**NISTIR 6242**

# ANNUAL CONFERENCE ON FIRE RESEARCH
## Book of Abstracts
## November 2-5, 1998

Kellie Ann Beall, Editor

Building and Fire Research Laboratory
Gaithersburg, Maryland 20899

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**United States Department of Commerce**
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**Intermediate Species Profiles in Low Pressure Methane/Oxygen Flames Inhibited by 2-H Heptafluoropropane: Comparison of Experimental Data with Kinetic Modeling**

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The U.S. Navy has selected 2-H heptafluoropropane (HFP, HFC-227ea) to replace Halon 1301 for some of its near term fire protection needs. HFP has a lower suppression efficiency compared to Halon 1301. It is important to understand the suppression behavior of this compound in order to optimize its performance. Of particular importance is the relative contribution of fluorine chemistry to suppression as opposed to the physical effects of the agent's addition to the flame.

A comprehensive mechanism for $C_1$ and $C_2$ fluorohydrocarbon agents has been developed at the U. S. National Institute of Standards and Technology (NIST) [1]. Recently, our laboratory has measured profiles of several intermediate species in premixed low-pressure methane/oxygen flames containing each of the fluoromethanes [2]. The experimental data were compared to predictions of the NIST fluorohydrocarbon mechanism with the $C_1$ hydrocarbon chemistry modeled using GRI-Mech [3]. Some refinements to the kinetics were suggested by this work on the basis of validation against the low pressure species profile data. Comparison of flame speed predictions of the modified mechanism to atmospheric pressure measurements indicate that the modifications do not substantially alter the mechanism's performance for stoichiometric to slightly fuel rich flames. Here we extend this work to include HFP inhibited flames.

For the present study, the experimental apparatus and procedures were identical to those used in our study on flames containing fluoromethanes [2]. We recorded profiles of H, OH, CH, CF, $CF_2$ and C.F., derived from LIF intensities, in 10 torr premixed flat flames of methane/oxygen (1:2 molar ratio) inhibited by 4% mole fraction of HFP. The previously reported flames contained the series of fluoromethanes at concentrations corresponding to the same fluorine loading as 4% HFP. All of the data were taken under the same conditions so that direct comparisons can be made on relative mole fractions of intermediate species produced from the different agents. The HFP flame data were not previously reported as a suitable $C_3$ fluorohydrocarbon kinetic mechanism was not available. Hynes *et al.* [4] have recently published a kinetic mechanism for the initial breakdown of HFP into $C_1$ and $C_2$ fragments. When added to the NIST HFC mechanism describing the subsequent chemistry of decomposition products, the HFP sub-mechanism permits kinetic modeling of the HFP-inhibited flame.

We compared the predictions of the HFP kinetic mechanism with our species profile data. The data for $CF_2$ is presented in Figure 1. Both the location and magnitude of this specie are well predicted by the Hynes et al. mechanism. Similar agreement was observed for the other species studied. We also compared the experimental profiles for the flame inhibited by HFP to data for flames containing $CHF_3$ and $CH_2F_2$ under the same conditions of stoichiometry and flux of fluorine atoms. Under these conditions, profiles of temperature and of H and OH mole fraction are identical between the flames containing HFP and $CHF_3$. The flame inhibited by HFP, however, is much more luminous than the flames containing the $C_1$ fluorohydrocarbons. The model points out that thermal decomposition, not

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radical attack, dominates HFP destruction. This is in contrast to the conditions of Hynes *et al.* in a low temperature hydrogen/air flame where radical attack predominated.

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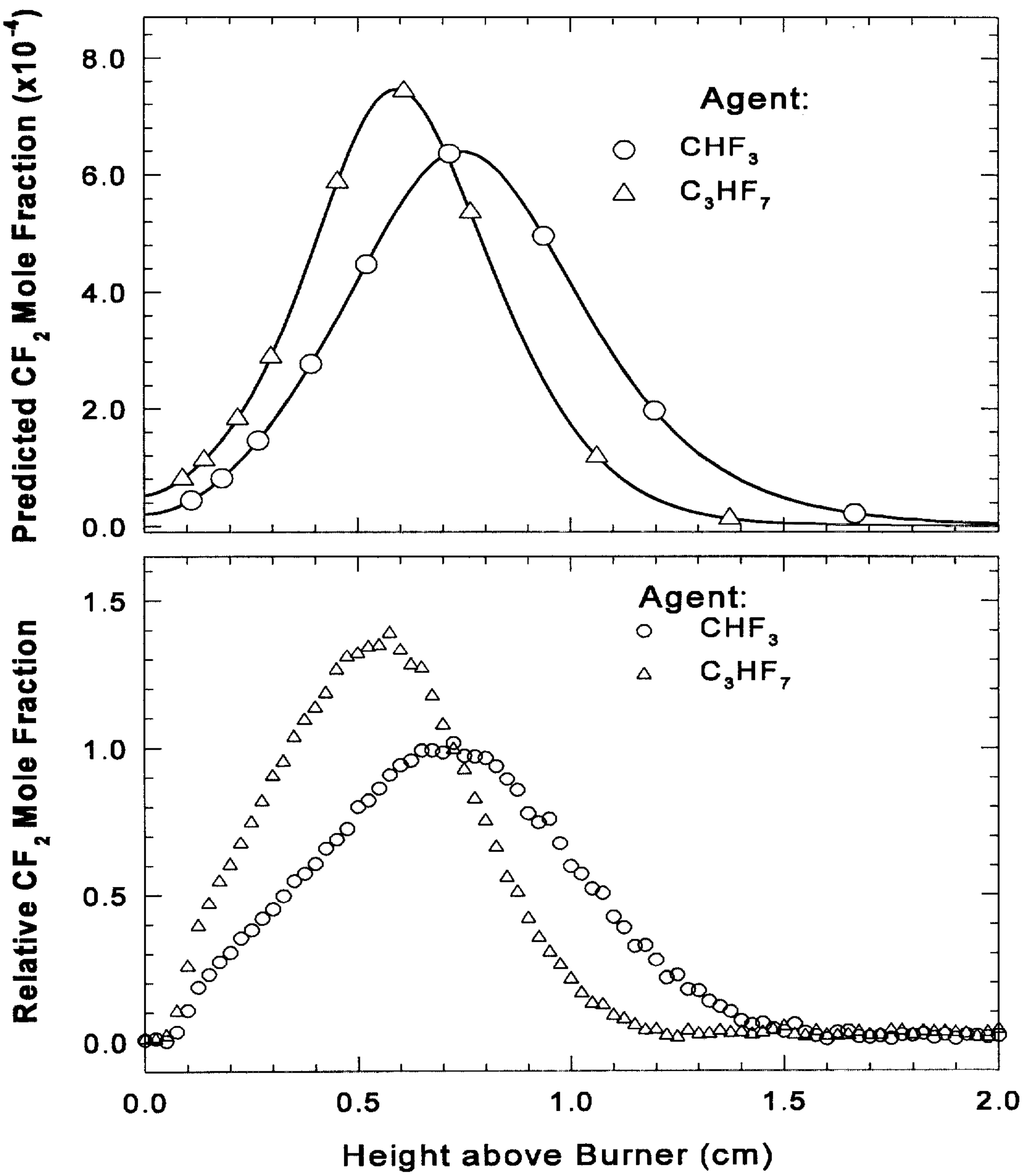


FIGURE 1. Calculated (top) and measured (bottom) profiles of $CF_2$ in a 10 Torr premixed $CH_4/O_2$ (1:2 mole ratio) flame containing 4% 2-H heptafluoropropane (triangles) or 8.9% $CHF_3$ (circles).