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13. ABSTRACT (Maximum 200 words)

This research involved theoretical studies of the chemical and fluid-mechanical phenomena which make turbulent combustion in high-speed flows different from such combustion in low-speed flows. Finite-rate chemistry plays a significant role in high-speed flows because of the small ratios of flow times to chemical times. The studies addressed ignition and extinction phenomena in nonpremixed turbulent combustion of hydrogen-air systems by both numerical and asymptotic methods. Efforts were made to provide a firmer foundation for the modeling of high-speed turbulent reacting flows, to aid in the development of a formulation which gives results that can be compared with experiments on turbulent combustion. It was shown that turbulent combustion occurs in the reaction-sheet regime in hypersonic propulsion, and the correspondingly needed critical ignition and extinction conditions for hydrogen-air systems were determined from fundamentals.

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THEORIES OF TURBULENT COMBUSTION IN HIGH SPEED FLOWS

1. INTRODUCTION

Uncertainties about turbulent combustion in hydrogen-air systems have an impact on our abilities to achieve successful designs of supersonic combustion devices for the National Aerospace Plane, for example. As a step toward addressing problems in this area, a research program on theories of turbulent combustion in high-speed flows was started at the University of California, San Diego. Prior to initiation of this research, it was not known whether the combustion was more likely to occur in reaction-sheet or distributed-reaction regimes, and in common practice was to assume the latter and employ laminar chemical kinetics in routines based on computational fluid mechanics. In the course of this research, estimates suggest that this is a poor procedure since the reaction-sheet regime is likely to be more prevalent than the distributed-reaction regime. Therefore, much of the research was directed towards determining regimes more firmly and developing improved methods for accounting for the chemical kinetics of the combustion in reaction-sheet regimes.

2. RESEARCH OBJECTIVES

The objective of this research has been to improve understanding of the chemical kinetics and fluid dynamics of turbulent combustion in high-speed flows. Supersonic combustion in hydrogen-air mixtures was addressed by theoretical approaches that distinguish between reaction-sheet and distributed-reaction regimes. The work sought 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.

3. EXECUTIVE SUMMARY OF ACCOMPLISHMENTS

The major accomplishments of the present work are summarized in the list of publications given below. The first nine of these twelve publications already are readily available, and the last three, all now accepted for publication in Combustion and Flame, soon will be readily available. Together, these twelve publications provide a complete record of the accomplishments of this program.

As a brief summary, it is of interest to indicate here the general thrust of each of the twelve publications. The aerospace-plane application dictated the selection of hydrogen-air systems for study, and it was reasoned [3,7] that in such systems the turbulent combustion is likely to occur in the reaction-sheet regime. For this regime we investigated flamelet structure, extinction and ignition [4-6, 8,11, 12] and compressibility effects [1,9], paying attention to approaches to modeling [2,10]. The research was mainly in combustion theory, employing both numerical and analytical methods, but also completed were experiments on extinction of laminar counterflow flames to test our theory [8].The general result was a greatly improved knowledge of flamelet structures in hydrogen-air systems, of useful reduced chemistry for describing flamelets, and of how to include flamelets properly in descriptions of turbulent reaction flows.

Besides the principal investigators, various visiting scientists participated in the research. These included K.N.C. Bray from England, M. Champion from France, E. Guthiel, F. Mauss and D. Trees from Germany, A. Liñán from Spain, C. Treviño from Mexico, and M.D. Smooke from Yale. F.A. Maury, from France, completed a Master's degree at USCD and returned to France. G. Balakrishnan completed his PhD at UCSD under this program and accepted an Assistant Professorship at Virginia Polytechnic Institute. Finally, J.S. Kim, who completed his PhD earlier at UCSD, participated in the research as a Postdoctoral Research Scholar at UCSD. All of these participants have co-authored one or more of the publications.

4. TURBULENT COUNTERFLOW COMBUSTION

Illustrative of how improvements in descriptions of turbulent combustion have been obtained from this work is the paper [10], soon to be published, on turbulent counterflow flames.

It is generally recognized that the greatest advances in both understanding and predicted capability are realized when close coordination of the experimental, theoretical and computational aspects of combustion research is achieved. However, this ideal is rarely attained. Nevertheless flames in stagnating turbulence provide a situation which permits this close coordination; we report here on our research devoted to these flames in nonpremixed systems.

