Unclassified
SECURITY CLASSIFICATION OF THIS PAGE

AD-A236 652

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION: Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; distribution is unlimited.
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S): AFOSR-TR- 91 0505
6a. NAME OF PERFORMING ORGANIZATION: University of California, San Diego — 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION: AFOSR/NA
6c. ADDRESS (City, State, and ZIP Code): La Jolla, CA 92093-0310	7b. ADDRESS (City, State, and ZIP Code): Building 410, Bolling AFB DC 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: AFOSR/NA — 8b. OFFICE SYMBOL (If applicable): NA	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: AFOSR-89-0310
8c. ADDRESS (City, State, and ZIP Code): Building 410, Bolling AFB DC 20332-6448	10. SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. 61102F; PROJECT NO. 2308; TASK NO. A2; WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)
(U) Theories of Turbulent Combustion in High Speed Flows

12. PERSONAL AUTHOR(S)
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13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Annual Technical	FROM 90/4 TO 91/4	91/4/2	6

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Turbulent Flames, Diffusion Flames, Supersonic Combustion

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Since Damköhler and Reynolds numbers over the range of conditions relevant to supersonic hydrogen-air combustion were found to be consistent with the combustion occurring in the reaction-sheet regime, detailed numerical integrations were performed on the structures of counterflow hydrogen-air diffusion flames, for pressures from 0.5 to 10 atm and air temperatures from 300 K to 1200 K, at a hydrogen temperature of 300 K. The results showed extinction to occur at high enough rates of strain in most cases, but no extinction for air temperatures above about 1000 K. Nitrogen chemistry was shown to have a negligible effect, and reduced chemical-kinetic mechanisms were developed for simplifying the computations. The computed extinction strain rates were found to be in excellent agreement with newly performed experiments. Compressibility effects are being taken into account, and the results are being worked into methods for describing turbulent combustion in high-speed flows.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT: ☒ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☒ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION: Unclassified
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DD Form 1473, JUN 86 — Previous editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE
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INTRODUCTION

Supersonic combustion in turbulent hydrogen-air systems is a topic of current interest because of its relevance to applications such as the development of one-stage-to-orbit vehicles that employ air-breathing propulsion. Previous research in the present program established that in applications of this type the combustion often occurs in the reaction-sheet regime. Current work has therefore been focused on determining the structures and combustion limits of reaction sheets in these hydrogen-air systems. Influences of different descriptions of the chemical kinetics of combustion are being investigated with the objective of identifying the simplest kinetic scheme that gives results that are sufficiently accurate for use in engineering computations for the combustors of applied interest. In addition, the compressibility effects are being studied in various geometrical configurations.

RESEARCH OBJECTIVES

The objective of this research is to improve understanding of the chemical kinetics and fluid dynamics of turbulent combustion in high-speed flows. Supersonic combustion in hydrogen-air mixtures is being addressed by theoretical approaches that distinguish between reaction-sheet and distributed-reaction regimes. The work seeks to identify effects of compressibility in turbulent combustion, methods for including compressibility in theoretical analyses, and reduced chemical-kinetic mechanisms appropriate for supersonic combustion. The results may help to enhance capabilities of reasonable computations of high-speed turbulent reacting flows.

ACCOMPLISHMENTS

Boron Combustion

Although boron combustion is not part of the present program, the AFOSR grant preceding the present one concerned boron combustion, and publication of results from that work is being completed under the present grant. Items 1-3 of the list of publications concern articles on results of the research on boron combustion.

In the most recent work on this subject attention was focused on including low-temperature oxidation of boron with a liquid oxide present on the particle. Although diffusion of B through the liquid layer was established to be most important at higher temperatures, detailed consideration of Russian experimental results strongly suggested that at lower temperatures the diffusion of O_2 becomes more important. An expression was derived for the temperature at which this change-over in the controlling mechanism occurs. The principal accomplishments of our previous work can be summarized as follows:

A description of ignition and combustion of boron particles was developed with the aim of obtaining a theory that is as simple as possible yet consistent with available data. For the ignition stage the model involves equilibrium reactive dissolution of B in the thin $B_2O_3(\ell)$ layer to form dissolved BO, surface attack of BO by $O_2(g)$ and by $H_2O(g)$ to form $BO_2(g)$, and HOBO(g), respectively, vaporization of B_2O_3, and reaction of H_2O with $B_2O_3(\ell)$ to form HOBO(g). For the combustion stage the model involves clean-surface attack of B by $O_2(g)$ and $B_2O_3(g)$ followed by a gas-phase diffusion flame between B and O_2. Values of relevant rate constants were identified that achieved agreement with experiments. Early laser-ignition experiments, not previously explained quantitatively, were employed for obtaining needed dry-gas rate parameters. New experiments on ignition and combustion of boron suspensions in hot combustion products of a flat-flame burner

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were performed to test adopted values of wet-gas rate parameters. Results provide a basis for calculation of ignition and combustion of boron in propulsion applications.

