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COMBUSTION PHENOMENA IN CHEMICAL LASERS

FINAL REPORT

1 May 1974 - 30 September 1977

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This final report briefly recapituates the problems studied, the results obtained, and the documents published under the subject project. Attention was focused on the modeling of "pumping" phenomena (i.e., the formation of activated product gas HF^*) in diffusion-type continuous (CW) chemical lasers of hydrogen-fluorine technology. The geometry examined was the "basic building block" of conventional CW lasers, essentially the plane parallel mixing → over

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20. Abstract (Continued)

layer formed by coflowing streams of diatomic hydrogen and monatomic fluorine. (Aside from one task involving the two-step symmetrical chain reaction, in which the hot slow chemical reaction and the cold fast chemical reaction were considered, only the case of high dissociated fluorine was examined.) The nature of reported unsteadiness in the lasing portion of the cavity was reviewed, in order to discern whether introduction of time-averaged modeling of turbulent diffusion flames is warranted for quantitatively accurate description of pumping. Because of the low pressure required in the cavity to prevent too rapid collisional deactivation of activated product gas, it is concluded that models developed for very-large-Reynolds-number, "conventional" aerodynamic flows with rapid burning of initially unpremixed gases, are probably inappropriate for the description of pumping phenomena. It is suggested that effectively laminar models, with appropriate starting conditions, may suffice to describe the preponderance, if not all, the lasing zone.

FINAL REPORT*

I. Participants in this Project

Participants in this project, in addition to Francis Fendell (principal investigator), were Phillip Feldman (TRW, numerical analysis), George Carrier (Harvard University, consultation on fluid dynamics), and William Bush (University of California, San Diego, consultation on approximate analysis).

The participants are grateful for encouragement and guidance from Charles Harmon, James Murray, and Robert Singleton of the Engineering Sciences Division, U.S. Army Research Office, Research Triangle Park, North Carolina; they wish to express their gratitude to William Martin, U.S. Army Missile Command, Redstone Arsenal, Alabama for technical input and detailed review of the work executed under this project.

II. Publications under this Project

1. Carrier, G. F. & Fendell, F. E. 1976 The effect of strain rate on diffusion flames. II: Large straining. SIAM J. Appl. Math. 30, 515-527.
2. Bush, W. B. & Fendell, F. E. 1975 On diffusion flames in turbulent shear flows — the two-step symmetrical chain reaction. Combust. Sci. & Tech. 11, 35-48.
3. Bush, W. B. & Fendell, F. E. 1976 On diffusion flames in turbulent shear flows: modeling reactant consumption in a mixing layer. Combust. Sci. & Tech. 13, 27-54.
4. Bush, W. B., Feldman, P. S., & Fendell, F. E. 1977 Comments and replies. In Special Issue on Turbulent Reactive Flows, ed. by F. V. Bracco. Combustion Sci. & Tech. 13, 22-23, 50-54, 74-75, 95-97, 144-147, 165-168, 253-255.

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*The findings in this report are not to be construed as an official Department of the Army position, unless so designated by other authorized documents.

5. Bush, W. B., Feldman, P. S., & Fendell, F. E. 1977a On diffusion flames in turbulent shear flows — modeling reactant consumption in a planar fuel jet. AIAA Paper 77-96, 22 pp.

6. Bush, W. B., Feldman, P. S. & Fendell, F. E. 1977b On diffusion flames in turbulent shear flows — modeling reactant consumption in a planar fuel jet. Combust. Sci. & Tech., to appear.

7. Bush, W. B. & Fendell, F. E. 1977 Analytic modeling of turbulent shear flow with chemical reaction, 26 pp. In Turbulent Combustion, ed. by L. Kennedy (vol. in Progress in Astronautics and Aerodynamics, ed. by M. Summerfield), to appear. New York, New York: AIAA. (Preliminary version presented at the ARO-BRL Workshop on Mathematical Modeling in Combustion, 23-24 February 1977, U.S. Army Ballistic Research Laboratories, Aberdeen Proving Grounds, Maryland.)

III. Problems Studied and Major Findings

A. *An Engineering Overview*

Theoretical prediction of power output of a diffusion-type continuous chemical laser, involving (very rapid direct one-step irreversible exothermic) reaction between unpremixed diatomic hydrogen and monatomic fluorine, remains a major goal of Army laser technology. An evaluation of existing predictive techniques characterizes them as semiempirical; extrapolation to new design parameters readily incurs errors of factors of two or more in power-output predictions. This project was concerned with trying to improve the predictive capability for power output.