Laminar flames in various opposed and impinging configurations have provided and continue to provide important fundamental results on the fluid mechanics and chemical kinetics of combustion phenomena. Thus, for example, one configuration studied extensively involves a fuel stream flowing opposite to an oxidizer stream setting up a flat laminar flame in the neighborhood of the stagnation plane. As a second example an

oxidizer stream inpinges on either a solid or liquid fuel. Finally, two identical streams of premixed reactants flowing opposite to one another result in two or three reaction zones depending on the stoichiometry of the two mixtures.

An important feature of all of these flames relates to the possibility of altering in a simple fashion the ratio of the flow time to the chemical time, i.e., to cover a range of Damköhler numbers. For purposes of discussion assume that the chemical time in each of these flows is fixed by the chemical composition, the temperature and the pressure. Now for fixed geometry the flow time depends on the velocity of the streams exiting from the jets so that by altering these velocities the Damköhler number can be continuously changed. Thus the entire range of chemical behavior from that corresponding to chemical equilibrium to frozen flow can be covered in one experimental set-up.

The other advantages of these flows relate to relative ease of their theoretical and computational treatment and thus to the possibilities they afford for the close coordination among the three aspects of combustion research discussed earlier. In particular, if attention is focused on the neighborhood of the axis, appropriate expansions in terms of the radial coordinate r reduce the partial differential equations characterizing conservation of mass, momentum, energy and species to a set of *ordinary differential equations* with the axial coordinate z as the sole independent variable. Thus the scope of the calculations dealing with the entire domain from one jet exit to the other in the case of opposed flows or from the jet exit to the wall in the case of impinging flows is significantly reduced.

Each of the laminar flames discussed here have their turbulent counterparts. The modification of the experimental set up to investigate turbulent flames involves installing a turbulence generating grid or baffle in each jet with the length scale of the turbulence depending on the geometry of the generator.

The experimental, theoretical and computational advantages attributed to laminar flames apply as well to these turbulent flames. Thus the entire range of an appropriately defined turbulent Damköhler number can in principle be covered in one experimental set-up and the related theoretical and computational efforts are significantly simplified by introduction of appropriate expansions of the turbulence quantities in terms of the radial coordinate. The possibility of studying extinction in turbulent flames is especially important since at the present time the theory of turbulent reaction flows exhibiting chemical equilibrium is well founded but the same is not the case for flows involving finite chemical kinetic effects, e.g., flows either undergoing extinction and ignition or producing minor species as a consequence of slow chemistry.

Experiments on turbulent flames in stagnating flows have been carried out and are presently underway in various laboratories in the United States, Western Europe and

Japan. Most of this experimental work has related to the premixed system but the group headed by Whitelaw at Imperial College published in 1992 the results of an experimental investigation of a turbulent nonpremixed flame in counterflowing fuel and oxidizer streams. The fuel is essentially methane and air is the oxidizer. These flames were found to be sensitive to rates of strain, i.e., could be established only for relatively low rates of strain, a feature which has significant theoretical implications.

Under our AFOSR contract we have for the first time studied theoretically the nonpremixed flames. A primary motivation for our research is the comparison of theory and the Whitelaw data. In this regard we note that although there have been several theoretical studies of premixed flames in stagnating turbulence no comparison with experiment has been made. Preliminary consideration of the experimental results establishes that because of the low rates of strain involved, the flame in question occupies a *significant fraction* of the space between the two opposed jets. As a consequence the applicability of the thin flame approximation used exclusively for previous analyses of premixed flames in stagnating turbulence is called into question. Accordingly, a new theory describing the entire flow from one exit plane to the other was developed, here for the nonpremixed system but the same approach should be applied to the whole spectrum of flames in stagnating turbulence.

In this first attempt at a theory for these nonpremixed flames in opposed fuel-oxidizer streams the k - ε theory is used to describe the fluid mechanics and a presumed pdf method and an equilibrium assumption is used to describe chemical behavior. The description of the chemistry is believed to be, and indeed is found to be, satisfactory but the k - ε theory is known to be inaccurate for the description of stagnating turbulence; in brief it does not predict accurately the anisotropy of the turbulence.

