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# Report on "An Experimental and Theoretical Study of Radiative Extinction of Diffusion Flames," NASA grant no. NAG3-1271

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by

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## ABSTRACT

The objective of this work is to investigate the radiation-induced rich extinction limits for diffusion flames. Radiative extinction is caused by the formation of particulates (e.g., soot) that drain chemical energy from the flame. We examine $\mu g$ conditions because there is a strong reason to believe that radiation-induced rich-limit extinction is not possible under normal-gravity conditions. In normal- $g$, the hot particulates formed in the fuel-rich flames are swept upward by buoyancy, out of the flame to the region above it, where their influence on the flame is negligible. However, in $\mu g$ the particulates remain in the flame vicinity, creating a strong energy sink that can, under suitable conditions, cause flame extinction.

## 1. PROGRESS FOR THE PERIOD JAN. 1, 1993 - DEC. 31, 1993:

### Simplified Radiation/DF Model:

We have found that a relatively simple model of radiation/DF interaction contains many features of more complex models. Thus, we have focused on the "top hat" soot-zone heat-loss profile. For the "top-hat" profile, four conditions must be met: (i) optically thin soot layer, (ii) soot density approximately constant across soot layer, (iii) the factor $T\left(T^4 - T_0^4\right)$ can be replaced by $T_R\left(T_R^4 - T_0^4\right)$ in the heat-loss term, where $T_R=''$ characteristic radiation layer temperature, and (iv) the soot mass fraction $Y_s$ also has a "top hat" profile, zero outside the soot layer and constant (positive) within. In addition we neglect gaseous radiation (from, e.g., $CO_2$ and $H_2O$) and do not examine a separate species equation for the soot. There is much evidence that soot mass fractions are rather small and that its influences on fuel (and oxidizer) mass fractions is also quite small. Consequently the influence of the radiating soot layer is primarily thermal: the fuel and oxidizer profiles are essentially unaltered but may be changed through their relation to T, which is directly influenced by the soot layer.

Unless the soot layer overlaps with the flame zone there is essentially no influence of the soot layer on the flame chemistry. The use of standard AEA techniques reduces the governing equations to $\Phi_{\eta\eta} = \left(\Phi^2-\eta^2\right)exp\left[-\left(\Phi+a_R\eta\right)/b_R\right]$, $\Phi_\eta(\pm\infty)=\pm1$. Here $\Phi$ is the perturbation to the temperature/heat loss profile, and $a_R$, $b_R$ are defined in a manner similar to Linan (1974). However, because of radiant losses $a_R$ is larger and $b_R$ smaller than it otherwise would be. These influences, we note, act in concert to facilitate extinction. That is, they are complementary influences producing the same thing...a weakened -- perhaps extinguished -- flame. Interesting deductions are:

1) The increase of $a_R$ over $a$ (its value without radiation) is achieved by decreasing the temperature gradient on the oxidizer side while increasing it on the fuel side. This is exactly what the soot layer does.

2) Because the temperature gradient on the oxidizer side can decrease only so much without becoming negative (a physical impossibility for ordinary DF's), the quantity $N_1\Delta Z_{soot}=N_R\left(Z_+-Z_-\right)$ has an upper sound. Here $N_R$ is the ratio of heat losses by radiation to heat generation by reaction. Thus, if $N_R$ increases, through increased $T_R$, the soot layer can become thinner ($\Delta Z_{soot}$ decreases) without diminishing the radiative heat losses.

Our work on this project has been accepted for publication in Combustion and Flame under the title "On the Influence of a Fuel-Side Heat-Loss ("Soot") Layer on a Planar Diffusion Flame" by I.S. Wichman. The article is being revised slightly to be resubmitted in final form in early January, 1994. The revisions are cosmetic.

### Pyrolysis Model for Soot Formation:

The PI has extensively studied a reaction mechanism for the pyrolysis of cellulosic materials, the so-called "Broido mechanism," that cogently and elegantly describes the essential features of the breakdown of the cellulose molecule to form tar (volatile gases) and char.

Basically, the cellulose breaks down to an intermediate or "active" compound that may follow one of two routes (tar or char) depending on the temperature, T.

The analogy to the soot formation process is very strong. Here, intermediate ("precursor") species like $C_2H_2$, $C_2H_4$ ... are formed from some of the fuel; these species either become soot or enter the diffusion flame as trace amounts of secondary fuel. The goal is to exploit the bifurcational tendency of the Broido-like model to describe this mechanism.

Our progress in this area has been in the detailed examination of the Broido mechanism. We have submitted the following articles on this subject:

> Wichman, I.S. and Oladipo, A.B., "A Comparison of Three Common Reaction Schemes for Cellulosic Materials," presented at the Winter Annual Meeting of the ASME, New Orleans, Dec. 2, 1993.
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> Wichman, I.S. and Oladipo, A.B., "Examination of Three Pyrolytic Reaction Schemes for Cellulosic Materials," submitted to the 1994 International Association for Fire Safety Science Symposium in Ottawa, Canada.

## 2. GOALS FOR THE PERIOD JAN. 1, 1994 - DEC. 31, 1994:

We have three goals for this period.

(1) Extend the simplified model to the case with convection and thermophoresis, since these two processes seem to be important in the overall analysis. We wish to make some comparisons with experimental results, since our previous work (to be published in C & F) has generated formulae that can estimate practical quantities (like soot-zone thicknesses, etc.)

(2) Perform the 2-D azimuthally-symmetric droplet burning computation, using the low-Re $\mu g$ theory developed in: Wichman, I.S. and Baum, H.R., "A Solution Procedure for Low Reynolds Number Combustion Problems Under Microgravity Conditions," Proceedings of the Winter Annual Meeting of the ASME, No. HTD - Vol. 269, pp. 111 - 117 (1993). For the geometry and conditions that we shall examine, a computational method of solution will be developed.

(3) Formulate and thoroughly examine a soot formation mechanism based largely on the Broido scheme already discussed. We shall also include nucleation criteria, physical growth processes (coagulation, etc.) and other mechanisms like oxidation, etc. Models already exist for nucleation and coagulation etc. in the aerosol literature, and the oxidation model may, for the time being, remain rather primitive. What we wish to establish is a reasonable, working model for the breakdown of the fuel to a certain set of "precursors" that in turn allow the sooting mechanism to occur. The model must be simple enough to be understandable and instructive yet complex enough to be descriptive and useful.

Budget (1/1/94 - 12/31/94)

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| Salaries | |
| Indrek Wichman, Principal Investigator<br>27% Summer | $5,292 |
| Graduate Assistant<br>Level II, 1/2 time | $16,454 |
| Undergraduate Student Hourly | $6,890 |
| TOTAL SALARIES | $28,636 |
| Fringe Benefits | |
| Faculty Summer @ 7.5% | $397 |
| Graduate Assistant Tuition Waiver* | $2,001 |
| TOTAL FRINGE BENEFITS | $2,398 |
| TOTAL DIRECT COST | $31,034 |
| Indirect Cost @ 45% MTDC | $13,966 |
| TOTAL COST | $45,000 |

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*Tuition Waiver to be charged to grant for Summer and Fall 1994 semesters. Spring 1994 semester tuition to be paid from account 61-2760.