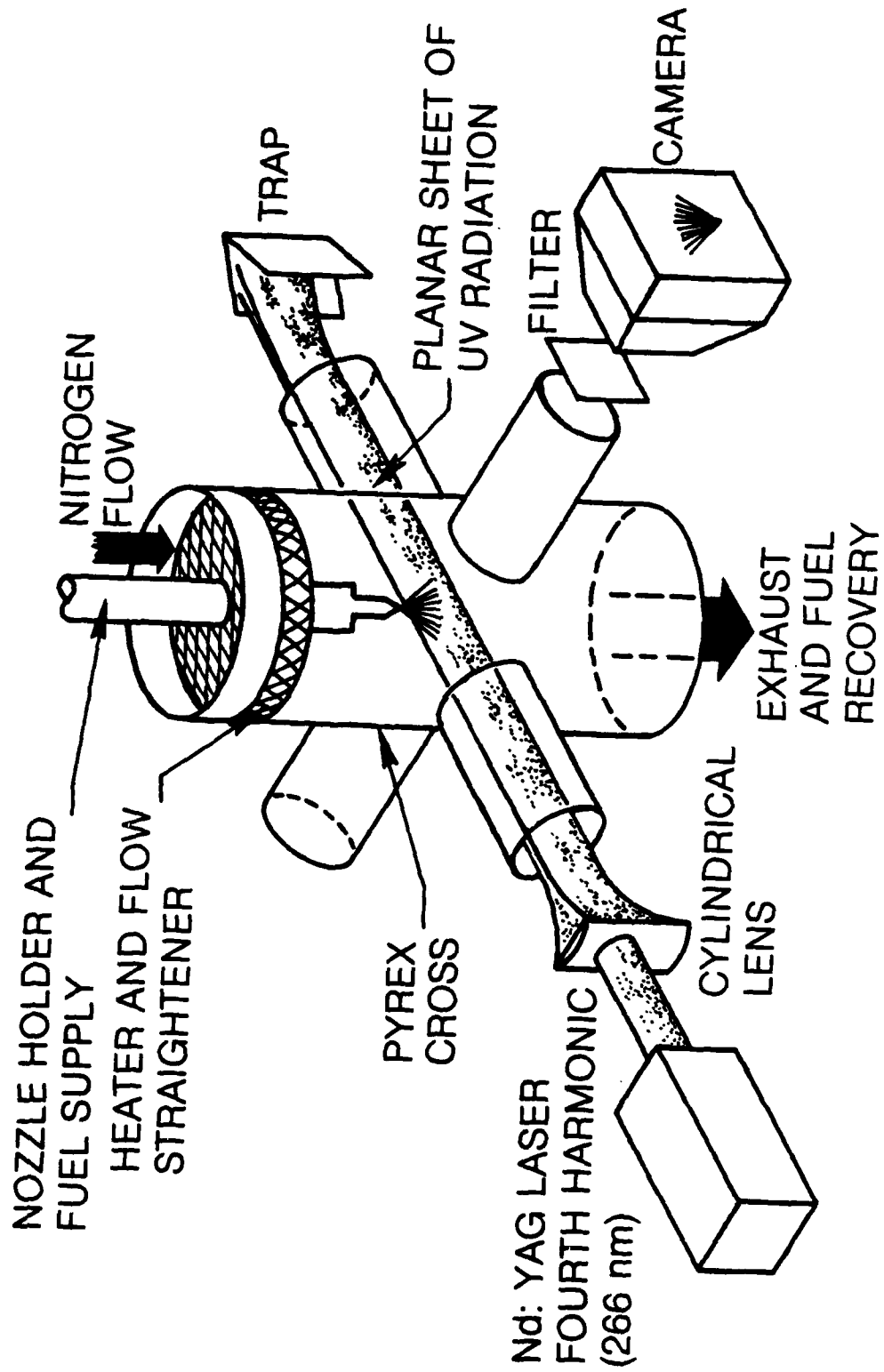
The important features of the experiment are drawn in Figure 2. The conical fuel spray, coflowing with heated nitrogen, is irradiated with a planar sheet of 266 nm radiation (fourth harmonic of a pulsed Nd:YAG laser). The fluorescence induced by this laser beam is photographed at 90 degrees to the beam, through appropriate filters to select the desired fluorescent emission. Color photographs of the combined liquid and vapor spray, liquid alone, and vapor alone will be shown. Single-shot (10 nanosecond pulse duration) photographs are presented in Figure 3. Clearly, the fuel flow is frozen in time in these photographs and the development of the liquid sheet breakup into droplets is evident. More recent analysis of the data present in these photographs, including some semi-quantitative characterization by means of computer generation of density contour maps and three dimensional perspectives will be presented.

# REAL TIME, 2-D SPRAY/VAPOR MONITORING VIA EXCIPILEX FLUORESCENCE



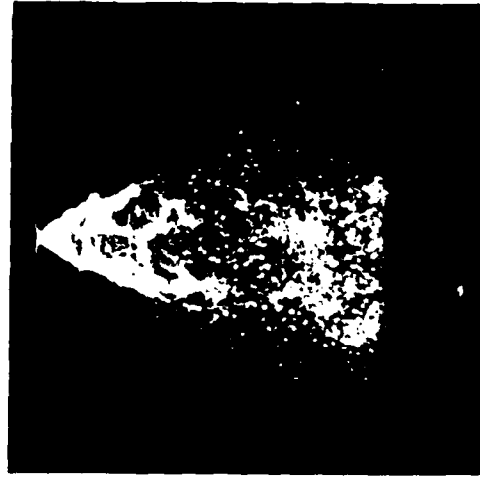
## Concept

- ①, ④ Laser excitation of monomer in liquid or vapor
- ② Exciplex (excited complex) formation, liquid phase only
- ③ Exciplex fluorescence occurs in green
- ⑤ Monomer fluorescence occurs in blue

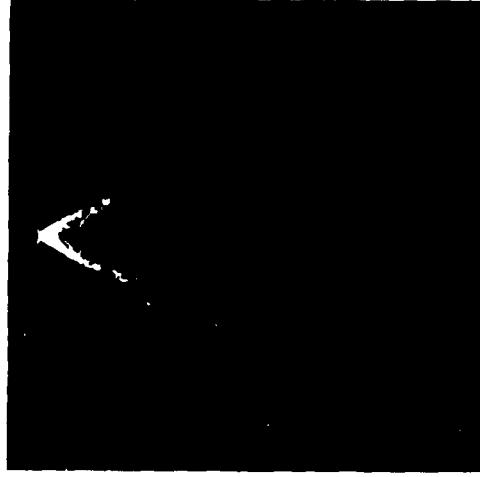


# LASER-INDUCED EXCIPILEX FLUORESCENCE FROM CONICAL FUEL SPRAY

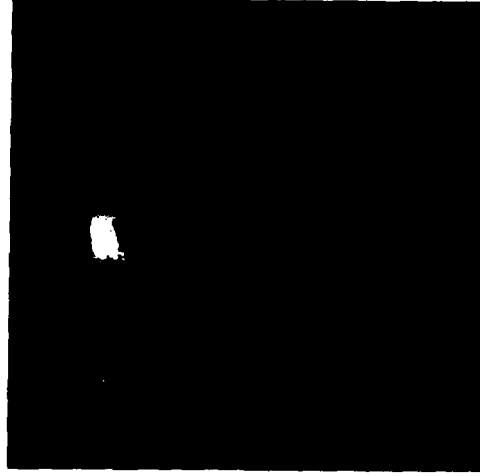
## Experimental results



Liquid and vapor



Liquid only



Vapor only

- Commercial nozzle operating with cetane doped with naphthalene/tetramethyl phenylene diamine (TMPD)
- Single, 10 nanosecond, fourth harmonic (266 nm) Nd:YAG laser excitation
- Two-color fluorescence separated with absorbing glass filters

# VAPORIZATION/FUNDAMENTAL COMBUSTION STUDIES OF LIQUID FUELS

(ONR Contract No. N00014-81-K-0384)

Principal Investigator: Frederick L. Dryer

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## SUMMARY/OVERVIEW:

This program is developing better understanding of the relationship of vaporization/combustion properties of fuels to fuel composition and combustion environment through the study of isolated free droplet vaporization/combustion experiments and bubble nucleation/growth experiments. Present efforts are devoted to:

- 1) determination of the mechanism of liquid phase coking of fuel droplets during vaporization/combustion and its relationship to:
  - a) low volatile and aromatic fractions
  - b) fuel contaminants (heavy metals, sodium, sulfur, oxygen, additives)
  - c) environmental parameters (gas composition, pressure, temperature)
  - d) droplet parameters (Reynold's number, etc.)
- 2) Investigation of the vaporization/combustion properties of distillate-type fuels, fuel components, and fuel emulsions under atmospheric and high pressure, at low and high relative gas convective conditions, and under vaporizing and combusting conditions. Current efforts are addressing the effect of distillation curve properties on vaporization/combustion, droplet generation effects on combustion phenomena, and the effect of relative gas convective on the secondary atomization of water-in-fuel emulsions and binary paraffin solutions.

## PROGRAM OBJECTIVES:

The interaction of combustion performance and emission characteristics of propulsion and other energy conversion systems with the physical and chemical properties of the fuel used empirically defines a range of fuel characteristics over which acceptable operation can be obtained. In the last decade, the supply/demand character of petroleum itself has pointed to difficulties in achieving suitable fuel supply. While reduced overall demand as well as new discovery and increased production have resulted in at least a temporary respite, strategically, the problem remains no less severe. Domestic resources continue to dwindle and more importantly, strongly depend on advanced secondary and tertiary recovery technology which typically result in heavier, more asphaltic and more highly contaminated crudes, larger aromatic content, and a continuing desire to extend acceptable range of fuel boiling point. Finally, although import sources appear more politically stable, the free world countries as a whole appear to remain nearly as susceptible to political manipulation of energy supplies. From a strategic point of view the development and interdiction of synthetic fuel liquids from alternate energy sources continues to be of significant importance.

Improved fundamental understanding of the relationship between vaporization/combustion behavior of fuel liquids, physical/chemical properties of the fuel itself, and the aerodynamic and environmental conditions are an integral part to each of the issues mentioned above. The present program is a continuation of work which has been underway at Princeton to develop new qualitative and quantitative insight to the vaporization/combustion properties of multicomponent, multiphase fuel structures through the study of isolated free droplet phenomena. Earlier free droplet studies were primarily concerned with the secondary atomization phenomena which can be pro-

duced in liquid fuel droplets by internal vaporization of liquid components within the droplet interior. While some effort has continued on this area of interest under this effort, and a parallel program on the combustion behavior and application of secondary atomization technology (through both internal vaporization and explosive chemical decomposition) on slurry fuels has been initiated (AFOSR, Contract No. F49620-82-K-0011) the research under this contract has been primarily interested in developing a better understanding of the relationship of fuel properties to the production of particulate through liquid phase reaction within fuel spray droplets during vaporization. This is a likely source of larger size particulate emissions in high pressure combustion of even mid-distillate range fuel components. While understanding the fundamentals of this issue continues to be important to extending the acceptable fuel specifications of existing and future propulsion systems, it is also technology which is relevant to improvement of gas turbine pattern factor itself, since the burnout of larger particulate matter often defines perceived "flame length" as well as erosion/corrosion. Finally, new efforts recently begun show promise of improving understanding of the effects of pressure and aerodynamic environment (Reynolds Number) on liquid droplet vaporization/combustion phenomena in general.

## RECENT RESULTS

### Liquid Phase Coking Phenomena

The combustion of heavy multi-component oils is characterized by qualitatively similar phenomena when burned in either a suspended or free droplet mode. During the first 40% of the lifetime of a free droplet the droplet burns quiescently. The droplet experiences disruptive burning (swelling of the droplet and ejection of material from the droplet) over the following 30% of its lifetime, after which it burns quiescently. This disruption is believed to be the result of the nucleation of some of the lighter fuel components within the droplet. Then in the final 9% of the droplet burning time the droplet again undergoes disruptive combustion. This second period of disruption is terminated by the appearance of an insoluble coke particle. The burnout of the carbonaceous cenosphere comprises the remainder of the combustion history. Dilution of the residual oil with a more volatile No. 2 fuel oil does not alter the nature of the droplet combustion. Although free and suspended droplets exhibit qualitatively similar combustion behavior, the presence of the solid surface continues to cause some question regarding the value of quantitative results obtained from suspended droplet experiments.

The droplet remains completely soluble in an organic solvent throughout the initial 91% of its lifetime at the end of which an immature coke particle exists. This cenospheric particle contains one or more blowholes and has considerable structural strength although it is still soluble in an organic solvent. It is not until the last 9% of the droplet lifetime that the thermal cracking and condensation reactions which transform the oil into an insoluble material become significant. It is these reactions which account for the ejection of gases from the droplet during the final stages of the droplet combustion. This off-gasing results in the blowholes observed in both immature and mature coke particles.

The mass of a coke particle is directly related to the fraction of heavy oil contained in the initial droplet. Residual oil droplets containing between 0% and 60% No. 2 fuel oil were found to form coke particles whose mass was a constant fraction of the mass of heavy oil in the initial fuel. For the residual oil employed, this conversion factor was approximately 3%. The addition of the more volatile No. 2 fuel oil to the residual oil serves only to reduce the fraction of heavy oil in the fuel. It has no apparent effect on the liquid phase pyrolysis of the heavy oil through a change in the droplet temperature history.

The fraction of heavy oil converted to coke is not influenced by the initial droplet diameter for droplets initially between 260 and 600 microns in diameter. Coke was observed to form within the last 9% of the droplet's lifetime i.e., within 10 to 20 msec. It is not likely that the conversion of oil to coke will be influenced by



the initial droplet diameters until droplets with burning times of this order are encountered.

It is not sufficient to correlate the relative coking tendencies of various oils strictly on the basis of asphaltene content. The contribution to the mass of the coke particle from the maltenes may vary among different oils and it can be significant. In the experiments reported here approximately 40% of the mass of the coke particle was attributable to the maltenes. Therefore correlations based solely upon asphaltenic content may be misleading.

The direct dependence of coke particulate production on the fraction of heavy ends in the fuel implies that practical combustors operating on heavy oils will necessarily form coke particles. Dilution of the oil with a lighter component or improved atomization, while changing the fashion in which the coke is distributed, will probably not change the mass of the coke formed in the combustion of a given amount of heavy oil. It does not seem possible to eliminate the formation of coke particles. However, it is possible to reduce the emission of these particles. This may be accomplished by enhancing the burning rate of the coke so that the particles are consumed within the combustor. Techniques such as the dilution of the heavy oil with a lighter component, improved atomization and the addition of water as an emulsion to the oil increase the surface area of the coke and hence its mass burning rate. The addition of organometallic compounds to the oil is also known to increase the mass burning rate of coke. However, it is important to remember that these approaches depend upon improving the rate of combustion of the coke and not on the suppression of coke formation. As a result they all require that the coke particles have a sufficiently long residence time in the hot environment of a combustor operating with excess air.

#### Effects of Aerodynamics and Pressure on Droplet Vaporization/Combustion

In the past several years, there has been much discussion of the effects of gas droplet relative velocity and environmental pressure on the vaporization and combustion characteristics of droplets. In the case of multicomponent fuels, high relative gas-droplet velocity has again been suggested by Law (1) to drive the interior of the droplet to be homogenous in chemical composition, i.e., the droplet would behave as a small batch distillation system. Since the droplet interior temperature can never exceed the surface temperature, and the surface temperature will increase only as the more volatile components are depleted from the drop. Under such conditions, the interior of the droplet can never reach a condition for nucleation and internal vaporization, and only explosive decomposition would remain as a plausible mechanism for producing secondary atomization. However the thermal ignition temperature of the compound would for the same reasons be limited to temperatures well below its saturation temperature, or otherwise the compound would be depleted by vaporization before it could decompose. On the other hand it has been proposed that large gas-droplet velocity results in the development of a Hill's vortex circulation within the droplet. Sirignano and his collaborators have pursued this hypothesis theoretically, and have also produced observations of high convection effects on (low temperature) vaporization of multicomponent droplets (2). The basic result of such a proposal is thought to result in rapid internal heating of the droplet through internal convection, but regions of the interior for which mass diffusion still partially govern the depletion of the more volatile components remain. The experimental work performed in this laboratory under this contract are the first experimental observations known to the principal investigator on the effects of high gas-droplet relative velocity on isolated droplet combustion phenomena.