The comparison of our theoretical predictions with the experimental data of Whitelaw is somewhat flawed with responsibility divided in an uncertain fashion between the two elements; as indicated our fluid mechanical description can be improved and in the future we intend to apply a Reynolds stress description to this flow with the same treatment of the chemical behavior. However, the details of the experiment severely compromise the comparison; particularly troublesome is the nonuniformity of the flows exiting from the jets, a feature which calls into question the validity of the radial dependencies of the various dependent variables arising in the theory. In addition the long-standing difficulty relating to Favre-averaging versus conventional averaging arises here. The theory is based on the former averaging scheme whereas the experimental data for velocity is obtained from a LDA system while the state variables are obtained by thermocouples and sampling probes. It is believed by experimentalists that the LDV system results in statistical information

intermediate between Favre and conventional averaging but the state variables are believed to be close to conventional averages.

Thus we are not satisfied with the comparison of theory and experiment for the velocity characteristics but recognize that more satisfactory results require improvements in both elements involved. Somewhat surprising is the rather satisfactory agreement achieved for the mean molal concentrations of species; in particular the location and width of the reaction zone is quite well predicted but given the uncertainties in the fluid mechanical data this agreement may be fortuitous. The results of our studies has been accepted for publication in Combustion and Flame [10].

5. CHEMICAL KINETICS

In a study directed at determining the regimes in which turbulent combustion occurs for Aerospace-Plane applications employing hydrogen as fuel, calculations of the relevant Damköhler and Reynolds numbers were completed [7]. Flight Mach numbers M_f from 1 to 25 were considered at altitudes from 11 to 80 km, with the U.S. standard atmosphere. An average diffuser efficiency of 95% (recommended by engine manufacturers) was employed, with combustor air Mach numbers of $M_f/2$ for $M_f \leq 4$ and $M_f/2 - 1$ for $M_f > 4$, fuel stream Mach numbers from 1 to 4, temperatures from 300 to 1200 K, and a characteristic combustor dimension of 0.3 m. Resulting combustor static pressures range from 0.3 to 5.0 atm. The results showed that Damköhler numbers always exceed unity, so that the reaction-sheet regime is the appropriate one. These results directed our subsequent research to the reaction-sheet regime.

One of our first tasks was to evaluate all data on rates of relevant elementary reactions for the hydrogen-air combustion system. A set of 21 key elementary steps was identified, and their rate parameters were determined [7]. This work provides the most up-to-date (and now entirely sufficient) information on elementary rates. In particular, persistent significant uncertainties about the H + O_2 branching step have now been resolved. It is strongly recommended that our rate data, some non-Arrhenius, be used in subsequent investigations. Unfortunately, too few researchers update their data in this way, and many still use inferior data.

Having determined the combustion regime and elementary rates, we analyzed the external compressible flow to define needed boundary conditions for the flamelet analysis [1]. In particular, 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. The problem of computing the flowfield was reduced to the solution of a

single integral equation, which was accomplished numerically. The ratio of specific heats γ was taken as a parameter of the solution, and parametric results were calculated from $\gamma =$ 1.0 to 1.67. The flow exhibits 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, as mentioned above.

In further clarification of the flamelet structure, asymptotic methods were used to evaluate the relevant characteristic diffusion time (the reciprocal of the so-called "scalar dissipation rate") for counterflow diffusion flames. Attention was restricted to the practically important limit of small values of the stoichiometric mixture fraction, which results in large values of the stream function at the reaction sheet, a quantity that was employed as a large expansion parameter. Three distinct layers were identified inside the viscous layer: (i) a convective-diffusive layer on the oxidizer side of the reaction sheet, (ii) a rotational inviscid layer on the fuel side of the reaction sheet, and (iii) a fuel-product mixing layer in the vicinity of the stagnation plane; all three of these layers were analyzed and matched. The matching produces analytic expressions for the stream function and mixture fraction at the reaction sheet and corrects formulas for the characteristic diffusion time previously derived on the basis of constant-density-flow or nonreactive-mixing-layer assumptions. Comparisons between analytical and numerical results demonstrated that the analytical results obtained provide accurate expressions for the characteristic diffusion times that are needed in analyses of flame structure and extinction. These results are being used in all of the subsequent analyses of the subsonic portions of the flamelets. They provide a very useful and accurate simplified strain-rate formula that is now employed extensively by the investigators.