By 1974, two observations were widely, but (in retrospect) probably unwarrantedly, interpreted to imply that "pumping phenomena" (i.e., the formation of activated hydrogen fluoride HF^*) occurred under turbulent conditions. For the plane-parallel-mixing-layer geometry that forms the basic building block of more conventional CW lasers, these observations were as follows: (1) the effective thickness of the mixing layer, as indicated by the presence of product gas HF^*, appeared to grow linearly after a given distance downstream; and (2) transverse injection of diluent (later, of reactant) from the "splitter plate" enhanced power output by apparently augmenting mixing of the gaseous combustibles. However, enhanced mixing does not necessarily imply transition is effected by the transverse injection, although injection became widely referred to as "tripping." Perhaps a degree of unsteadiness does occur in the laser portion of the cavity, but experience with wake-type flows suggests that the lasing-zone conditions are incompatible with transition to well-developed turbulence familiar from aerodynamic-type flow. The lasing-zone portion of the cavity, which is about 3 in long, is characterized by Mach number 1 to 4.5; Reynolds number 2000/in to 20,000/in; pressure 5 to 30 torr. The major contribution of this program was to identify this misconception and then to challenge the use of conventional aerodynamic phenomenology for fully developed turbulence in modeling pumping phenomena. Such extrapolative procedure was at least partly responsible for overestimates of CW laser performance by existing computer codes, together with inadequate provision for collisional deactivation in some cases.

In fact, TRW is currently achieving adequate prediction of CW laser power performance on the basis of an essentially laminar model, with proper initial conditions. What has been prohibitively expensive to compute in the past, by use of the Navier-Stokes equations, is the flow in the viscous hydrogen nozzle and in the viscous fluorine nozzle from throat to exit. Hence, proper starting conditions for the laser cavity flow have rarely been available, to initiate analysis of the pumping phenomena. Monte-Carlo computer simulation of molecular motion in the low-density nozzle flows now presents a viable alternative method for obtaining suitable initial conditions for laser-cavity-analysis computer codes as **LAMP**. Thus support of such Monte Carlo calculations is advocated here as the CW laser modeling activity most deserving of support at this time.

Finally, the principal investigator wishes to bring attention to the fact that the preponderance of turbulent reacting flow problems arising in engineering design entail turbulent diffusion flames. That is, rapidly reacting, initially unmixed combustibles are preferred, for reasons of safety and control, by designers. Overly intricate formulations of mixing and of chemical mechanisms introduce so many unknowns that these models may incur greater expense, but may achieve little more validity, than more rapidly analyzed, more readily interpreted models with explicit, low-order closure. For the preponderance of engineering flows, in which the rate of product formation is inviscidly controlled through macroscale mixing (as opposed to microscale diffusion and kinetics), key information relating performance to alteration in controllable input parameters is often furnished adequately by simple closure. Thus, this project on chemical lasers also provides a case in point that overly elaborate computer codes do not always justify the expense incurred, in that simpler models guide design just as adequately. Adding some refinements, while still omitting others of comparable importance, results in intricate models with little net improvement in predictive capability.

B. Specific Analysis Carried Out

Very brief description is now given of specific analyses executed under this project; further details are available in the publications themselves.

First, the enhancement in rate of product-gas generation for unpremixed combustibles in an unsteady flow field is related to (1) the augmented area of exposure of fuel to oxidant, and to (2) increased transport to the reaction zone per unit area; the augmentation occurs provided the rate of straining does not outstrip the rate of reaction, and provided one reactant is not locally depleted [1].

Next, it is pointed out that unpremixed reactants are especially segregated under the two-step symmetrical HF chain, such that the role of diffusion (omitted in early CW laser models) is nonnegligible; poor CW laser performance on the chain is linked to the reduced rate of the hot step, and to enhanced deactivation rates [2].

A plausible, simple time-averaged description of reactant consumption, and hence of product generation, at the downstream end of the mixing-lasing region, is given as a function of velocity and temperature differential of the two bounding streams, of the stoichiometry of the reaction and the richness of the bounding streams, of the Schmidt number, etc. [3]. While the results are no less plausible than those of more elaborately conceived alternatives [4], still, in the absence of experimental data for the mixing layer, it adds confidence to demonstrate the ability of the same simple model to recover experimental data that is available for turbulent-fuel-jet diffusion flames [5,6].

The problem now warranting attention is establishing valid starting conditions for the velocity, temperature, and mass fraction fields at the laminar upstream end of the mixing-layer geometry [7]; since the lasing zone (preponderantly, if not entirely) consists of developing flow, not selfsimilar flow, sensitivity of results to starting conditions is large.

Finally, work on modes of interdiffusion of initially separated gases, initiated under another ARO program, was brought to completion during this project [8].