The existence of disruptive behavior for multicomponent fuel droplets subjected to high relative gas-droplet velocities has been conclusively demonstrated. In particular, detailed observations on the combustion behavior of isolated free droplets of a 50 vol. % hexane/5- vol. % hexadecane solution revealed a preferential direction of ejection of liquid from the droplet shoulder normal to the droplet motion ("shoulder oriented disruption"). Time from ignition-to-disruption was observed to be decreased

substantially (by about a factor of 4) by imposing a high relative gas droplet velocity approaching 20 meters per sec. Furthermore, the fractional increase in ignition-to-disruption times due to larger initial droplet size was found to be significantly less for a highly convective environment as compared to a stagnant environment.

Observations are entirely consistent with the vortex model description for the droplet interior set forth by Sirignano et al. and refute the plausibility of a "well mixed" or "rapid mixing limit" description suggested by other investigators. Moreover, micro-explosive behavior of water-in-n-hexadecane emulsified free-droplets for high relative gas-droplet velocity conditions, has been experimentally established. The occurrence of micro-explosive combustion of these emulsified fuels despite the more readily available supply of water particles to the droplet surface as a result of the internal convective motion, indicates that water and fuel are not vaporizing independently of each other.

A reduction of the ignition-to-micro-explosive-event-time was observed when subjecting the emulsified droplets to a strong convective atmosphere. For the low (9 vol. %) water content emulsion the distributed disruption collapsed into one micro-explosive event under high relative velocity conditions. The absence of any apparent penalties in the existence and violence of the micro-explosive event of the emulsified fuels considered here, warrants the consideration of these fuel types for practical applications.

#### FUTURE WORK

Further work under this program will address the following three general areas: complete some additional studies on secondary atomization phenomena, including the nucleation character of multicomponent solutions. Continue and extend the existing efforts on the liquid phase coking of multicomponent fuels. Investigate the effects of aerodynamics and pressure on the vaporization/combustion characteristics of multicomponent and multiphase fuel droplets.

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## ORGANIC AZIDES AS JET FUEL ADDITIVES

(ONR Contract No. N00014-83-K-0207)

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### SUMMARY/OVERVIEW

The present program aims to (1) synthesize and formulate organic azides and their solutions/emulsions with pure fuels and fuel blends; (2) determine their thermochemical properties; (3) quantify and maximize the droplet burning intensity of these azido fuels, especially the potential of droplet micro-explosion through internal decomposition; and (4) provide guidance for their optimum chemical structure and mixture composition for enhanced combustion in compact ramjets. Preliminary experimental results on azido- and diazido-alkanes show significantly reduced droplet lifetime due to faster droplet burning rates as well as earlier onset of micro-explosion. These beneficial effects, however, are reduced when they are mixed with conventional hydrocarbon fuels. Analytical modeling and in-depth understanding of the governing physico-chemical phenomena are also temporarily handicapped by the lack of essential thermochemical data of these azides.

### TECHNICAL DISCUSSIONS

The present program was initiated with the suggestion that the potential to achieve and intensify micro-explosion of droplets of jet fuels can be significantly enhanced through the addition of small quantities of organic azides, which upon heating will decompose to release heat and  $N_2$ . The occurrence of micro-explosion shortens the droplet lifetime, promotes mixing, and facilitates the complete gasification of broad-specification fuels.

Two series of experiments are being conducted simultaneously. The first studies the vaporization, combustion, and micro-explosion of free droplets of azido fuels in a high temperature, normal or high pressure, oxidizing or inert environment; schematic of the apparatus is shown in Fig. 1. The second measures the droplet temperature at micro-explosion by immersing the test droplet in a heated glycerin column with an upwardly-oriented positive temperature gradient through which the droplet slowly rises due to buoyancy; schematic of this apparatus is shown in Fig. 2.

For the organic azides tested, the present investigation shows that the addition of azides in conventional hydrocarbon fuels enhances the intensity of micro-explosion, although the instant of its occurrence is only slightly advanced. This is due to the unexpectedly high micro-explosion temperatures of these azido mixtures. We are currently exploring possibilities of modifying the mixture properties to facilitate the onset of micro-explosion.

Testings involving droplets of pure azides show dramatic reduction in the

droplet lifetime and thereby enhancement of the burning intensity. This is accomplished by the significantly faster droplet burning rates and sometimes earlier occurrence of micro-explosion. Preliminary results also indicate that azido-alkanes and diazido-alkanes have different combustion characteristics. That is, droplets of azido-alkanes tend to burn quiescently while those of diazido-alkanes exhibit severe distortion followed by micro-explosion. A probable explanation for this difference could be that the decomposition temperature is higher than the boiling temperature for azido-alkanes but is lower for diazido-alkanes.

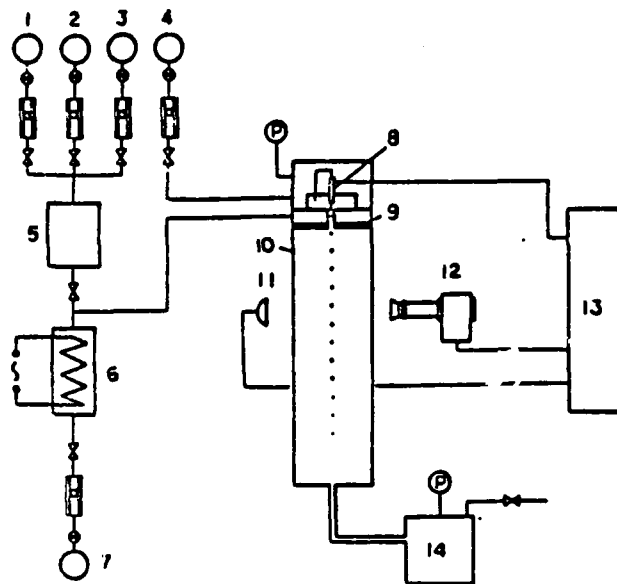


Figure 1

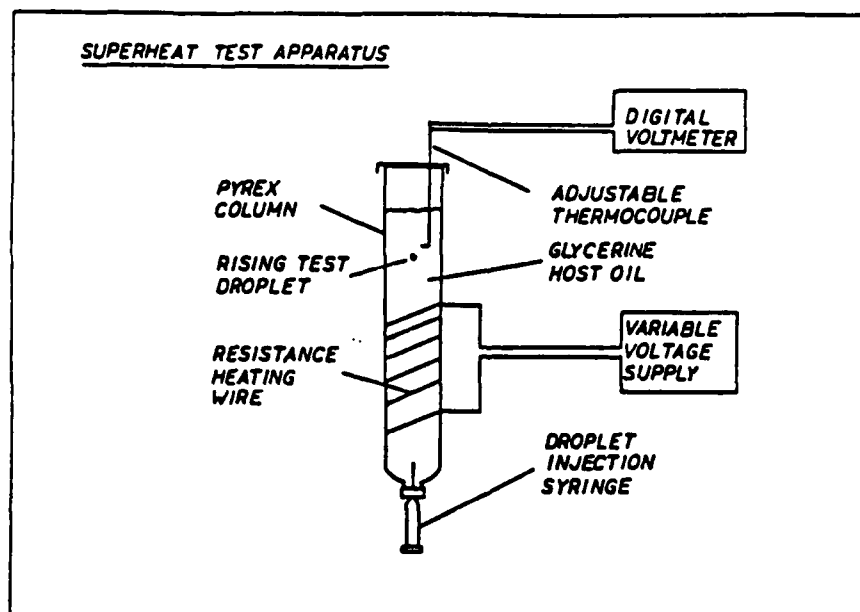


Figure 2

## PARTICLE AND VAPOR MASS TRANSPORT THROUGH NON-ISOTHERMAL COMBUSTION GASES

AFOSR Grant No. F49620-82K-0020

Principal Investigator: Daniel E. Rosner

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### SUMMARY/OVERVIEW\*:

The performance of gas turbine (GT) engines in dusty atmospheres, at very high turbine inlet temperatures, or when using jet fuels from non-traditional sources (e.g., shale, or coal-derived), and the performance of ramjets burning slurry fuels (leading to condensed oxide aerosols), will depend upon the formation and transport of small particles across non-isothermal combustion gas boundary layers. Moreover, even engines burning "clean" fuels can experience soot formation/deposition problems, including combustor liner burnout, accelerated turbine blade erosion and "hot" corrosion. Accordingly, our research is directed toward providing propulsion systems design engineers with quantitative information on important interfacial rate processes at high temperatures.

An interactive experimental-theoretical approach is used to understand and develop rational engineering correlations of performance-limiting chemical, and mass/energy transfer phenomena at interfaces. This includes the development and exploitation of laboratory flat flame burners (see, e.g., Fig. 1), and flow-reactors, along with novel diagnostic techniques. Resulting experimental data, together with the predictions of comprehensive asymptotic theories, are then used as the basis for proposing and verifying simple viewpoints and effective engineering correlations.

### TECHNICAL DISCUSSION

The dominant role of thermophoresis (particle drift down a temperature gradient) in determining the deposition rate of submicron particulate matter from combustion gases<sup>1,2</sup>, has recently been demonstrated in our laboratory by using three independent "real-time" experimental methods:

1. small thermocouple (TC) response to the amount of deposit<sup>3</sup>
2. laser-reflectivity (LR) of deposition target<sup>4</sup>
3. laser-scattering from surface deposit (LSSD).

Here we focus on methods 1. and 3. (applied to carbonaceous soot), which we have developed since the 1983 Contractors' Meeting. Each of these experimental techniques has been applied, to date, under conditions of low particle mass loading<sup>1</sup>, and negligible particle inertia<sup>5</sup>. We conclude with a brief description of our recent theoretical results on particle mass transport across non-isothermal combustion gas turbulent boundary layers<sup>6</sup>.

When a TC bead is immersed in soot-laden combustion products (say, downstream of a water-cooled flat-flame burner) soot deposition mass fluxes can be inferred

\* 1984 AFOSR/ONR Contractors Meeting on Combustion, 20-21 June, 1984, Pittsburgh, PA.

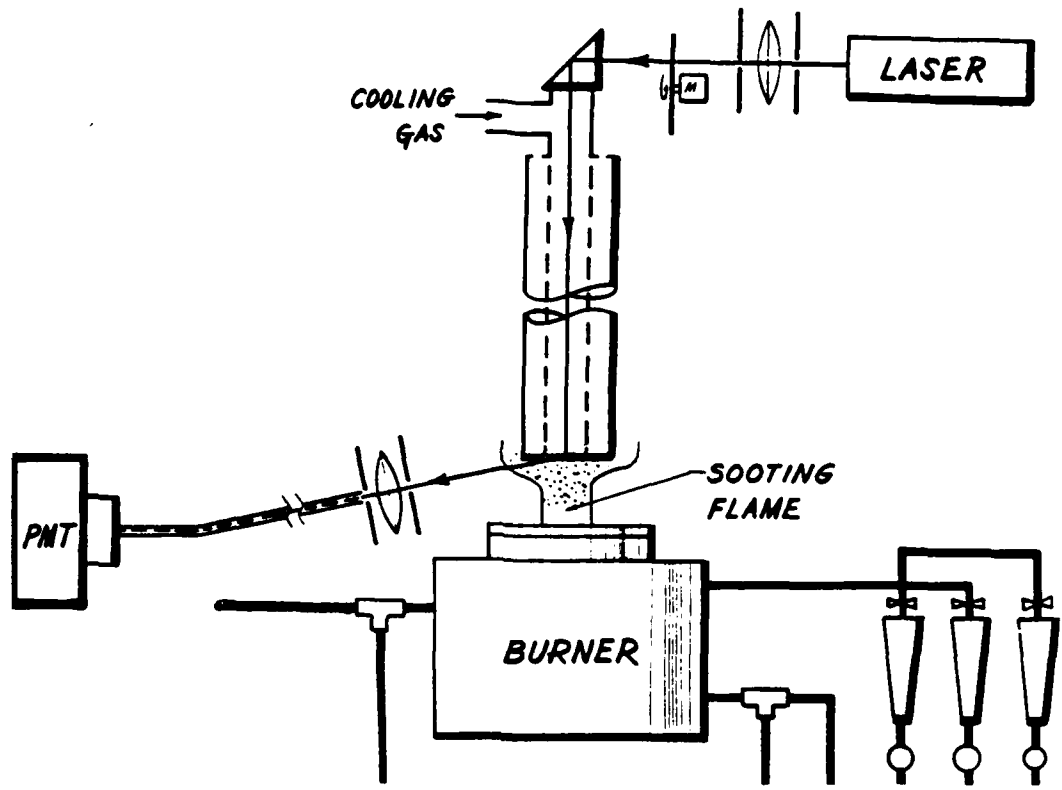


Fig. 1

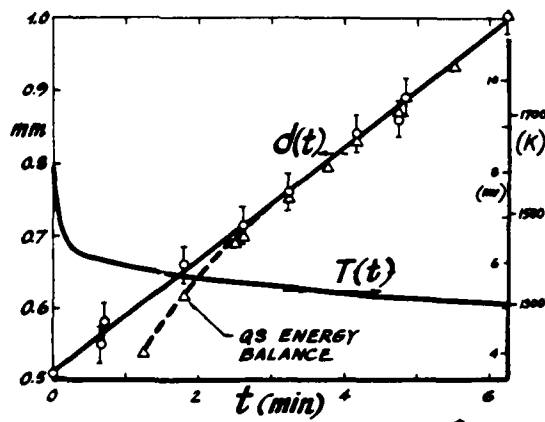


Fig. 2

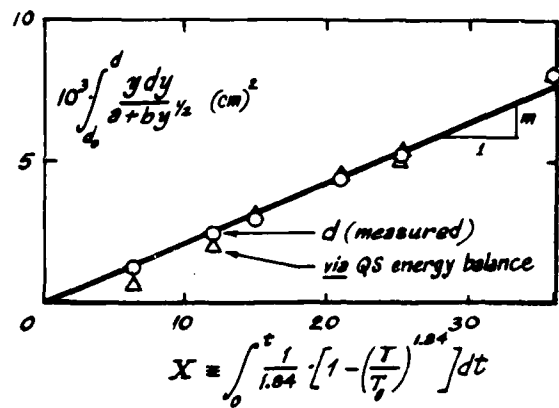


Fig. 3

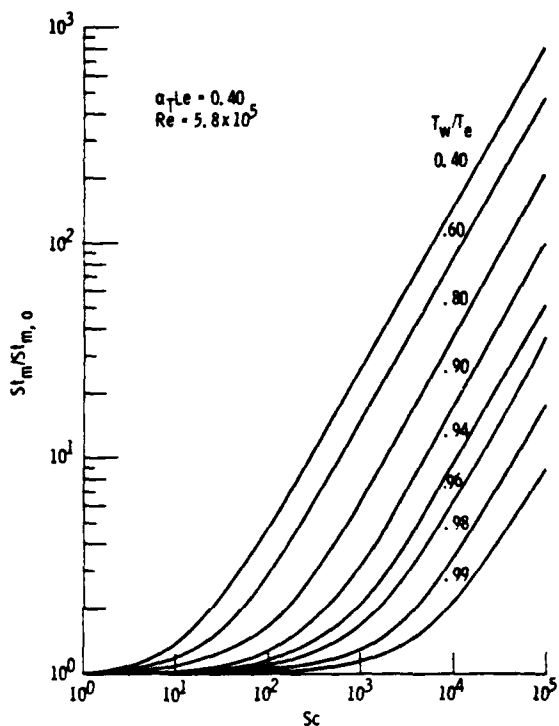


Fig. 4a

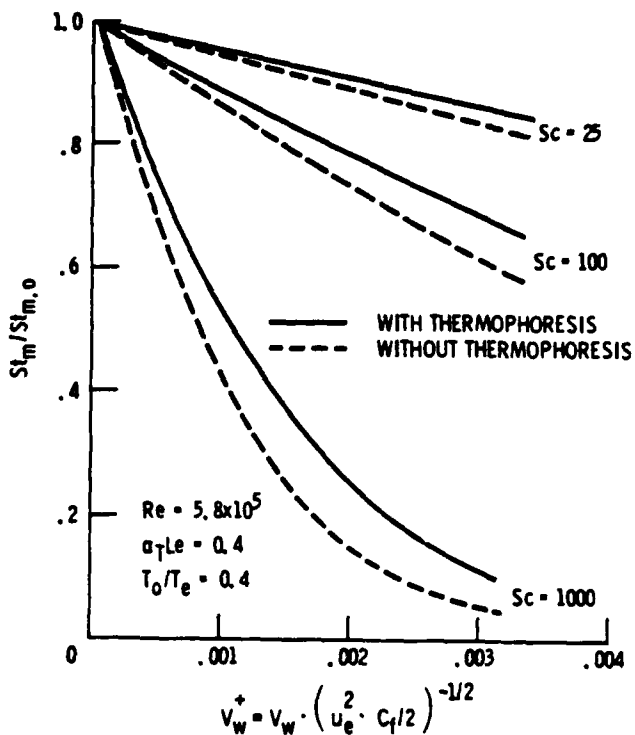


Fig. 4b

photographically, as well as estimated via a quasi-steady energy balance and the TC bead's thermal response to the growing deposit (Fig. 2). Our results have been compared to a theory of particle thermophoresis in the gas thermal boundary layer (BL) surrounding the TC target; a theory which suggests straight line plots (Fig. 3) whose slope should be proportional to the local soot volume fraction. When the TC bead is immersed in a series of different soot-laden flames its response indeed correlates with the flame soot-loading, as inferred via our in situ laser beam extinction measurements. We conclude that:

a) observed soot deposition mass fluxes are several orders-of-magnitude greater than those expected based only on Brownian (concentration) diffusion at the prevailing Reynolds numbers

b) knowing the particle size-insensitive thermophoretic diffusivity, the local soot loading can be obtained via the slopes of linear plots (cf. Fig. 3) constructed exclusively from our experimental thermocouple temperature response information. Accordingly, this technique should be useful in probing three-dimensional combustor flows, in which the application of line-of-sight laser techniques is inadequate

c) the dependence of soot deposition rates on the temperature "contrast" between the gas and target is in accord with proposed thermophoretically dominated mass transport theory (cf. straightness of data points in Fig. 3)

d) the behavior of submicron soot particles in non-isothermal combustion products is strongly influenced by thermophoresis, with important implications for understanding rates of soot nucleation, growth, coagulation, burnout and deposition.