Finally, the chemical kinetics within the flame itself were addressed numerically for both full and reduced chemistry [12]. The structure, extinction and ignition of counterflow hydrogen heated-air systems were investigated for pressures and temperatures of interest in high-speed aerospace applications. A critical assessment of the recent literature was made to reverify that our chemical-kinetic scheme is applicable for the aforementioned conditions of interest. Numerical integrations were performed for various strain rates using a continuation code which handles the singularities in the Jacobian matrix at critical strain-rate parameters. The numerical results with the detailed chemical scheme were compared with results obtained from a four-, three- and two-step reduced chemical-kinetic scheme. Although good agreements for extinction and ignition strain rates were obtained, the two-step mechanism provides rather poor predictions of minor-species concentrations. Thermal

diffusion was found to play an important role in diluted flames at high oxidizer temperatures and low fuel temperatures but to be relatively inconsequential at high fuel temperatures or in pure hydrogen-air systems. These results provide the community with the needed chemical-kinetic aspects of the hydrogen diffusion flamelet structure.

It is always satisfying to test theoretical and computational predictions against experiment. G. Pellet at NASA Langley has been trying to complete the relevant experiments for nearly ten years now. Unfortunately he always works with low aspect ratios, for which the theories are inaccurate and for which much more complicated computational methods would be needed. The theories apply at high aspect ratios. For this reason, we performed experiments on diffusion-flame extinction at high aspect ratios in our laboratory [8]. The agreements with the results of the computations were excellent and truly satisfying. This provided further indication that we had indeed solved the chemical-kinetic problem that we had set out to address.

6. PRESENTATIONS

"The Role of Theory in Combustion Science," Hottel Plenary Lecture, Twenty-Fourth International Symposium on Combustion, Sydney, Australia, July 6, 1992.

"The Role of Turbulence Modeling in Combustion," Center for Turbulence Research, Stanford University, July 23, 1992.

"Theory of Premixed Turbulent-Flame Propagation in Reaction-Sheet Regimes," Euromech 294, University of Bristol, Bristol, England, September 2, 1992.

"Advances in Modeling of Turbulent Combustion," Sixth Toyota Conference, Mikkabi, Japan, October 12, 1992.

"Hydrogen Diffusion-Flame Studies for High-Speed Propulsion," ICASE, NASA Langley, Hampton, VA, October 23, 1992.

"Theories of Turbulent Combustion in High-Speed Flows," AFOSR Contractors' Meeting, Atlantic City, NJ, June 14, 1993.

"Asymptotic Analysis of Stoichiometric and Lean Hydrogen-Air Flames," International Workshop on Mathematics in Combustion, Santiago de Compestela, Spain, July 24, 1993.

"Autoignition of Nonuniform Mixtures in Chambers of Variable Volume," 14th International Symposium on Dynamics of Explosions and Reactive Systems, Coimbra, Portugal, August 3, 1993.

"Reduced Chemistry for Hydrogen-Air Supersonic Combustion," Department of Chemical Engineering, UCLA, Los Angeles, CA, November 22, 1993.

"Turbulent Combustion," Department of Aerospace and Mechanical Engineering," University of Southern California, Los Angeles, CA, April 7, 1994.

"Combustion Theory and Conditional Moment Closure Modeling," Zel'dovich Memorial International Conference on Combustion, Moscow, Russia, September 13, 1994.

"Free Boundary Problems in Nonpremixed Combustion," ESF/FBP Workshop on Free Boundary Problems in Combustion, Arcachon, France, March 24, 1995.

7. INTERACTIONS

There have been continuing interactions with groups at Cambridge University, England and Poitiers, France on theories of turbulent combustion. These interactions have led to joint research publications.

There have been continuing interactions with the group of M.D. Smooke at Yale. These interactions have led to joint publications on hydrogen-air diffusion-flame structures.

There have been interactions with the group of C.K. Law at Princeton, particularly with Dr. T. Kreutz of that group, concerning hydrogen-air diffusion-flame structures. These interactions became contentious when the present research established that the results of Kreutz on diffusion-flame ignition in hydrogen-air systems are unexplained physically and possibly erroneous.