Turbulent Combustion Regimes in Supersonic Combustion

In previous work, calculations had been completed of Damkölhler and Reynolds numbers for the anticipated range of supersonic combustion conditions showing turbulence Reynolds numbers to range from 10^3 to 10^7 and Damköhler numbers from 10 to 10^4. The latter results motivated the present focus on the reaction-sheet regime.

Counterflow Hydrogen-Air Flame Structure

The structure and extinction of counterflow diffusion flames of hydrogen and air were investigated for pressures from 0.5 to 10 atmospheres and for initial temperatures from 300 K to 1200 K as described in items 4 and 5 of the publications. Numerical integrations were performed for air-side strain rates from 60 s^{-1} to extinction. The numerical results were compared with predictions of an asymptotic analysis that involved reduction to one-step chemistry through introduction of steady-state and partial-equilibrium approximations. Reasonable agreement was found for concentrations in the main reaction zone at low strain rates.

When these flame-structure computations were first completed and extinction predictions were compared with available experimental results (from the NASA Langley facility), it was found that the predicted strain rate at extinction exceeded the measured value by nearly a factor of two. However, our computational results motivated refined experiments at Langley that produced the revised experimental extinction strain rates, for different hydrogen mole fractions X_{H_2} in hydrogen-nitrogen fuel mixtures, as listed in Table 1. Also shown in Table 1 are predictions of two other computational groups. It is seen in Table 1 that our predictions are in excellent agreement with experiment and that our agreement is better than that achieved by the other groups. We attribute this success to our careful selection of the best elementary rate constants available in the current literature. It seems especially noteworthy that for the hydrogen-air system our prediction preceded experiment and was subsequently confirmed.

X_{H_2}	Experimental	Dixon-Lewis	Issac Ho	Present Work
1.00	8250	13000	7750	8140
.80			7700	
.75				7100
.70	7580			
.60	6750		5900	
.50	5550	8600		4710
.40	3360		2750	3285
.35	2480			
.30	1850		1400	
.25	1100			1140
.21	660	1520	925	

Table 1: Comparison between experimental and one-dimensional numerical evaluations of extinction strain rates (s^{-1}) at atmospheric pressure with the feed streams at 300 K.

In the application of flamelet models to turbulent flames it may be valid and certainly efficient to consider simplified descriptions of both the chemical kinetic and the fluid mechanical processes. Therefore as an effort complementary to that described earlier an analysis of hydrogen-air flames in counterflowing configurations with reduced chemical kinetic and simple transport descriptions is underway. Programs permitting the limiting cases of frozen and equilibrium as characterized by the flame sheet approximation are completed and incorporation of a reduced mechanism to deal with finite rate chemical effects is presently underway. The results of these simplified descriptions will be compared with the full calculations discussed earlier in order to assess the possible errors in applications to turbulent flames. In this same regard attention is being devoted to the special features associated with the incorporation of flamelet models into turbulent flames in high speed flows in particular with the influence of fluctuations of temperature and pressure in the two streams. A review which includes some comments on these studies is to appear soon as publication 5.

In a more recent study we have employed asymptotic methods (publication 6) to analyze the displacement effects produced by heat release in counterflow flames. This work addresses the significant corrections called for to interpret properly experimental results in such flames, in particular on extinction strain rates. Introduction of these corrections was shown to bring theory and experiment into good agreement.

In even more recent work we have included nitrogen chemistry in our computations because we learned at the previous AFOSR contractor's meeting that concerns existed about the possibility of nitrogen chemistry significantly influencing flame structure and extinction. Our recent results demonstrate these influences to be negligible. For example, the effect on the maximum temperature, which we find to be greatest when we add 10^{-3} ppm of NO to a hot air stream, is always less than a 30 K change at a temperature in the range of 2800 K. For these reasons we do not currently plan to study effects of nitrogen chemistry further. Instead, our current direction seeks greater simplification in kinetics.

Extinction computations were performed with all H_2O_2 chemistry removed from the system, and the influence was found to be negligible. Recently computation schemes with four-step and with three-step reduced mechanisms have been implemented in our calculations. Preliminary results indicated that both of these reduced mechanisms yield excellent agreement with results of computations based on the full mechanism. Work is proceeding to test three-step and two-step approximations for achieving maximal simplicity. We already know that a one-step scheme will not give good extinction results.