A new laser probe method has been developed to measure the intensity of light scattered from particles depositing on an immersed transparent gas-cooled (back side) sapphire disk (see Fig. 1). This LSSD method, which we find to be extremely sensitive to the amount of material deposited, enables us to study the effects of thermophoresis at  $T_w/T_e$ -values much lower than 0.7 (previously studied using our reflective Pt-ribbon targets (method 2)). Although these experiments are in progress, our preliminary evidence for soot acquisition on the target surface is consistent with the abovementioned conclusions concerning the dominance of thermophoretic particle transport.

We have also extended the underlying mass transfer boundary layer theory to include the important case of turbulent dusty-gas boundary layers on transpiration-cooled surfaces<sup>6</sup>. For impermeable surfaces (cf. Fig. 4a) even the slightest temperature contrast (e.g., wall temperature only one percent less than mainstream temperature) is associated with order-of-magnitude increases in the convective mass transfer coefficient for particles with Schmidt numbers greater than  $10^5$  (ca.  $d_p > 0.2 \mu\text{m}$  particles). However, thermophoresis reduces, but by no means eliminates, the fouling rate protection offered by transpiration using a dust-free cooler gas (cf. Fig. 4b). This "effusion" technique can therefore be used to minimize particle deposition within cooled combustion gas sampling probes.

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NUMERICAL AND EXPERIMENTAL STUDIES OF INJECTION,  
ATOMIZATION, IGNITION AND COMBUSTION OF LIQUID  
AND SLURRY FUELS IN HIGH-SPEED AIR STREAMS

AFOSR Grant 82-0159B

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SUMMARY:

Transverse injection of liquid or slurry jets into high speed airstreams finds application in several propulsion systems. For supersonic air flows, these include thrust vector control and external burning as well as scramjet engines and for subsonic airstreams, "dump" combustors and afterburners, in addition to conventional ramjets. All these cases involve physical processes associated with gross penetration, jet breakup and atomization, and some involve chemical processes. The numerical studies at VPI are examining the effects of ignition and combustion on jet break-up. The experimental investigations are concerned with the unsteady features of atomization using a charge-coupled-device (CCD) and the important question of the distribution of injectant mass across a spray plume cross-section.

TECHNICAL DISCUSSION:

The experimental studies of injection across high speed streams are run in the 23 cm x 23 cm wind tunnel at Mach 3.0,  $P_t = 4$  atm. and  $T_t = 300$  K. One important feature of the flow that we have studied is the distribution of injectant mass across the spray plume at a given downstream station. The method of measurement is to withdraw timed samples through an aspirated probe. Both liquids and slurries have been considered. Detailed results were presented in AIAA Paper 84-0041. Figure 1 here shows the distribution of liquid injectant to air mass ratio across the spray plume at  $x/d = 30$ . It can be seen that the flow over most of the plume cross-section is very fuel rich indicating problems for efficient combustion. Figure 2 shows some results for injection of an initially 30% loaded slurry jet. The local loading increases smoothly in the  $+z/d$  direction from  $z/d = 2$  to 10 then jumps sharply at  $z/d = 12$  to almost triple the value at  $z/d = 2$ . This increased loading is due to the heavier particles following paths with greater radii of curvature due to their greater inertia and thus separating from the liquid plume consistent with our visual observations. Perhaps unexpectedly the same phase separation was noticed side-to-side in the  $y/d$  direction at  $z/d = 2$  and 10. Our numerical work is based upon the volume-of-fluid (VOF) extension of the marker-and-cell (MAC) method developed at Los Alamos. We have previously extended that work in various directions. The complex effects of rapid mass transfer and the attendant high heat transfer at a liquid/gas interface have been included. This involved significant additions and modifications to the basic equation system and the interface boundary conditions. Recently, we have included models of ignition and finite-rate chemistry to enable studies

of the effects of those processes on jet break-up. The details are given in AIAA Paper 84-1180. One representative result is given here as Fig. 3. Lastly, the spray plume created by the cross-stream injection of a liquid jet is characterized by time dependent motions over a range of characteristic frequencies associated with liquid column fracture, clumb break-off and plume "whipping", etc. Some of these motions were quantified by our work this year. Complete details are in AIAA Paper 84-1319. High-speed measurements of the droplet size distribution were made using the Fraunhofer diffraction technique in conjunction with a CCD solid state video camera. Details of the periodic fluctuations in the droplet size distribution at various plume locations were obtained. The period of these oscillations centered around 1 msec although much variance was noted. The oscillations were characterized by the relatively brief occurrence of large droplets in the plume. Downstream of the jet breakup, the severity of the fluctuations declined markedly as the jet became atomized. One set of results is shown in Fig. 4 for a 2.5 msec sample time. This time produced the largest fluctuations in the distribution profiles. Three sets of distributions are shown. The sets were taken 3 seconds apart; the distributions within each set were measured at time intervals of 2.5 msec. At some instants, only 1% of the droplets were in the 7-15 micron bin, with 53% in the 20-35 micron group and 25% larger than 40 microns. During the other extreme, 41% were in the 7-15 micron bin, while 24% and 12% in the 20-35 and 40-100 micron groups respectively. In some cases, the three major groups can be readily identified (Fig. 4a); at other times the divisions become blurred (Fig. 4b).

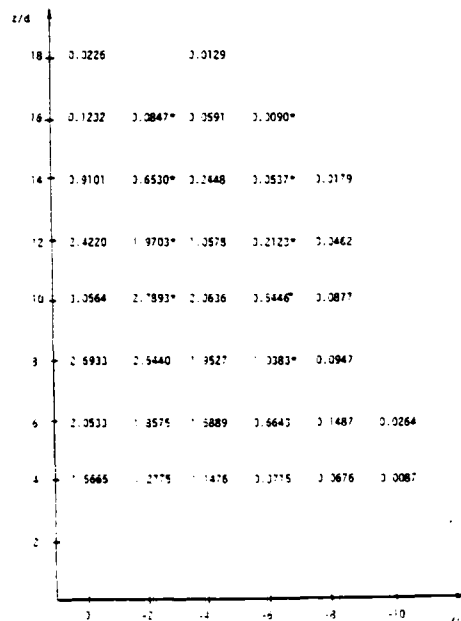


Fig. 1 - Deduced liquid injectant to air mass flux ratios at  $x/d = 30$ .

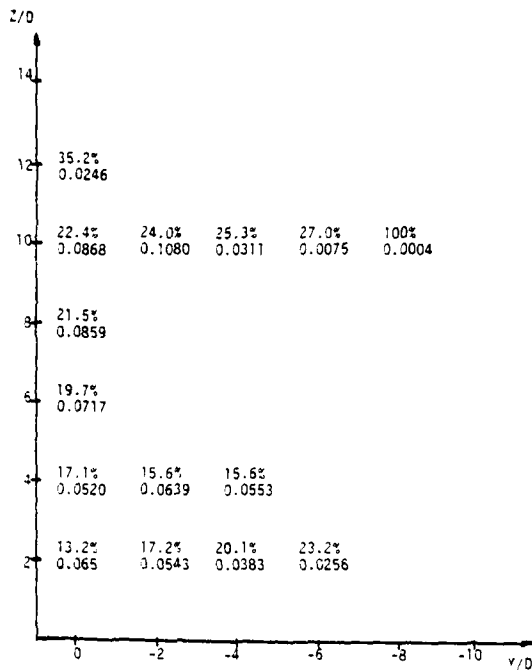


Fig. 2 - Local total (solid plus liquid) mass flux values and local loading (in percent) for slurry jet injection at  $x/d = 30$ .

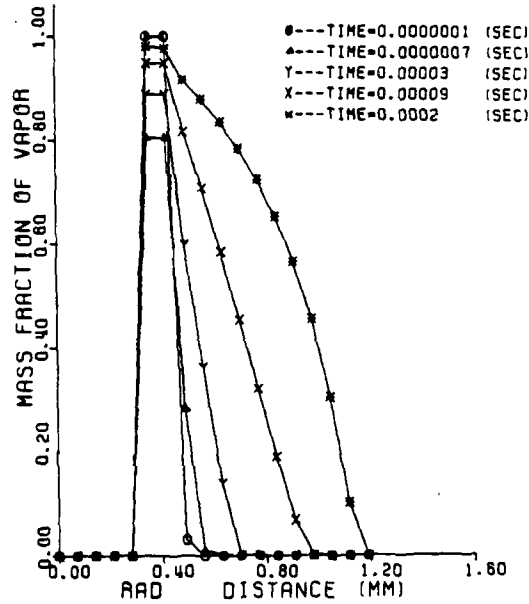
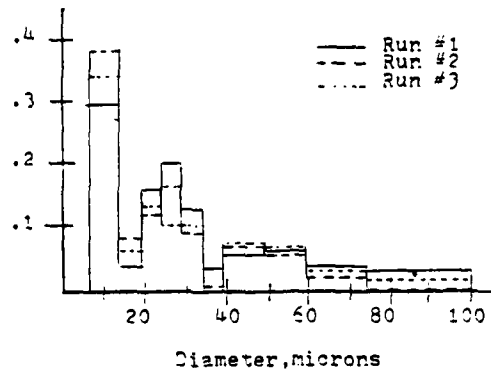
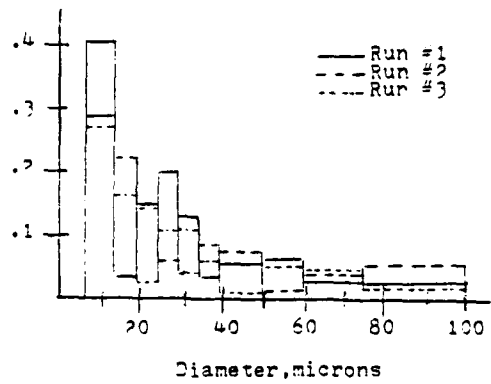


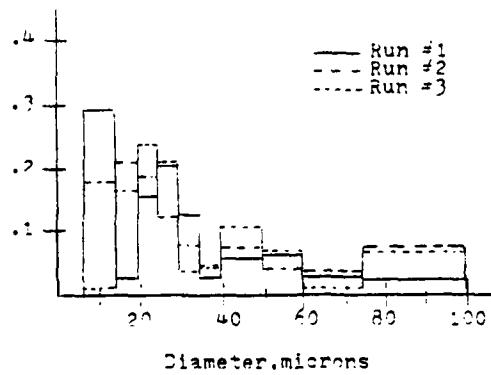
Fig. 3 - Fuel vapor concentration profiles in the radial direction out from the trough at various times with combustion.



a



b



c

Fig. 4 - Variation of droplet size distribution as a function of time.  
 $x/d = 24$ ,  $z/d = 12$  and  $\bar{q} = 12$

# MECHANISMS OF EXCITING PRESSURE OSCILLATIONS IN RAMJET ENGINES

AFOSR-80-0265

Principal Investigators: F. E. C. Culick  
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## SUMMARY/OVERVIEW:

In order to sustain large amplitude pressure oscillations in fluid dynamic systems, a source of energy is required to replace energy lost from the acoustic field due to various mechanisms. In combustion chambers, this requirement usually means that the heat released in the combustion process must have a periodic component which has the appropriate phase relationship to the pressure fluctuations. Our understanding of combustion instabilities in air breathing propulsion systems is poor principally because we do not understand how the acoustic field interacts with the combustion process to produce this feed back of energy to the acoustic field. The purpose of the theoretical and experimental work being carried out under this contract is to obtain an understanding of the important mechanisms by which this feedback can occur. Once this understanding is in hand, strategies for eliminating combustion instabilities in air breathing propulsion systems can be developed in a rational manner.

## TECHNICAL DISCUSSION:

### I. EXPERIMENTAL STUDIES OF COMBUSTION INSTABILITIES

The experiments are being carried out in a simple burner which is supplied with a premixed, prevaporized fuel-air mixture. The burner is a straight duct with a bluff body flameholder and the flow is two-dimensional. When the combustion is stable, the flow in the shear layer produced by the flame holder has many of the well known characteristics of isothermal shear layers such as the small scale vortices which grow by pairing and move down stream at some fraction of the gas speed. In our system, the shear layer is not visibly affected by the presence of strong pressure oscillations in the system which do not produce a large velocity fluctuation at the flame holder lip.

In contrast, when the combustion instability occurs, a pressure oscillation is present in the system which does have a large velocity fluctuation at the flame holder lip. Large vortices are formed in the shear layer near the flame holder lip with the same frequency as the large velocity and pressure oscillations. They

grow rapidly as they drift downstream with a velocity which depends on the amplitude of the fluctuations. Thus, the instability mechanism is not directly associated with the vortical structures present in a normal shear layer. Rather, we believe that the self excited oscillations result from a coupling between the vortex production mechanism, i.e., the velocity fluctuation at the flame holder lip which accompanies the pressure fluctuation, and the nonsteady heat addition produced by time dependent combustion in the vortex.

The general objective of the experimental part of this program is to obtain a better understanding of this combustion phenomena in as general a manner as possible. Although the systems used in this study is a simple model of a dump burner configuration, such as that which would be used in a ram jet system, we believe that the experiments will lead to a fundamental understanding of an important, unsteady combustion process and will be generally applicable to many combustion system.

The experiments are being carried out in a small blowdown facility and the combustion chamber is a rectangular duct 2.6 cm high, 7.6 cm wide and from 40 to 100 cm long. The flame holder spans the 7.6 cm dimension of the chamber and vycore windows on the 2.6 cm sides allow observation of the two-dimensional flow. Instrumentation includes time and space resolved measurements of the pressure and the intensity of radiation from the flame. Flow visualization techniques include the use of shadowgraph photographs with either single photographs obtained with a microsecond duration spark light-source or high speed movies.

Experimental parameters include the velocity and fuel-air ratio of the mixture entering the combustion chamber, the geometry of the system and the fuel type. Changes in the geometry and acoustic damping of various parts of the supply system allow us to change the natural frequencies of the acoustic modes of the system and thereby determine the response of the combustion process to pressure perturbations over a range of frequencies between 200 and 500 hz.

Simultaneous measurements of fluctuations in radiation intensity and pressure, obtained at a number of positions in the duct, have been coordinated with shadowgraph photographs of the flame taken at the same time. Based on this information we have obtained a good qualitative picture of the interaction between pressure and heat release fluctuations, and we are in the process of developing a quantitative description of the elements of the instability mechanism. The dependence of the process on the fuel properties and the fuel-air ratio of the mixture is also under investigation.