There have been interactions with T. Gatsky at NASA Langley on simulation of turbulent diffusion flames and with M. Hussaini and others of ICASE, at the same location, on the use of reduced chemistry for hydrogen-air systems in turbulent simulations and modeling.

There have been interactions with H. Chelliah and others at the University of Virginia on use of reduced chemistry in modeling turbulent combustion.

There has been continuing interaction with A. Liñán and co-workers at the University of Madrid in Spain on the theory of the structure of hydrogen-air diffusion flames. These interactions have led to joint publications.

There have been continuing interactions with the group of N. Peters at the university RWTH in Aachen, Germany on development of reduced mechanisms for describing the chemistry of diffusion flames. These interactions also have led to joint publications.

There have been interactions with the group under P. Moin at the Center for Turbulence Research of Stanford University on the use of reduced chemistry in turbulence simulations of reacting flows. These interactions have led to their adoption of some new simulation methods.

There have been interactions with W.T. Ashurst and others at the Sandia Combustion Research Facility in Livermore, California. These interactions, too, have led to modifications in methods of simulation of turbulent reacting flows.

8. INVENTIONS

None.

9. PERSONNEL

Principal Investigators: P.A. Libby and F.A. Williams

Graduate Students: G. Balakrishnan and F.A. Maury

Post-Doctoral Researchers: J.S. Kim

Visiting Researchers: N.K.C. Bray, M. Champion, E. Guthiel, A. Liñán, F. Mauss, M.D. Smooke, D. Trees, C. Treviño.

See Section 3 for a more thorough discussion of personnel.

10. PUBLICATIONS

1. G. Balakrishnan, A. Liñán, and F.A. Williams. Compressibility effects in thin channels with injection. *AIAA Journal*, 29(12):2149-2154, December 1991.

2. K.N.C., Bray, M. Champion, and P.A. Libby. Premixed flames in stagnating turbulence: Part I. the general formulation for counterflowing streams and gradient models for turbulent transport. *Combustion and Flame*, 84:391-410, 1991.

3. G. Balakrishnan. *Studies of Hydrogen-Air Diffusion Flames and of Compressibility Effects, Related to High Speed Propulsion.*. PhD thesis, University of California San Diego, September 1992.

4. G. Balakrishnan, C. Treviño, and F. Mauss. Asymptotic structure of hydrogen-air diffusion flames. *Combustion and Flame*, 91(3-4):246-256, December 1992.

5. E. Guthiel, G. Balakrishnan, and F.A. Williams. Structure and extinction of hydrogen-air diffusion flames. In N. Peters and B. Rogg, editors, *Reduced Kinetic Mechanisms for Application in Combustion Systems*. Springer Verlag, Berlin, 1993, Chapter 11, pp. 177-195.

6. J.S. Kim and F.A. Williams. Structures of flow and mixture fraction fields for counterflow diffusion flames with small stoichiometric mixture fractions. *SIAM Journal on Applied Mathematics*, 53(96):1551-1566, December 1993.

7. G. Balakrishnan and F.A. Williams. Turbulent combustion regimes for hypersonic propulsion employing hydrogen-air diffusion flames. *Journal of Propulsion and Power*, 10(3):434-436, May-June 1994.

8. G. Balakrishnan, D. Trees, and F.A. Williams. An experimental investigation of strain-induced extinction of diluted hydrogen-air counterflow diffusion flames. *Combustion and Flame*, 98 (1-2):123-126, 1994.

9. K.N.C. Bray, P.A. Libby and F.A. Williams. High Speed Turbulent Combustion. In P.A. Libby and F.A. Williams, editors, *Turbulent Reacting Flows*, Academic Press, London, to appear, 1994, Chapter 10, p. 609-638.

10. F.A. Maury and P.A. Libby. Nonpremixed flames in stagnating turbulence. Part I. The k - ε theory with equilibrium chemistry for the methane-air-system. *Combustion and Flame*, to appear, 1995.

11. K.N.C. Bray, M. Champion and P.A. Libby. Premixed combustion in laminar Couette flow. *Combustion and Flame*, to appear, 1995.

12. G. Balakrishnan, M.D. Smooke, and F.A. Williams. A numerical investigation of the ignition and extinction limits in laminar nonpremixed counterflowing hydrogen-air streams. *Combustion and Flame*, to appear, 1995.