Compressibility Effects

In previous work on this project a theoretical analysis of the inviscid flow between a porous plate and a parallel impermeable plate was performed for small values of the ratio of the plate separation distance to the lateral extent of the plates, for both planar and axisymmetric geometries, as described in item 7 of the publications. The problem of computing the flow field was reduced to the solution of a single integral equation, which was accomplished numerically. The ratio of specific heats γ was a parameter of the solution, and parametric results were obtained from $\gamma = 1.0$ to $\gamma = 1.67$. The flow exhibited choking at a critical value of the lateral extent of the plate, in the vicinity of which the Mach number approaches unity. The results are needed in providing external boundary-layer conditions for studying the flame structure in the viscous region between two counterflowing streams when compressibility is important.

It was observed that the same formulation that was employed in this study also can be applied to a model for the flow field in a laterally burning rocket motor. For this reason, such an extension was completed, although it is somewhat peripheral to our central objective. The results are presented in publication 7. Future work on compressibility effects is intended to return to counterflow-like configurations, considering structures that may arise in vortices.

SUMMARY

These continuing studies are helping to improve our understanding of structures of reaction zones in high-speed flows. Effects on descriptions of turbulent combustion remain under active consideration. In addition, investigations of compressibility effects and of reduced chemical-kinetic mechanisms continue to be pursued to improve understanding of turbulent supersonic combustion.

PUBLICATIONS

1. S.C. Li , "Optical Measurement of Size Histories of Boron Particles in Ignition and Combustion Stages in a Flat-Flame Burner," Combustion Science and Technology, to appear, 1991.

2. S.C. Li and F.A. Williams, "Ignition and Combustion of Boron in Wet and Dry Atmospheres," Twenty-Third Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, to appear, 1991.

3. S.C. Li and F.A. Williams, "Ignition and Combustion of Boron Particles," Second International Symposium on Special Topics in Chemical Propulsion: Combustion of Boron-Based Solid Propellants and Solid Fuels, Lampoldshausen, West Germany, 1991.

4. E. Gutheil and F.A. Williams, "A Numerical and Asymptotic Investigation of Structures of Hydrogen-Air Diffusion Flames at Pressures and Temperatures of High-Speed Combustion," Twenty-Third Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, to appear, 1991.

5. P.A. Libby, "Comments on the Interaction of Turbulence and Chemical Kinetics," Proceedings of the ICASE/NASA Combustion Workshop, October 1989 (to appear).

6. J.S. Kim, P.A. Libby and F. A. Williams, "On the Displacement Effects of Laminar Flames," Western States Section, The Combustion Institute, Boulder, CO, March 19, 1991. (To be submitted to Combustion Science and Technology.)

7. G. Balakrishnan, A. Liñán and F.A. Williams, "Compressibility Effects in Thin Channels with Injection," AIAA Journal, to appear, July, 1991.

8. G. Balakrishnan, A. Liñán and F.A. Williams, "Inviscid Flow in Laterally Burning Solid-Propellant Rocket Motors," Western States Section, The Combustion Institute, San Diego, CA, October 14-16, 1990.

PERSONNEL

		Percentage Time
Professor P.A. Libby	Principal Investigator	15%
Professor F.A. Williams	Principal Investigator	15%
Mr. S.C. Li	Postgraduate Research Engineer	50%
Mr. G. Balakrishnan	Ph.D. Student	100%

INTERACTIONS

Related talks/contributed papers by the PIs at meetings during the reporting period are:

"Considerations of the Structure of Premixed Hydrogen Flames," July 20, 1990, International Workshop on Flame Structure, Department of Engineering, Cambridge University, Cambridge, England.

"An Experimental and Theoretical Investigation of the Dilution, Pressure and Flow-Field Effects on the Extinction Conditions of Methane-Air-Nitrogen Diffusion Flames," "A Numerical and Asymptotic Investigation of Structures of Hydrogen-Air Diffusion Flames at Pressures and Temperatures of High-Speed Combustion," "Vortex Modification of Diffusion Flamelets," "Ignition and Combustion of Boron in Wet and Dry Atmospheres," July 22-27, 1990, Twenty-Third International Symposium on Combustion, University of Orléans, Orléans, France.

"Do Flames Really Penetrate Vortex Cores?", July 28-29, 1990, Tenth International Workshop on Mathematics in Combustion, University of Poitiers, Poitiers, France.

"Swirl Effects on Flame Structure," seminar, November 5, 1990, Technological Institute, Northwestern University, Evanston, Illinois"

"Some Advances in Combustion Theory Bearing on Fire-Safety, Energy-Production and Environmental Issues," keynote talk, March 21-22, 1990, 3rd ASME-JSME Thermal Engineering and ASME-JSME-JSES Solar Energy Conferences, Reno, Nevada.

INVENTIONS

None.