Some of our current conclusions are: First, the processes involved in the formation, growth and motion of the large vortices formed in the shear layer are important features of the instability mechanism. The rate of growth and the velocity of the vortices in the downstream direction depend on the magnitude of the pressure oscillations and only weakly on the mean gas speed at

the flame holder lip. Second, large amplitude acoustic disturbances are most easy to excite at one of the acoustic modes of the system, and the mode selected by this instability is one which produces a large amplitude velocity fluctuation at the flame holder lip. The fluctuation produces the disturbance in the shear layer which leads to the formation of the large vortices. Third, the experiments suggest that unsteady combustion in the vortex produces the pressure fluctuation which is required to drive the acoustic oscillation. Positive feed back can occur when the frequency of the fluctuations lies with a band of acceptable frequencies. Fourth, the frequencies observed correspond to acoustic modes of the system and are independent of the gas speed and fuel-air ratio although both influence the regimes in which the instability is observed. Fifth, acoustic modes which do not produce large velocity fluctuations at the flame holder lip are observed to be excited to large amplitudes; they do not produce the vortex shedding and are driven by a different process.

## II. ANALYTICAL STUDIES OF FLOW IN RAMJET ENGINES

A major purpose of this work is to analyze unsteady motions in the low frequency range of longitudinal motions. Steady and unsteady flows in both the inlet and a dump combustor are being treated. The results are intended to serve as a basis for assessing linear and nonlinear stability of devices; to aid in the interpretation of experimental data; to help design experiments; and eventually to provide guidelines for use in design of full-scale devices.

### Steady Flow Field in the Combustor

Because we are primarily concerned with unsteady motions, the analyses to date have been based on a simple model of a two-dimensional flow field. The volume is divided into three zones: the upstream unreacted flow; the downstream flow of combustion products; and a recirculation zone. An infinitesimally thin shear layer and a flame sheet separate the zones. The shapes of the shear layer and flame sheet are computed as part of the solution.

### Steady Flow Field in the Inlet

Throughout this work we assume that the shock system in the diffuser is represented by a single normal shock. For much of the work on oscillations we have assumed further that the flow is uniform in the inlet. The unsteady behavior of the shock is represented by an acoustic admittance function.

During the past year we have constructed a numerical analysis of the inlet flow in order to handle large amplitude unsteady motions. A finite difference scheme has been used to compute the flow with a normal shock, including approximation to the effects of the viscous boundary layers. The analysis will also accommodate injection and vaporization of liquid fuel in the inlet duct. The results are limited to cases in which flow separation does not occur. Good agreement for the pressure distribution has

been obtained upon comparison with data taken at the McDonnell-Douglas Research Laboratory.

### Unsteady Motions

We have analyzed a wide variety of cases of increasing complexity for comparison with experimental results. In all instances we have assumed the unsteady motions to be quasi-one-dimensional. Both axial and lateral dump configurations have been treated.

The simplest calculations are based on uniform steady flow in the inlet and in the combustor. All combustion is assumed to occur in an acoustically compact region at the dump plane. The shock wave is represented as a linear acoustic admittance. Calculated distributions of pressure amplitude and phase show quite good agreement with data for many cases studied at the Naval Weapons Center. Successful comparison has also been made with some data taken in the experiments at Caltech, described above.

The finite difference analysis, with a shock-fitting algorithm, has been used to study large amplitude unsteady motions in a diffuser. Responses to both upstream and downstream disturbances have been calculated. In the extreme circumstance of very large downstream pressure oscillations, the shock wave periodically propagates through the throat, to reappear downstream. For lesser amplitudes, the average position of a  $v$  shock is changed, and the analysis provides a means of estimating the loss of static margin due to longitudinal oscillations.

A numerical analysis has also been carried out for lateral dump combustor, approximated as a one-dimensional duct. The combustion process is approximated as a stirred reactor followed by reacting plug flow. The distribution of unsteady pressure seems to agree well with observations; the amplitude is about 25% below the experimental value found in work at the Naval Weapons Center.



# TRANSIENT COMBUSTION DYNAMICS

(AFOSR Grant 82-0222)

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**SUMMARY/OVERVIEW:** The objective of this program is to study the interaction of the pressure oscillation at the inlet of a dump combustor and the various existing vortices in the flow field. Such mutual interactions lead to a low frequency combustion instability in the form of large amplitude, coherent pressure oscillation in the chamber which disrupt the operation of the combustor. As a part of this study a feedback control system is to be proposed which can sense the onset of the combustion instability and by means of either gas jets or mechanical actuators destroy the coherent structure of the vortices and thereby minimize the effect of combustion oscillation. This study is aimed at understanding the fundamental causes of vortex-induced combustion instability and investigating a novel concept of minimizing its effect.

**TECHNICAL DISCUSSION:** Experiments at USC and elsewhere show that coherent vortex shedding at the dump plane due to the inherent instability of the shear layer induces a low frequency pressure oscillation in the combustion chamber. Also if one is able to change the characteristics of the shear layer, rough burning ceases. This observation is the basis of the proposed feedback control system for minimizing the effect of combustion oscillation.

During the last grant period it was found that the interaction of vortices showed a "beat" phenomenon on the p-t history of the chamber. When the beating was reinforced by the induced pulsing, combustion instability resulted. By using a bandpass filter the distribution of beat frequencies were obtained by photographic means. At a given flow velocity the beat frequency distribution associated with the vortices at the step depends upon the step height and the chamber geometry. For the present 2-D chamber under cold flow conditions, the beating originates from frequencies in the neighborhood of 1.9 khz (fig. 1). The resulting mean of the frequency distribution is in the range of 70-100 hz and it coincides with the observed critical pulsing frequency. No beating was observed without the step (e.g. with only a flat plate). The amplitude of pressure increased with the step height (maximum at  $\frac{1}{4}$ " for the chamber) and then decreased. For a 3" axisymmetric chamber, the beats originate from frequencies near 2.3 khz and the amplitude reaches a maximum at a step height of  $\frac{1}{4}$ ". The air supply also causes beating originating in the frequency range of about 430 hz. Induced pulsing at the mean of the distribution of frequencies ( $\sim 350$  hz) did not result into rough burning indicating that the beating caused by the sudden expansion step is the primary cause of rough burning. Figures 1, 2 and 3 are sketches which further elaborate the results obtained thus far.

Work on the vortex interaction as well as the control system is continuing during the remainder of the grant period.

2-D CHAMBER,  $\frac{1}{2}$ " STEP

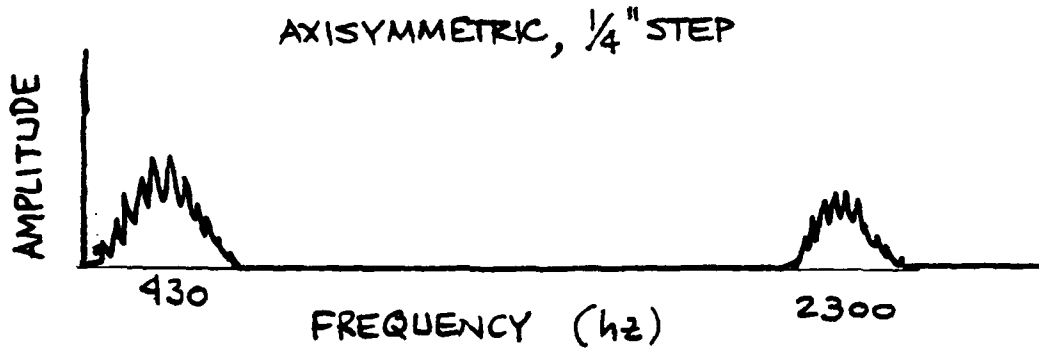
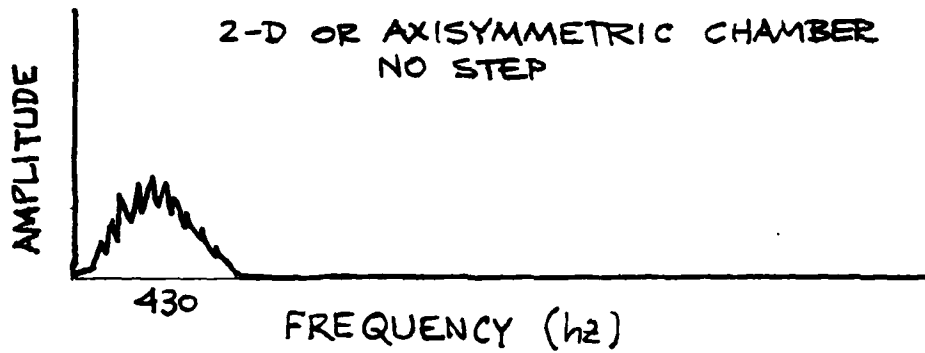
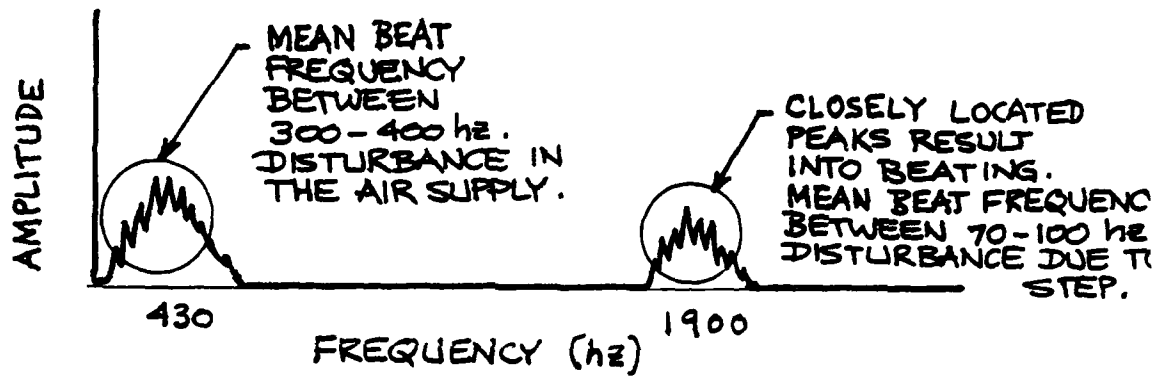


FIGURE 1. SKETCHES OF TYPICAL DISPLAYS FROM A FREQUENCY ANALYZER. COLD FLOW.

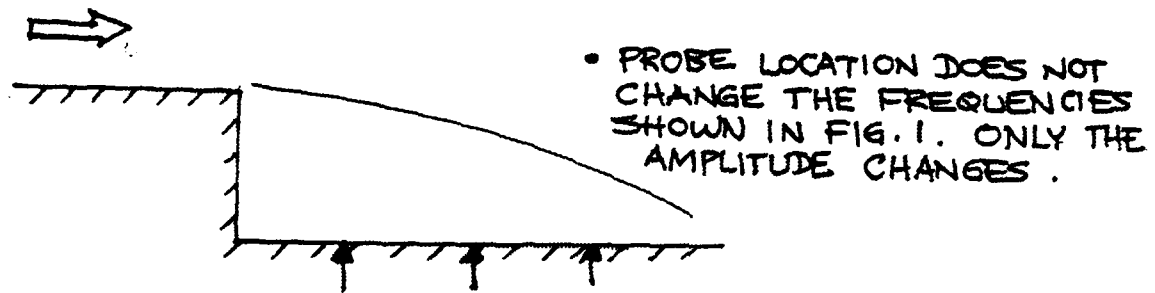


FIGURE 2. THREE DIFFERENT RELATIVE LOCATIONS OF THE PRESSURE TRANSDUCER.

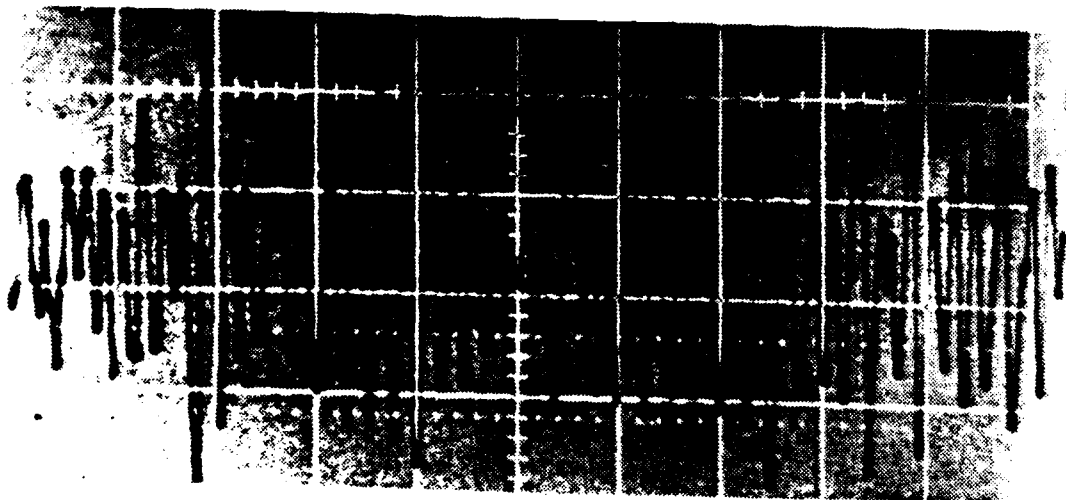


FIGURE 3. A TYPICAL  $p-t$  TRACE SHOWING "BEAT" DUE TO THE STEP. 5 ms/DIVISION; .03 PSI/DIVISION; 200 ft/sec. HOT FLOW.

# THE ROLE OF LARGE- AND SMALL-SCALE MIXING ON FUEL-RICH PLUME COMBUSTION

AFOSR MIPR 84-0014

Principal Investigator(s): K. C. Schadow and M. J. Lee

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## SUMMARY/OVERVIEW:

The purpose of this research program is to study experimentally the basic structure of an initially turbulent jet shear layer. The understanding of the large scale structures that constitute the shear layer, their evolution and relation to small scale eddies is important to be able to manipulate and control the mixing layer of a plume in a combustion process. Nonreacting tests with a hot-wire anemometer, and combustion tests with thermocouples and photographic observation are being performed to characterize the shear layer dynamics and their effect on fine-scale and large-scale mixing, as well as auto-ignition and combustion. The findings provide an improved understanding of the effect of turbulence on the initiation of combustion in the extreme fore-end of a coaxial mixing region, and quantitative data needed to enhance combustion in this part of the mixing region, which is decisive for the overall heat release in the fuel-rich plume.

## TECHNICAL DISCUSSION

Several airbreathing propulsion concepts utilize after-burning of fuel-rich reaction products in air. To optimize the heat release, it is important to initiate auto-ignition in local mixing regions with near-stoichiometric mixture ratios. This is necessary to achieve highest possible (near-stoichiometric) local combustion temperatures and therefore highest reaction rates. This is especially critical in systems with particulate fuels such as carbon and boron. In the latter case, high temperatures are required to free the boron particles from an inhibiting oxide layer.

In a coaxial mixing region, with overall above-stoichiometric air-to-fuel ratios, or equivalence ratios less than one ( $\phi < 1$ ), near-stoichiometric mixture ratios exist in the extreme fore-end of the mixing region.

In the previous year, experiments with boron particle-laden fuels and a coaxial mixing region without dump showed that, especially at low pressure, combustion did not occur in the extreme fore-end of the mixing region and the combustion temperatures were significantly below the near-stoichiometric temperatures. This was the result of excessive air mixing with the fuel-rich plume which had already taken place before combustion was initiated. Under these conditions, the heat release (combustion efficiency) was low<sup>1</sup>.

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<sup>1</sup>M. J. Lee and K. C. Schadow. "Detailed Flow Measurements in Fuel-Rich, Particle-Laden Plumes." Proceedings of the 20th JANNAF Combustion Meeting, Monterey, Calif., October 17-20, 1983.

During this reporting year, experiments were performed in a coaxial mixing region with dump. The objectives were to determine detailed radial and axial combustion temperature profiles in the presence of a recirculation zone behind the dump. The characteristics of the recirculation zone were varied by injecting ethylene or oxygen through the dump plane (see Figure 1). It may be seen from this figure that in the presence of a recirculation region, the combustion temperature at  $x/D = 1.4$  (for example) decreased compared to test conditions without ethylene injection. The temperature decreased because the plume mixed initially with air whose oxygen content is reduced as a result of the reaction in the recirculation zone.

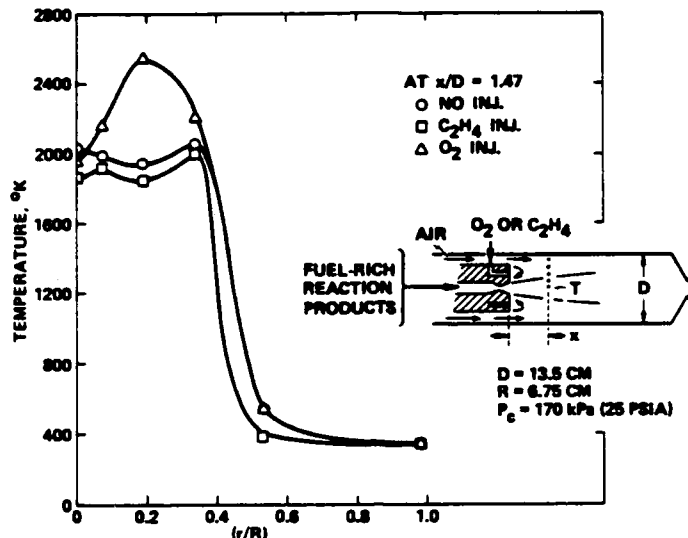


FIGURE 1. Radial Combustion Temperature Profiles.

The test results support the earlier conclusion that a coaxial mixing region without dump provides the potential for optimum heat release of a fuel-rich plume if auto-ignition can be initiated in the extreme fore-end of the mixing region.

It is generally assumed that ignition in the fore-end of the mixing region is delayed because of limited mixing on the molecular scale in the presence of large-scale vortices. Therefore, a detailed study of the vortex structure of a shear layer and its effect on the combustion process is necessary.

Tests with elliptic nozzles were continued with which enhanced mixing and combustion in the initial stages of the shear layer development was demonstrated<sup>2</sup>. The improvements were attributed to the elliptic vortices formed as a result of the initial instability of the jet. The elliptic vortices grew at a different rate in their major and minor axes as they were convected downstream. This motion was accompanied by the deformation of the vortices cross-section and development of azimuthal instabilities. As a result of these processes, small scale fluctuations were formed and small scale mixing was augmented in the initial region of the jet.

<sup>2</sup>K. C. Schadow, K. J. Wilson, M. J. Lee, and E. Gutmark. "Enhancement of Mixing in Ducted Rockets with Elliptic Gas-Generator Nozzles," AIAA Paper 84-1260, AIAA/ASME/SAE 20th Joint Propulsion Conference, Cincinnati, Ohio, June 1984.

In addition, various active methods of controlling the shear layer were tested. In one of them, the jet was issued from a variable length duct. Changes in the duct length produced different acoustic resonance frequencies inside the cavity. These frequencies were forcing the jet initial shear layers. As a result of the shear layer's typical amplification curve, which can be predicted from linear instability theory, the flow acted like a band-pass filter on the upstream forcing. The wide band multi-frequencies acoustic forcing was reduced in the shear layer to a limited frequency range of amplified disturbances. All other frequencies were attenuated. The filter's center frequency varied with the jet velocity.

Figure 2a shows the pressure spectrum of the upstream acoustic forcing of a 650 mm long duct leading to the jet nozzle. When the jet exit velocity was 50 m/s, the velocity fluctuations spectrum, measured at  $X = 5$  mm downstream of the nozzle exhibited a peak energy at  $f = 1787$  Hz (Figure 2c). Higher and lower frequencies had lower energy level. Fluctuations of  $f > 3000$  Hz were fully attenuated. At lower velocity ( $U_0 = 20$  m/s), the peak energy frequency moved to  $f = 775$  Hz. No fluctuations prevailed in the flow in a frequency higher than 2000 Hz (Figure 2b).

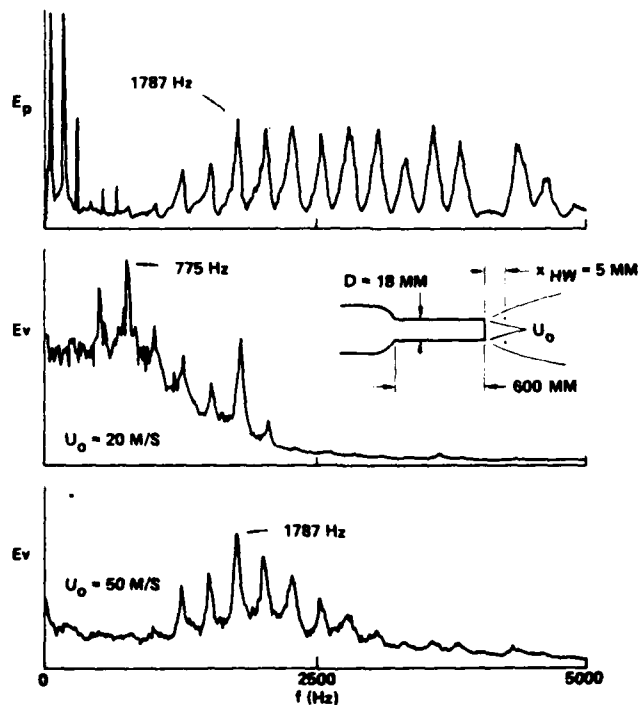


FIGURE 2. Duct Pressure and Shear Layer Velocity Spectra.

The upstream forcing of the jet when applied in the amplified frequencies range generated large scale structures in the flow and increased its overall mixing rate with its surroundings as shown by mean velocity profiles and Schlieren photography.

The large-scale flow data measured in the nonreacting tests is important to the combustion environment since the velocity fluctuation spectra contained also small scale turbulence which is critical to initiate combustion.

Since the jet flow was initially highly turbulent, small scale turbulence existed at the nozzle exit and was further increased when large-scale structures were formed by acoustic forcing. The energy increase of the small scale eddies was probably due to the stretching action of the large-scale vortices. Detailed combustion experiments with acoustic forcing will be performed to further explore the effect of shear layer forcing on the initiation of combustion in the extreme fore-end of a coaxial mixing region.

# LARGE EDDY STRUCTURES IN TRANSITIONAL AND TURBULENT FLAMES

AFOSR Contract No. 82-0266

Principal Investigator: Norman Chigier

Department of Mechanical Engineering  
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Pittsburgh, PA 15213

## SUMMARY/OVERVIEW:

The purpose of this research is the investigation of the fundamental mechanisms involved in the formation, development, and subsequent history of large eddy structures in jet flames. Propane, methane, and hydrogen flames are currently being studied. A second generation burner assembly which provides a uniform coflowing air stream but no physical enclosure around the flame has been constructed. Laser doppler velocimetry, Schlieren and high speed photography, and microthermocouples are presently being used in this study.

## TECHNICAL DISCUSSION

Work continues on the study of large eddy structures in flames. The second generation burner facility shown in Figure 1 has recently been completed and is now being used for measurements. Studies are presently concentrating on the 5 mm stainless steel nozzle described in previous reports.<sup>1</sup> Four Granger 4C448 shaded pole blowers mounted at the secondary air inlet provide the coflowing air stream. Each blower is rated at 465 CFM free air and 227 CFM across a 0.5" static pressure drop. The bottom plenum is 48" square and 14" high. Two perforated sheets, one mounted 11" above the bottom of the plenum and one mounted at the plenum exit, provide the flow resistance necessary to produce a uniform air flow. The perforated sheets are made from 20 gauge carbon steel and are perforated with 1/16" holes located on 3/16" staggered centers. The air then flows thru the center section, a round duct 3' in diameter and 14" high. The upper section, identical in size to the middle section, contains the secondary air flow straightener at its entrance. The flow straightener is composed of approximately 21,000 drinking straws, each 1/4" in diameter and 7 3/4" long, packed in the duct. At the exit of the flow straightener is a wire cloth stretched in a hoop frame. This screen, made from 304 stainless steel 55 mesh produces a fine scale turbulence which should decay before the secondary air flow reaches the nozzle exit. The unit is sized so that a 4' high flame will still be surrounded by the uniform air flow at the flame tip.

The studies are presently being conducted using laser doppler velocimetry, high speed and Schlieren photography and microthermocouples. The LDV uses a single component He-Ne laser. Seeding will use either  $Al_2O_3$  or  $TiO_2$ . Several prototype seeder designs have been tested using both of these materials in powder form. A seeder, which produces  $TiO_2$  from  $TiCl_4$ , designed at Wright-Patterson AFB<sup>2</sup> has recently been obtained on loan. The Wright-Patterson seeder has the capability of

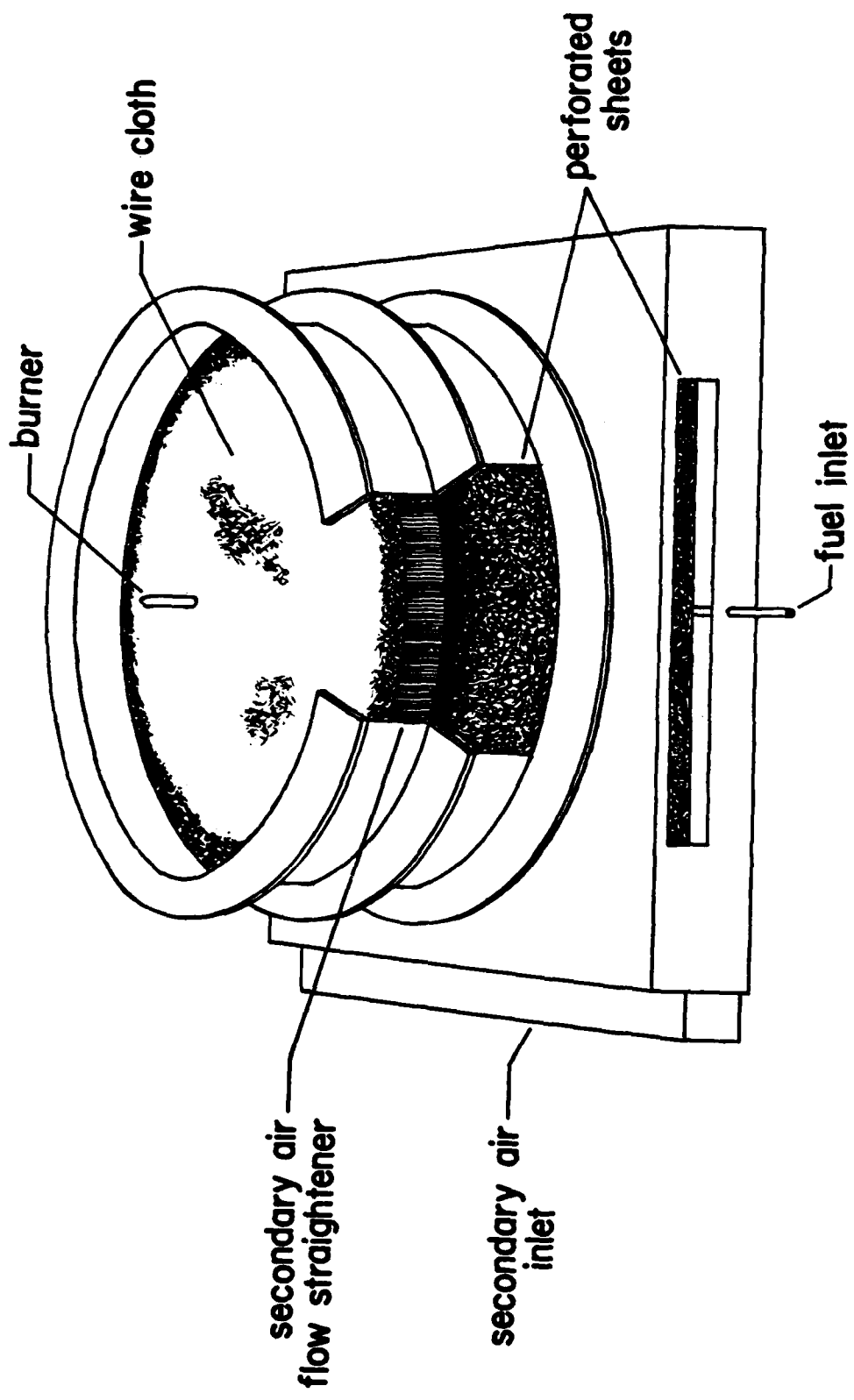
1. N. Chigier, K. Laskey, and T. Zsak, "Large Eddy Structures in Transitional and Turbulent Flames", First Annual Report to AFOSR, September 1983.
2. R.R. Craig et al, "A General Approach for Obtaining Unbiased LDV Data in Highly Turbulent Flows, Air Force Wright Aeronautical Laboratories, Wright-Patterson Air Force Base, Ohio



seeding the entire secondary air flow and may also be used for seeding the fuel. LDV data is obtained using a TSI 1980A analog signal processor, and the raw data is reduced immediately using software written for a MINC23 portable mini computer.

The Schlieren system makes use of two 12" diameter spherical mirrors, each with a 12' focal length. A 16ZW mercury arc lamp is presently being used as the light source. A rainbow aperture located at the focal point of the imaging mirror produces a color Schlieren image. The rainbow aperture consists of concentric rings of color. Colors in the Schlieren image result from the differing amount of light deflection through the flame and indicate density differences in the flame.

Microthermocouple work is using single wire, pulse heated platinum-platinum rhodium wire. The thermocouple wire in use ranges from 25 to 50 microns. Work is now in progress to provide temperature compensation on line using the MINC23 mini computer.



BURNER ASSEMBLY

MIXING, IGNITION AND COMBUSTION IN  
FLOWING, REACTING FUEL-AIR MIXTURES

(AFOSR Contract F 49620-30-C-0082)

Principal Investigators: R. B. Edelman & P. T. Harsha

SCIENCE APPLICATIONS, INC.  
Combustion Science and Advanced Technology Department  
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Chatsworth, California 91311

SUMMARY/OVERVIEW

The development of advanced volume and weight-limited airbreathing propulsion systems that can operate efficiently over wide operating limits is imposing severe requirements on combustor performance. This research program is concerned with the development of an improved understanding of flame stabilization and flame propagation in short residence time environments encountered in ramjet and ducted rocket combustors in which mixing and chemical kinetics can control the effective utilization of condensed phase fuels. The phenomena that have been studied in the program include fuel spray dynamics, chemical kinetics, boron combustion, turbulent transport and combustor model development. Modeling of fuel spray phenomena adopts an Eulerian approach, initially in the near-dynamic equilibrium limit, with fully-coupled finite rate chemistry. Chemical kinetics model development is concerned primarily with combustion of heavy hydrocarbon fuels in fuel-rich regions. Boron combustion modeling work is aimed at establishing boron particle combustion characteristics in the oxide-free limit, and is emphasizing temperature and pressure effects as well as the coupling of boron consumption with hydrocarbon carrier kinetics. Work on turbulent transport analysis has been carried out to investigate swirling flows using direct shear stress modeling, focusing on the effects of nonisotropic effective viscosity and of different types of swirl. Finally, combustor model development efforts have been concerned with two-phase flows (droplets and/or particles) in sudden expansion combustor environments and with the development of models for ducted rocket configurations. The objective of all of this work is to provide analytical insights into the variety of problems that affect combustion processes in propulsion systems, in order to aid in the interpretation of experimental results and in the development of advanced airbreathing propulsion systems. Future research will focus on ignition and flame stabilization in supersonic combustion and on the completion of the other elements of the current program.

TECHNICAL DISCUSSION

One major thrust of this research has focused on the development of a unique modular model approach. This concept provides for detailed analysis of the elementary flow and chemical processes while the modular model framework is structured to accommodate systematic coupling of these elementary processes to represent flames and combustors.

A significant aspect of this work has involved the development of a spray analysis that includes detailed chemical kinetics for the oxidation of realistic fuels. The quasiglobal chemical kinetics model developed under AFOSR support represented a major step forward in our ability to characterize the details of the combustion of realistic fuels, but was recognized to be deficient in its characterization of fuel-rich combustion. Recently an advanced quasiglobal model has been developed by SAI which removes this deficiency by incorporating modeling of fuel breakdown and pyrolysis, and under AFOSR support this model has been extended to the characterization of advanced ramjet fuels. The spray model that incorporates this chemistry has been used to develop comparisons of predictions with data obtained from controlled experiments. Figure 1 shows the predicted total liquid mass fraction contours for a vertical spray jet into a quiescent environment. The significance of this result is illustrated by contrast with the temperature contours shown in Figure 2 which shows that substantial mixing and vaporization of the fuel spray occurs prior to the development of a sustained high temperature flame zone. The result of the computations show that a complex physical and chemical structure develops in the near field in which droplet size distribution is continuously changing in the presence of finite rate pyrolysis and partial oxidation of fuel compounds prior to establishment of the flame. These predictions are in general agreement with the experimental observations and are providing insight on the importance of chemical transformations in the ignition and flame stabilization processes in spray flames.

The analysis of combustor processes using the modular approach has recently been directed toward establishing its validity in interpreting experimental data obtained from large scale test hardware. Figure 3 shows a comparison of predictions with typical overall performance data obtained from a sudden expansion ramjet combustor. While the agreement is good the analysis shows that in this case the performance trend is dominated by the fuel injection geometry and turbulent mixing process. Current research is focusing on the establishment of the range of applicability of this theory to generic ramjet combustor analysis and to bring this phase of research to a logical conclusion.

Future research will be directed toward high speed flow with emphasis on flame stabilization phenomena in supersonic combustion.

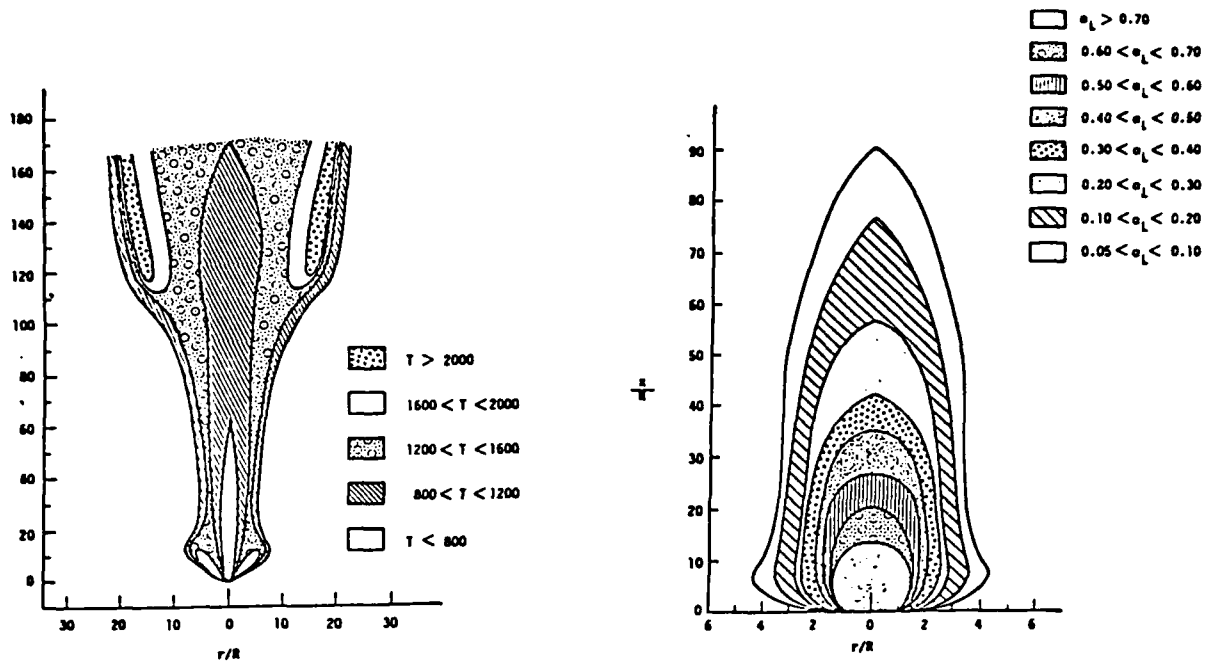


FIGURE 1. Droplet Total Mass Fraction (All Classes) Contours, Initial Spray Flame Region.

FIGURE 2. Temperature Contours in Initial Spray Flame Region.

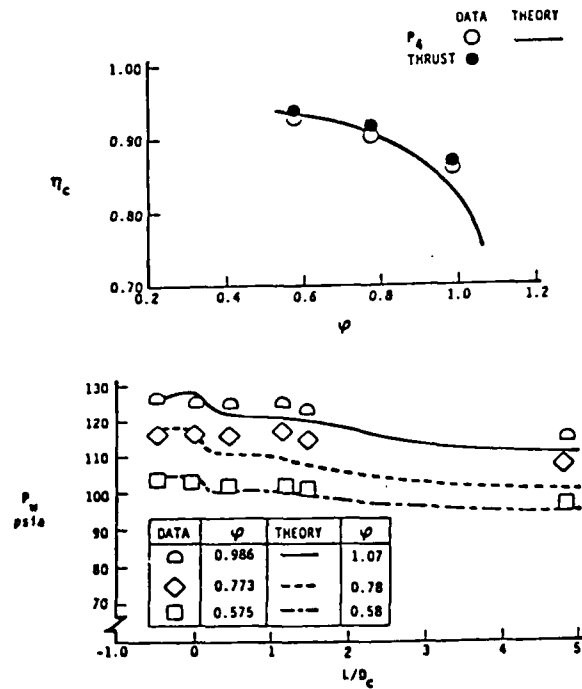


FIGURE 3. Combustor performance Prediction Compared with Experimental Data, Sudden Expansion Combustor, Wall Poppet Fuel Injection

# TEMPORAL DEVELOPMENT OF TURBULENCE-COMBUSTION INTERACTIONS

(AFOSR Grant No. 83-0373)

Principal Investigator: Tau-Yi Toong

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## SUMMARY/OVERVIEW:

Despite recent important advance in the study of turbulent combustion, physical understanding of turbulence-combustion interactions is still obscure. The main objective of this research is to determine and elucidate the mechanisms governing these interactions in different spectral regimes. Temporal development of spectral changes within the flame brush is examined as a quasi-laminar flame propagates into the wake region of a neighboring cylinder. It is hopeful that this study will help to advance our understanding of the physics of turbulence-combustion interactions and to provide sound guidelines for improving combustion efficiency and reducing emissions.

## TECHNICAL DISCUSSION

In order to elucidate the mechanisms governing turbulence-combustion interactions, temporal development of spectral changes in the thermal structure of premixed, rod-stabilized, lean methane-air V-flames is examined as a quasi-laminar flame (in the absence of grid-generated turbulence) propagates into the wake region of a neighboring cylindrical rod of four different diameters (1.6, 0.89, 0.64 and 0.41 mm). Spectral density distributions of apparent all-pass mean-square temperature fluctuations within disturbed flames are compared with those within undisturbed and turbulent flames (in the presence of turbulence-generating grids of corresponding mesh size) at different distances downstream from the cylindrical flameholder.

Figure 1 shows comparisons of the spectral density distributions\* within undisturbed, disturbed and turbulent flames at 3 and 35 mm downstream from the flameholder. The diameter of the disturbance rod in this case is 1.6 mm and is the same as that of the 4-mesh turbulence-generating grid in the study of turbulent flames. (This disturbed flame is thus designated as DF4.) The temperature fluctuations were monitored by the use of 25- $\mu$ m wire-diameter, frequency-compensated, Pt/Pt-10% Rh thermocouples at a position within the flame brush where the apparent all-pass RMS temperature fluctuations are the maximum. (Other conditions are specified in the captions.) Note that at 3 mm downstream (cf. Fig. 1a), the spectral structure within the disturbed flame resembles that within the undisturbed flame (UDF), while at 35 mm downstream (cf. Fig. 1b), the structure of DF4 approaches that of the corresponding turbulent flame (TF4), thus showing the temporal development of the disturbance effect from the neighboring cylinder. Note also that the structure within the undisturbed flame shows a peak at approximately 200 Hz, which corresponds to the predominant frequency observed in the velocity

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\* Integrated area under the curve between two specific frequencies represents the mean-square temperature fluctuations within the band pass.

fluctuations along the centerline of the 2.1 mm-diameter flameholder in the absence of the flame.

The spectral density distributions in the presence of disturbance rods of different diameters are also compared at different distances downstream of the flameholder. At 3 mm downstream, DF4, 6, 10 and 20 (with the respective disturbance-rod diameter equal to that of the turbulence-generating grid of corresponding mesh size) seem to give nearly the same structure in the high-frequency region. Farther downstream at 35 mm downstream, on the other hand, DF4 (in the presence of the largest disturbance rod) shows the highest spectral densities while DF10 and 20 give nearly the same structure and DF6 (in the presence of a disturbance rod of an intermediate diameter) begins to show some deviation in a limited spectral regime. These observations seem to imply that the effects of the disturbance rods on the spectral structure are due to interactions of rate processes which become more pronounced with increasing disturbance-rod diameter and with increasing time as the flow moves downstream.

Due to the presence of low-frequency fluctuations which would lead to slow motion of the flame across the temperature-monitoring station, the long-time signals obtained at a given spatial position in the laboratory-reference coordinates do not originate from a fixed position within the flame brush. In order to shed light on the nature of the higher-frequency components at different "instantaneous" mean temperatures within the flame brush, the signals should be analyzed within time intervals much shorter than the characteristic time of the low-frequency fluctuations. One can then relate these fluctuations to the chemical effect at a mean temperature pertaining to this time interval and the corresponding reaction rate and infer therefrom whether they are due to possible coupling between chemical kinetics and turbulence on the basis of our understanding of the instability mechanisms in reacting flows.

Temporal development of the RMS temperature fluctuations within the high-frequency region has been examined for undisturbed, disturbed and turbulent flames. Figure 2 shows comparisons at 3 and 35 mm downstream of the flameholder at different "instantaneous" mean temperatures (pertaining to a time interval of 25 ms<sup>\*</sup>). Consistent with the spectral density distributions shown in Fig. 1, the RMS values for DF4 are nearly the same as those for UDF at 3 mm downstream (cf. Fig. 2a). On the other hand, at 35 mm downstream, the RMS values for DF4 are much higher than those for TF4 (cf. Fig. 2b). Despite some scatter, Fig. 2 shows that the RMS values are the highest within the reaction zone and lower near the unburned and the burned regions, thus implying the possible role of chemical reaction rate in augmenting the higher-frequency fluctuations.

The high-frequency fluctuations are augmented to higher values in the presence of a larger disturbance rod, thus implying that the relevant interactions leading to the augmentation may also depend on the intensities and scales of turbulence generated by the disturbance rods. Coupled with the earlier observation on the chemical effect at different mean temperatures, one can expect that the interactions governing the augmentation of the high-frequency fluctuations may depend on the coupling between chemical kinetics and turbulence.

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\* A characteristic time of the observed low-frequency fluctuations is about 200 ms.

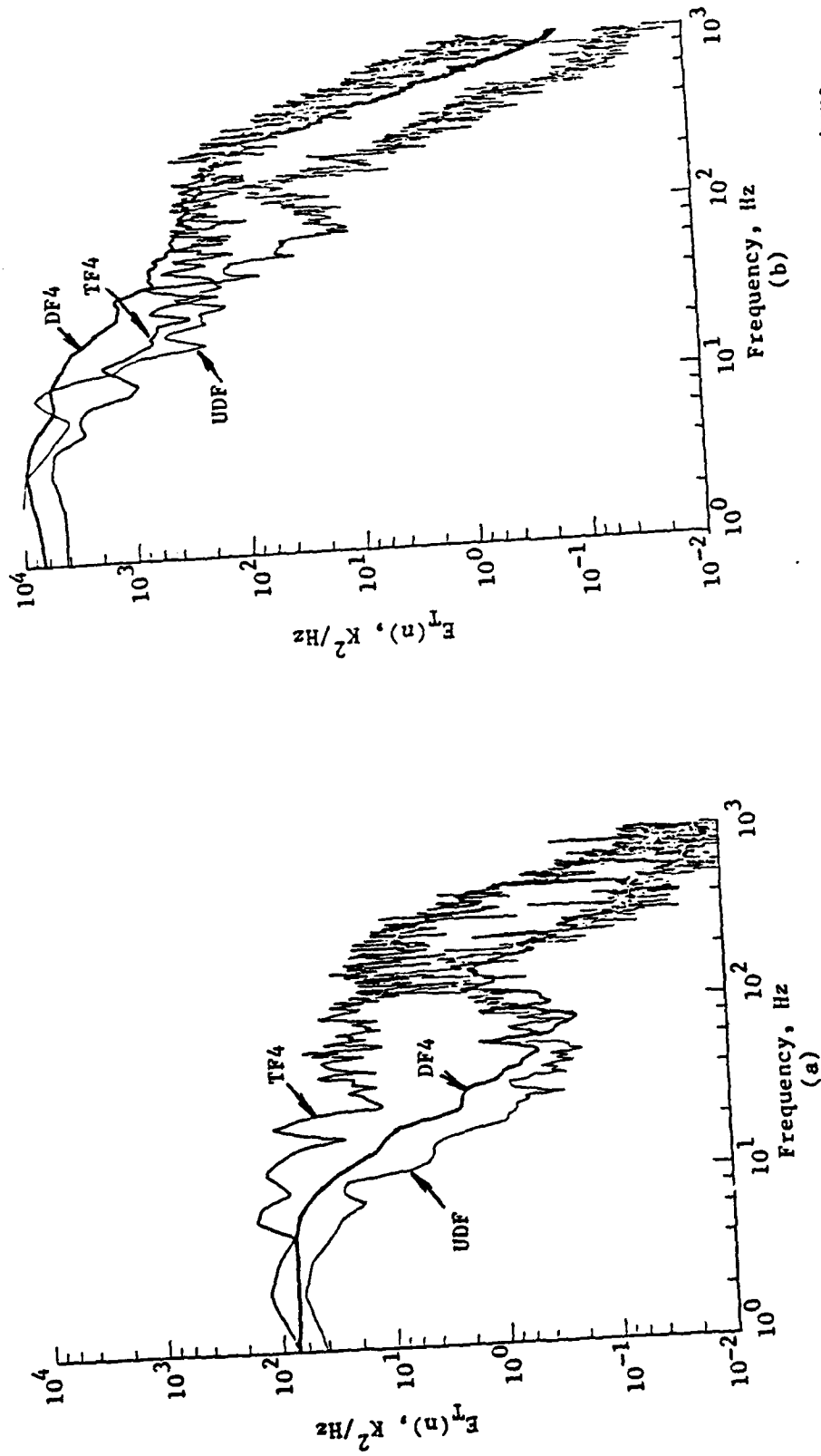


Fig. 1 Comparisons of spectral density distributions of apparent all-pass mean-square temperature fluctuations within undisturbed (UDF), disturbed (DF4 with 1.6 mm-diameter disturbance rod) and turbulent (TF4 with 4-mesh grid) flames at a position of maximum apparent all-pass RMS temperature of fluctuations; equivalence ratio, 0.75; mean mixture velocity, 2.4 m/s; (a) 3 mm downstream of 2.1 mm-diameter flameholder (b) 35 mm downstream



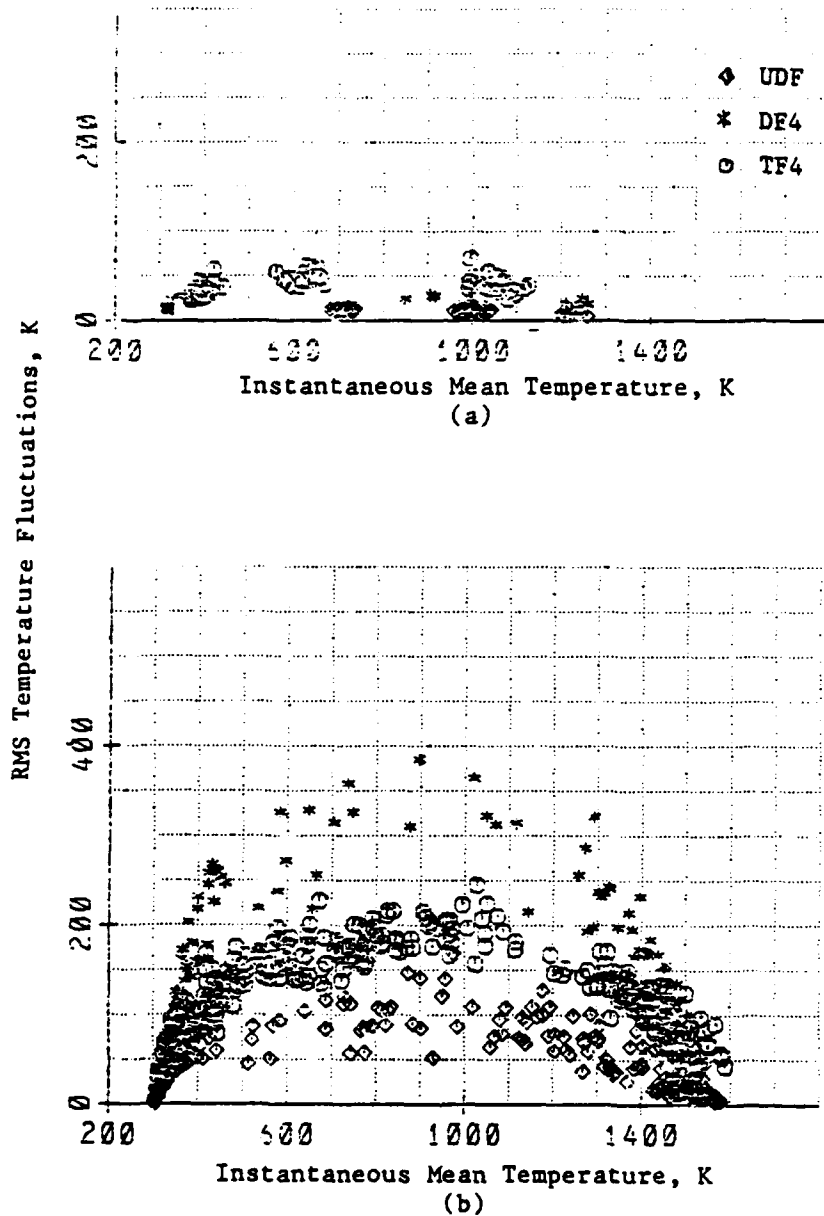


Fig. 2 Comparisons of RMS temperature fluctuations within high-frequency region at different "instantaneous" mean temperatures (pertaining to a time interval of 25 ms) for undisturbed UDF, disturbed DF4 (with 1.6 mm-diameter disturbance rod) and turbulent TF4 (with 4-mesh grid) at a position of maximum apparent all-pass RMS temperature fluctuations; equivalence ratio, 0.75; mean mixture velocity, 2.4 m/s; (a) 3 mm downstream of 2.1 mm-diameter flameholder (b) 35 mm downstream

FLAME PROPAGATION AND STABILIZATION STUDIES  
USING RAYLEIGH SCATTERING AND LASER VELOCIMETRY

(AFOSR Contract # F49620-80-C-0065)

Principal Investigator(s): L. Talbot and F. Robben

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SUMMARY/OVERVIEW:

The research program has continued in the investigation of the interactions between combustion processes and fluid mechanics in a V-shaped flame stabilized on a rod in a turbulent flow. Such a relatively simple flame is suitable for laboratory study and also representative of practical combustion systems. Non-intrusive laser-based diagnostics comprise the primary experimental techniques for the measurement of (a) velocity by laser Doppler velocimetry, (b) instantaneous fluid density by Rayleigh scattering, and (c) high speed photography (Schlieren and laser tomography using an oil aerosol). These experimental methods make possible a detailed characterization of this system and provide data which may be compared with the predictions of theoretical models and numerical simulations. Particular effort has been directed towards the generation of a flame front algorithm, the acquisition and reduction of scalar length and time scale data in the light of recently available models (1) and a study of the stabilization region of the V-shaped flame.

TECHNICAL DISCUSSION:

The experimental set-up has been described in detail elsewhere (2). Ethylene and methane have been used as fuels.

With the present experimental configuration the free stream turbulence can be varied by placing grids or pierced plates in the inlet flow. By means of high speed photography and laser tomography it has been possible to visualize the effect such changes have on flame structure. To aid interpretation of these results a numerical study of this system has been initiated. The wrinkled laminar flame observed experimentally has been modeled as a line of points which propagate normal to themselves into the unburnt flow by means of a Huygens-type construction and act as volume sources which simulate the effect of density changes during combustion. The impact of vorticity on this modeled flame front is presently under investigation utilizing the Random Vortex Method.

The stabilization region behind the flame holder is of practical and fundamental importance. Studies are in progress using single point Rayleigh scattering to measure density and laser tomography to provide two dimensional, qualitative flame front information. Preliminary results indicate that the flame in the shear layer between the free stream and the recirculation zone is laminar with slight wrinkling when the approach flow is turbulent. LDV will be used to give insight into the onset of instabilities in the shear layer and the recirculating eddies, and how they affect the flame.

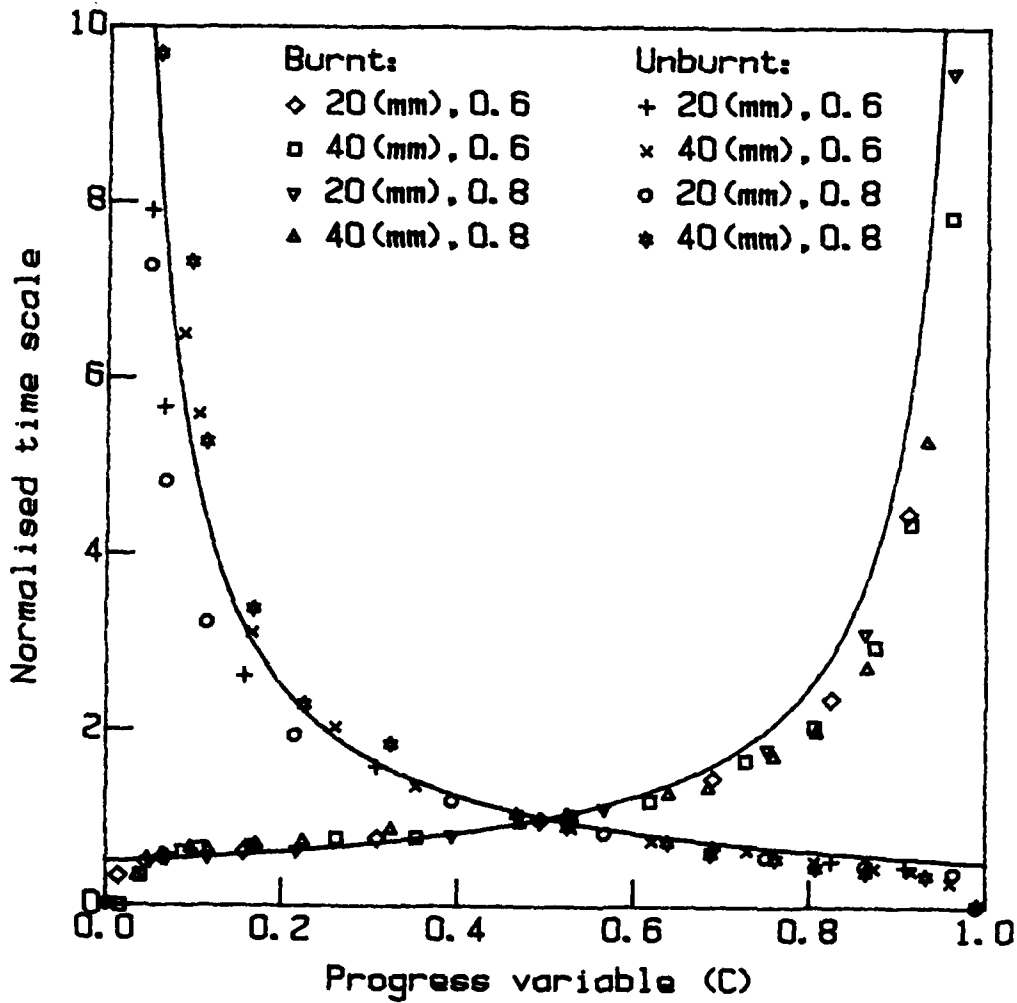
The Bray-Moss-Libby model of premixed turbulent combustion has recently been extended (1) to include such characteristics of the scalar field as time and length scales, autocorrelation functions and power spectra. The predictions of the model may be compared to suitably reduced single point Rayleigh data obtained previously. Figure (1) shows a comparison of normalized time scales between the model (solid line) and data obtained from a variety of flame conditions. Close agreement is also found for the autocorrelations and the power spectra. The two point Rayleigh data is currently being reduced to derive length scale information for comparison with model predictions.

Work has continued on the wrinkled laminar flame sheet model which describes the turbulent flame region in terms of the instantaneous flame-front position. Non-dimensionalizing the flame density profiles by a turbulent flame thickness derived from the maximum density gradient, all the data may be collapsed onto a simple error function plot: the solid line in Figure (2). In Figure (2) the unburnt fraction is derived from the mean density and is 1 in the unburnt gas and 0 in the products.

#### REFERENCES:

1. Bray, K.N.C., Libby, P.A. and Moss, J.B. to appear in *Combustion Science and Technology* (1984).
2. Namazian, M., Talbot, L., Robben, F. and Cheng, R.F.: *Nineteenth Symposium (Int'l) on Combustion*, p. 487, The Combustion Institute (1983).

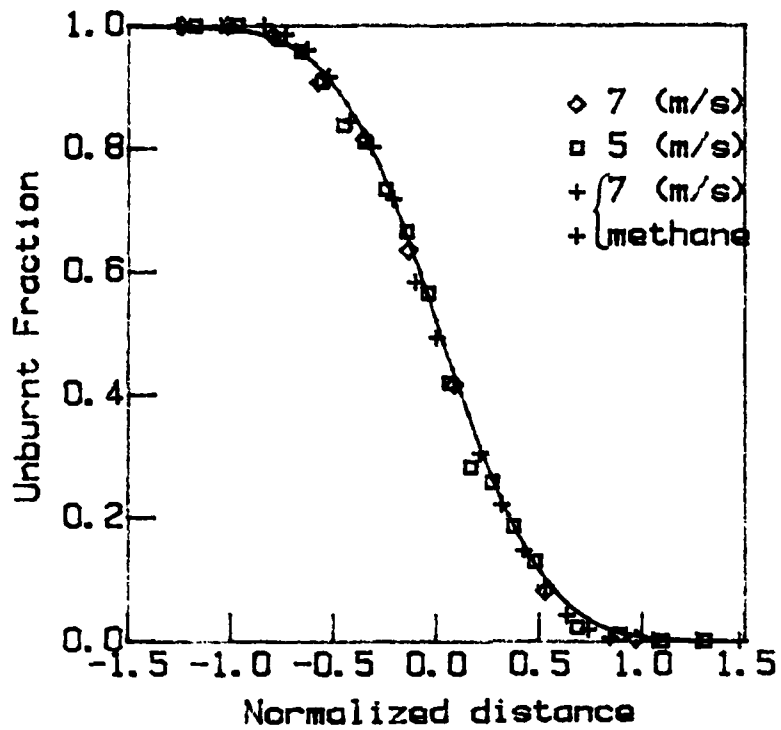
Flames: ZMT76, ZMT78  
 b20, a40. a20, a40



Normalized time scales of burned and unburned regions in turbulent methane/air flame plotted as a function of the progress variable C. Solid lines are the predictions of Bray and Libby. Flame conditions: 7 m/s velocity, grid turbulence, 20 mm, and 40 mm downstream of flame holder, and equivalence ratio,  $\phi = 0.6, 0.8$ .

Figure 1.

Flames:  $\Phi = 0.6$ ,  $x = 40$  (mm)



Flames:  $U = 7$  m/s,  $\Phi = 0.8$

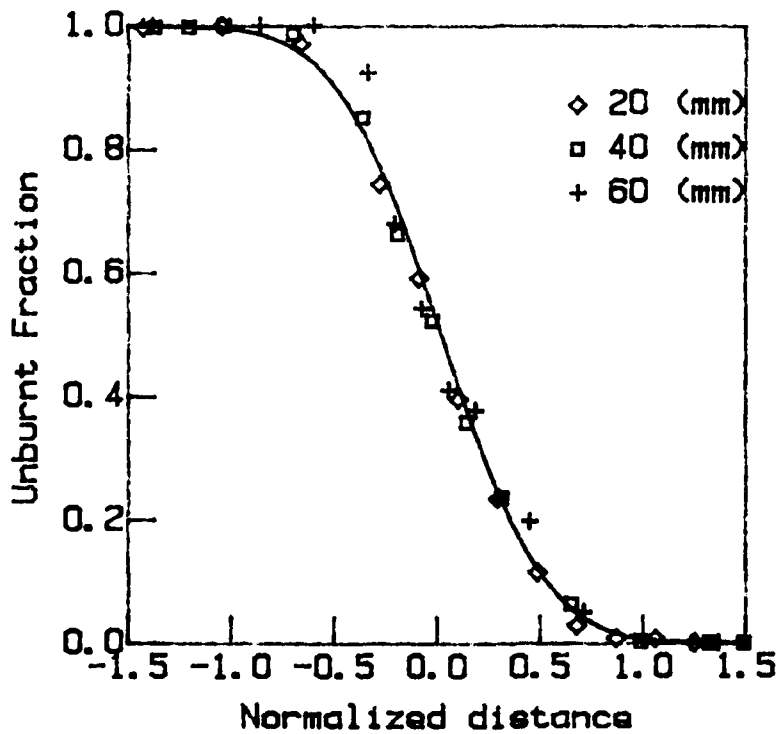


Figure 2.

# CHEMICALLY REACTING TURBULENT FLOW

(AFOSR-ISSA-84-00005)

William M. Pitts  
Takashi Kashiwagi

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National Bureau of Standards  
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## SUMMARY

This project is designed to study chemically reacting turbulent flows by systematically investigating the effects of density differences, temperature differences, and heat release on turbulent mixing. During the past eight months much time and effort has been spent on the continuing development of diagnostic techniques for real-time measurement of concentration and velocity in turbulent flow fields of variable composition. Experiments are also being planned which will allow real-time measurements of concentration along a line in a variable density flow. Both of these techniques will allow a more complete characterization of density effects on turbulent mixing than has been possible in the past.

## TECHNICAL DISCUSSION

### Introduction

This research program is a long term, systematic study of chemically reacting turbulent flow. This is the second fiscal year that this project has been supported by the Air Force Office of Scientific Research.

During the first year of the project we performed measurements of density effects on the centerline mixing behavior of an axisymmetric jet of one gas into a slow coflow of a second gas [1]. We also developed a technique combining the use of laser induced Rayleigh light scattering for concentration measurement and hot-wire anemometry for simultaneous measurement of concentration and velocity in variable density flows [2].

This research has shown that hot-wire and film anemometry can be applied to mixtures if the mixture composition is known. However, despite the wide spread use of these instruments and a great deal of previous research, it has been necessary to undertake a fairly detailed investigation of their response in different gases and mixtures in order to be confident of their behavior. These studies are described below. This work has been done in collaboration with Dr. Bernard McCaffrey of the Center for Fire Research.

Recently, we have received supplemental funding from the National Bureau of Standards to demonstrate line measurements of concentration in variable composition flows using Rayleigh light scattering. A short discussion of the proposed experiment is given.

### Hot-wire and Film Behavior in Different Gases and Mixtures

Both hot-wires and films have been used in our simultaneous concentration and velocity measurements. Originally, we used a simple King's law expression to fit the response of the instrument:

$$E^2 = A + B \sqrt{V}. \quad (1)$$

$E$  is the voltage drop across the wire and  $E^2$  is proportional to the heat loss of the wire,  $V$  is velocity, and  $A$  and  $B$  are parameters which depend on gas composition.

By empirically determining the behaviors of A and B as a function of molecular composition, we were able to use the hot-wire and film in combination with Rayleigh light scattering (used to determine concentration) to measure velocities in variable composition flows [2]. Measured centerline velocity behavior in an axisymmetric jet was consistent with previous literature measurements. However, it became clear that there were inaccuracies in our calibrations due to the use of Eq. (1). Furthermore, we were unable to predict the heated elements' responses to different gases with sufficient accuracy for calibration purposes using empirical heat transfer laws available in the literature.

For the above reasons, we have run a series of calibrations for the hot-wire and film in a number of gases covering a molecular weight range of 4 g/mole (He) to 149 g/mole (CF<sub>3</sub>Br). Measurements were made over a velocity range of ~ 50 cm/s to 900 cm/s. We have used a modified form of Eq. (1),

$$E^2 = A + BV^n, \quad (2)$$

to fit the data. The exponent n is chosen to give the best fit of the experimental data. Examples of such data fits are shown in figure 1 for a number of gases.

For the hot-wire we found that the exponent in Eq. (2) is nearly constant at  $n \sim 0.43$  for all gases except helium which had a much lower value. This implies that Eq. (2) can be used to compare different gases and mixtures. Unfortunately, the values of n for the film calibrations vary from 0.45 to 0.36 for the different gases. Errors will clearly be introduced if a constant value of n is assumed for the hot-film. We attribute the variation in n for the film to the different Reynolds number (Re) ranges over which measurements are made for the various gases. This conclusion is supported by the observation of a clear transition in heat transfer behavior at  $Re \sim 44$  which is due to the well known onset of vortex shedding from the heated filament. We have identified a previously unreported hysteresis in this flow transition region which demonstrates clearly the effect of this transition on heat transfer behavior.

In order to limit the number of calibrations necessary it is desirable to be able to predict the behavior of a hot-wire or film in a gas based on its known calibration in another gas. Usually, empirical heat transfer laws such as that of Collis and Williams [3] are used for this purpose. Such laws are based on the behavior of the heated filament Nusselt number (Nu) as a function of Re. This dependence can be written as

$$Nu = A' + B'Re^n \quad (3)$$

where

$$Nu = i^2 R_w / (\pi k_g L \Delta \theta) \quad (4)$$

and

$$Re = DV/\nu \quad (5)$$

The variables in these equations have their usual meanings. The factors which vary with gas composition are the gas thermal conductivity ( $k_g$ ) and the kinematic viscosity ( $\nu$ ).

For most hot-wires and hot-films the measured Nu is only an approximation since there is also heat transfer to the prongs holding the filament. In this case the subscript m is added to Nu indicating that it is an effective Nu. Figure 2 shows plots  $Nu_m$  versus  $Re^{0.43}$  for a hot-wire calibrated in several different gases. By comparing Figs. 1 and 2 it is clear that the data is partially correlated by Eq. (2), but that the correlation is not complete.

We now know that in order to adequately correlate the hot-wire and film data it is necessary to consider heat transfer to the prongs. We are currently developing expressions to allow such correlations.

Similar calibration measurements have been made in binary gas mixtures. The heat transfer in these mixtures is not predicted well by the extrapolated pure gas results. We have postulated that these differences are due to thermal diffusion effects in the mixtures and are using theories especially developed for this study in an attempt to quantitatively predict the magnitude of such effects.

The results of our calibration studies have highlighted the complexity and poorly understood nature of the response of heated filament anemometers. Such problems were not evident as we began our investigation. The results of this study have enabled us to understand hot-wire and film response in different gases much better. Such an understanding is necessary for accurate velocity measurements using our new technique. In a wider sense, we have learned a great deal about the behavior of these devices which should be of interest to workers who use heated filament anemometry in other types of experiments.

#### Concentration Line Measurements

There has been a great deal of recent interest in making line and two-dimensional measurements of concentration in turbulent flow fields [4-6]. These measurements combine laser based optical probes with the use of new and powerful solid state detector arrays. Very simply, the laser beam is passed through the flow as a beam (line measurement) or as a sheet (2-D measurement). The laser light interacts with the molecules of the gas in some manner (e.g., fluorescence, or Rayleigh or Raman scattering). These interactions result in light "emission" from the flow field in directions different from that of the laser beam. In general, the intensity of this "scattered" light is proportional to some scalar value (i.e., density or molecular species concentration) in the flow field. By imaging this "scattered" light onto a suitable detector, the spatial variation in the scalar can be recorded. Usually the spatially resolved light intensity pattern on the detector is digitized and stored in the memory of a computer for later analysis. Fluorescence, Raman and Rayleigh scattering, and Mie scattering from particles have all been employed in such studies.

The studies done thus far have yielded a great deal of information about turbulent flow fields and have demonstrated the vast potential of these techniques for contributing to an improved understanding of chemically reacting turbulent flow fields. However, it is fair to say that the technique is still severely limited by laser, detector, and computer constraints. For example, the measurements reported thus far have been single shot and measurement accuracy has been poor.

We are currently developing an experiment in which line measurements of concentration are to be made in a turbulent flow of two gases. The design goals of this experiment are (1) a 0.2 ms time resolution, (2) a 0.2 mm spatial resolution, and (3) a concentration accuracy of 4% for each individual measurement.

A system has been designed which should meet these goals and we have begun purchasing the necessary components for its construction. This new experiment will allow much more detailed studies of density effects on turbulent mixing.

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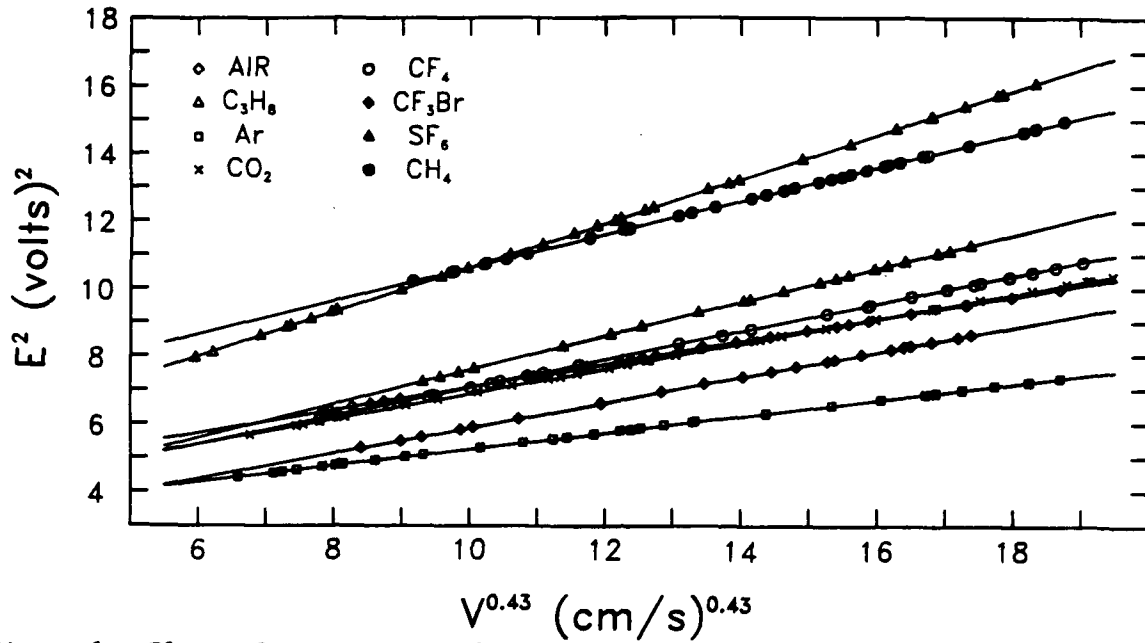


Figure 1. Plots of anemometer voltage squared versus flow velocity to the 0.43 power for the gases listed in the figure. Lines correspond to linear least square fits of the data.

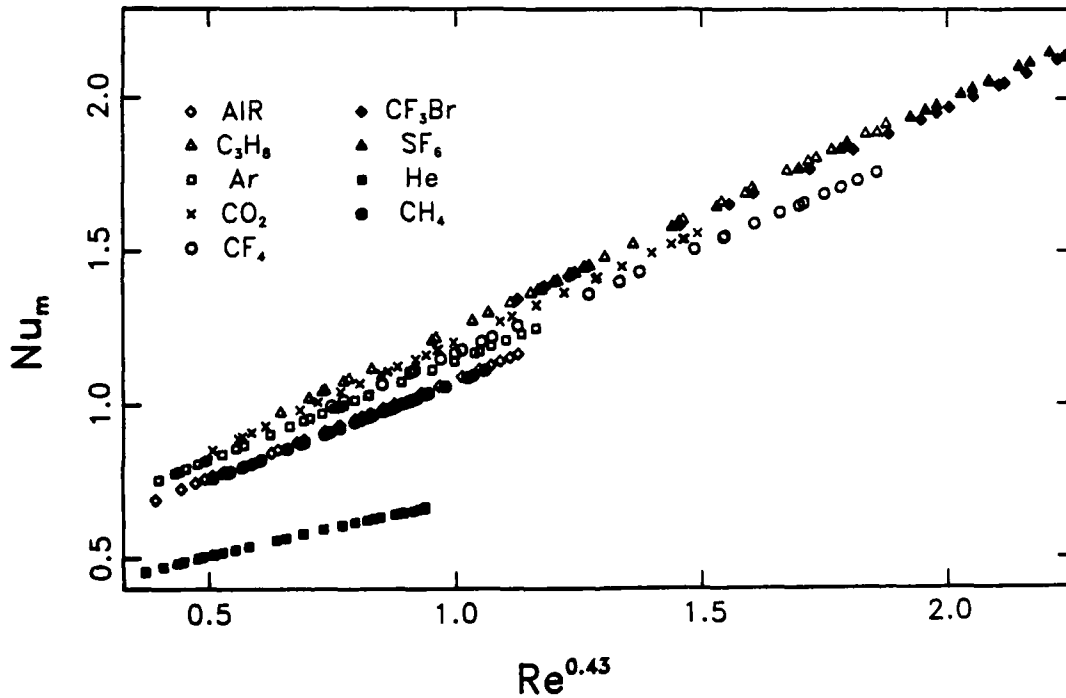


Figure 2. Plots of  $Nu_m$  versus  $Re^{0.43}$  for the gases indicated in figure. These values were obtained from the experimental data shown in figure 1 using eqs. (4) and (5).

## CHEMICAL REACTIONS in TURBULENT FLOWS

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Work is continuing in both gas phase and liquid phase mixing, chemical reactions and combustion, in moderate to high Reynolds number free shear turbulent flows. This is primarily an experimental investigation, closely supported by theoretical and modeling efforts (see Broadwell and Dimotakis 1984), as well as specific diagnostics developments, as dictated by the needs of the experimental program.

### 1.0 GAS PHASE SHEAR LAYER COMBUSTION.

The work described below was conducted in conjunction with the hydrogen-fluorine shear layer combustion facility.

#### 1.1 Reynolds number effects

Reynolds number effects upon the mixing and combustion process were investigated at high-speed stream velocities of  $U_1 = 13.5, 22.5, 44$  and  $85$  m/s, at a speed ratio of  $U_2/U_1 = 0.4$ . Preliminary results of this work were reported at last year's AFOSR Contractor's Meeting. We continue to observe the existence of large, hot structures that govern the flow dynamics at all speeds. The mean temperature profile is found to decrease modestly with increasing speed. The amount of chemical product (product thickness  $\delta_p$ ), as normalized by  $\delta_1$ , the 1% shear layer width, decreases by ~ 6% per factor of 2 increase in Reynolds number. Tripping the high speed boundary layer is also found to result in significant thinning (by as much as 30%) of the width of the layer and a slight increase in the peak mean temperature rise.

These results were recently documented by Mungal, Dimotakis and Hermanson (1984).

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### 1.2 Preliminary investigations of chemical kinetics effects

An exploratory effort was begun, which attempts to simulate the effects of slow chemistry in the turbulent reacting mixing layer. This is accomplished by systematically decreasing the amount of nitric oxide (the pilot or trigger gas), premixed with the  $H_2$  stream, while holding all other variables constant. For these runs, nominal concentrations of 8%  $H_2$  in  $N_2$ , on the high speed side, and 1%  $F_2$  in  $N_2$ , on the low-speed side were used. Three effects are observed as the NO concentration is decreased:

1. A loss in the total product formed.
2. A shift in the mean temperature profile towards a more symmetric shape, in spite of the large excess of hydrogen,
3. A change in the distribution in temperature within a given large structure.

These results are in qualitative agreement with the slow chemistry predictions of the Broadwell & Breidenthal (1982) model. We are presently attempting to compute the relevant Damkohler numbers for these runs using a detailed chemical kinetics analysis.

### 1.3 Heat release effects

Combinations of reactant concentrations up to 6%  $F_2$  and 16%  $H_2$  have been investigated, producing adiabatic flame temperatures of 900 K (600 K rise) and a maximum mean temperature rise across the layer of 370 K, corresponding to a maximum mean density reduction of more than 50% in the layer over the free stream value. The previously reported trend of layer thinning with heat release persists. A preliminary report was made at the American Physical Society, Fluid Dynamics 1983 meeting (Hermanson, Dimotakis and Mungal 1983).

Early results also suggest that an additional effect might be a change, with heat release, in the entrainment ratio in favor of the low speed fluid. Preliminary measurements from spark schlieren photographs also indicate that there is a decrease in mean large scale structure

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spacing caused by the heat release, of approximately the same amount as the fractional decrease in shear layer thickness.

A parallel effort has been initiated to investigate pressure gradient effects in a combustng shear layer.

### 1.4 Supersonic shear layer combustion study

An initial feasibility/design study was undertaken and a first cut at a test section design for a 2-D supersonic reacting shear layer was completed. A guideline in this design, in order to minimize cost and leadtime, was the decision to use as much of the existing HF combustion facility as possible with the apparatus upstream of the contraction section unchanged. This necessarily led to limits on the range of flow conditions and run times that could be expected, permitting, on the other hand, sufficient flexibility to allow high speed stream Mach numbers in the range of  $1 < M_1 < 3$ , and run times in the range of 1-3 seconds.

A serious problem was, however, identified. Along with the high heat release associated with the  $H_2 + F_2$  reaction, subsonic experiments performed to date have been in the fast chemistry, "diffusion-limited" regime. It became clear that, under the adopted constraints, we could not engineer a high Mach number flow that would also be free of finite kinetic rate effects; any results concerning the effects of compressibility on the combustion process could be confused with the effects of finite chemistry. It was decided that we should separately investigate the effects of small Damkohler number in initially subsonic flow. The pilot investigation in section 1.2 was initiated, in part, with this in mind.

### 2.0 GAS PHASE JET MIXING. RAYLEIGH SCATTERING MEASUREMENTS

Work to date has centered around the development of Rayleigh scattering techniques for concentration measurements in binary gas mixtures. We expect that this technique can be applied in a wide variety of turbulent flows. Based on performance calculations, we

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expect signal-to-noise ratios of the order of 50:1, with Kolmogorov scale time/space resolution, for jet Reynolds numbers of the order of  $5 \times 10^3$ .

As of this writing, a bench test experiment is under way. Using a small pressure vessel ( $0.4 \text{ ft}^3$ ) and specially designed optics and electronics, we intend to verify that we can meet our measurement performance specifications by changing the vessel pressure, laser power, filter bandwidth, sampling volume size and scattering cross-section of the gas. Preliminary results show good agreement between our bench test results and our performance calculations.

This work is co-sponsored, in part, by the Gas Research Institute.

### 3.0 LIQUID PHASE MIXING and CHEMICAL REACTIONS

These studies are undertaken to investigate Schmidt number effects in high Reynolds number turbulent mixing and chemical reactions, by comparison with parallel experiments in gas phase flows, and also to exploit the diagnostic power of (liquid phase) laser induced fluorescence techniques for those questions that can be answered independently of the fluid medium.

#### 3.1 Shear layer mixing and chemical reactions

Direct multi-point, high time/space resolution measurements of species concentration in a non-reacting layer allowed us to extract the probability distribution function (PDF) of the composition field across the width of the layer. The results, recently reported by Koochesfahani and Dimotakis (1984), showed that the mixed fluid composition is fairly uniform across the transverse extent of the mixing layer, and is biased in favor of the high speed stream fluid. This is also in good agreement with the recently reported (Dimotakis 1984) entrainment calculations for these flows.

## CHEMICAL REACTIONS in TURBULENT FLOWS

Measurements of the product concentration in a reacting liquid mixing layer indicate that:

1. The amount of chemical product in a liquid mixing layer is about 50% of that for a gas phase layer at comparable Reynolds numbers.
2. The mean concentration of the mixed fluid is essentially constant across the entire transverse extent of the layer. The value of this constant is biased in favor of the high speed stream fluid, in agreement with the results from the non-reacting layer.
3. The probability of finding unmixed fluid, in the center of the liquid mixing layer, for high Reynolds number layers, can be as high as 0.45.

### 3.2 Turbulent jet mixing and chemical reactions

Laser-induced fluorescence (LIF) techniques are used to make measurements of the concentration field in the far-field of reacting and non-reacting, liquid-phase, momentum-driven, axisymmetric turbulent jets. Of particular interest, in these measurements, is our observation of a large-scale nearly-periodic unsteadiness in the entrainment and mixing process, which we have shown plays a crucial role in determining how chemical reactions occur in the jet, as evidenced by observed nearly-regular fluctuations of reacting jet "flame" lengths (Dahm, Dimotakis and Broadwell 1984).

In addition, LIF digital imaging techniques, developed to make direct measurements of the concentration field in the plane mixing layer (section 3.1), have been adapted to permit similar measurements to be made in the far-field of turbulent jets. Thus far, we have used this technique to make measurements of the concentration PDF (simultaneously at 1024 points) along the jet centerline.

This work is supported, in part, by the Gas Research Institute.

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