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# SUMMARIES OF BFRL FIRE RESEARCH IN-HOUSE PROJECTS AND GRANTS, 1994

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Nora H. Jason, Editor

**NIST**

United States Department of Commerce  
Technology Administration  
National Institute of Standards and Technology

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Nora H. Jason, Editor  
Building and Fire Research Laboratory  
National Institute of Standards and Technology

October 1994



**U.S. Department of Commerce**  
Ronald H. Brown, *Secretary*  
**Technology Administration**  
Mary L. Good, *Under Secretary for Technology*  
National Institute of Standards and Technology  
Arati Prabhakar, *Director*





## PREFACE

The United States continues to have one of the worst fire loss records in the world. The annual life loss is still over 4000, direct property losses now exceed \$10 billion, and the total cost of fire to the nation is nearly \$128 billion. Fire is thus a significant threat to the population and a major constraint on the economy.

Improving this deplorable profile requires the concerted efforts of fire safety professionals. Change results from new fire safety practices and technologies, new fire-safe products, and an advanced approval process for bringing those products to market quickly and efficiently. The advent of these innovations offers both societal and commercial opportunities.

Much of the technical basis for a less fire-prone nation results from the National Institute of Standards and Technology (NIST)/Building and Fire Research Laboratory (BFRL) work. The BFRL Fire Research Program is nationally recognized as the focal point for fire research in the United States. BFRL has a state-of-the-art, multi-disciplinary technical staff that is supported by extensive laboratory and computing facilities and a definitive fire research library.

The BFRL pursues NIST's commitment to meeting the critical needs of the fire safety industries and the governmental and private fire protection communities. BFRL staff perform basic research to improve the understanding of the elemental phenomena of fire and applied research to develop or to adapt technological tools and procedures to address critical issues of fire safety. We work closely with industrial counterparts to promote the development of new materials and products that will reduce the impact of unwanted fires. In addition to our in-house program, the BFRL maintains a fire research grants program that supports most of the academic fire research in the United States. This was initiated under the Federal Fire Prevention and Control Act of 1974, which authorized the Secretary of Commerce to conduct a fire research program directly or through contracts and grants.

This report describes the fire research projects performed in the BFRL and under its extramural grants program during Fiscal Year 1993. Included are research performed both with funds appropriated to the BFRL Fire Research Program and under contract to outside organizations.

The BFRL Fire Research Program has directed its efforts under four program thrusts. The in-house priority projects, extramural grants, and externally-funded efforts thus form an integrated, focussed ensemble. This publication is organized along those lines:

Performance-based Fire Standards

Fire Safe Materials and Products

Advanced Fire Sensing and Suppression

Large/Industrial Fires

For the convenience of the reader, an alphabetical listing of all grants is contained in the Part 2.0.

Richard G. Gann, Ph.D.  
Chief, Fire Science Division  
Building and Fire Research Laboratory



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## **A. PERFORMANCE-BASED FIRE STANDARDS**





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

CARBON MONOXIDE PRODUCTION AND PREDICTION

Professional Personnel

William M. Pitts, Project Leader  
Nelson P. Bryner, Chemical Engineer  
Erik L. Johnsson, Mechanical Engineer  
George W. Mulholland, Research Chemist

Project Objective

To develop for the fire safety engineering community a fundamental understanding of the mechanisms of carbon monoxide formation in fires sufficient to produce an estimation model by July, 1994 and a detailed predictive model by July, 1998.

Scope

This program is designed to assess the importance of CO in fire toxicology (i.e., the levels of CO generated) and to provide the scientific background required to allow the prediction of CO in real fires. Efforts range from purely empirical studies such as assessments of CO production in full-scale fire tests to fundamental studies designed to improve the understanding of the chemically reacting turbulent flows which ultimately produce CO. New information which is generated is incorporated into existing BFRL models of fire behavior.

Technical Accomplishments

During FY94, work has focused on providing the input necessary to meet the major milestone of providing an engineering estimate of CO generation in enclosure fires. This work has been carried out as part of the overall priority project plan [see W. M. Pitts, "Long-Range Plan for a Research Project on Carbon Monoxide Production and Prediction," NISTIR 89-4185, October 1989].

Much of the earlier research in the project had been aimed at allowing an assessment of whether or not the global equivalence ratio (GER) concept offers a viable approach for the prediction of CO formation in real fire scenarios. The GER concept refers to the experimental observation that concentrations of major gas species, including CO, in the well-defined layers of combustion gases above simple fires can be correlated in terms of the GER. The GER is defined as the ratio of fuel to air available normalized by the ratio of fuel and air required for complete combustion to water and carbon dioxide.

The research has demonstrated that there are at least four mechanisms of CO formation in enclosure fires. Only one, the quenching of a fire plume in a rich upper layer, is considered by the GER concept. Other mechanisms for CO generation include mixing of oxygen directly into a rich high-temperature upper layer with subsequent reaction to form CO, approach to full thermodynamic equilibrium concentrations in a rich, high-temperature upper layer, and pyrolysis of wood in high-temperature, vitiated environments. A detailed summary of pertinent research and these formation

mechanisms is available. [W. M. Pitts, "The Global Equivalence Ratio Concept and the Prediction of Carbon Monoxide Formation in Enclosure Fires," *NIST Monograph 179* (July, 1994)]

## 1. Investigation of CO Formation in a Reduced-Scale Enclosure (Johnsson, Bryner)

Despite the importance of the problem, very few detailed investigations of CO production during full-scale fire tests are available. The principal reason for this lack of data is the high cost associated with full-scale testing. An approach which is often used is to perform experiments on a reduced scale where costs are lower and the tests are more easily manageable. A major drawback to this approach is that all the important fire parameters cannot be scaled simultaneously. Despite this, reduced-scale testing has contributed immensely to the understanding of fire behavior for conditions where the effects of scaling are properly understood. A reduced-scale enclosure (RSE) fabricated at NIST has been used to characterize CO formation for a variety of test conditions. The RSE is a 2/5-scale model of a full-size room having a single doorway which is used widely for fire testing. Measurements available include vertical profiles of temperature at locations in the front and rear of the RSE as well as CO, CO<sub>2</sub>, and O<sub>2</sub> concentrations for two locations in the front and rear of the upper layer formed by a fire in the enclosure.

Natural gas was used for over 140 test fires during FY 91-92. These tests showed that CO concentrations as well as the other products of combustion observed in the upper layer at the rear of the enclosure during underventilated burning were in good agreement with those predicted by the GER concept. However, in the front of the enclosure (i.e., nearest the doorway) upper-layer CO concentrations were roughly 50% higher. Analysis indicated that the higher CO concentrations were due to the direct entrainment of air into the upper layer where it reacted with the rich gases to generate CO in preference to CO<sub>2</sub>. As required by this explanation, the upper-layer local equivalence ratios were lower in the front than in the rear of the enclosure. Upper-layer temperatures were also higher in the front of the RSE as expected for the additional heat release.

In order to investigate whether changing fuel would dramatically affect the behavior of fires in the RSE, a series of fires have been burned within the RSE during the past year using heptane as fuel. Pools of heptane having diameters of 16, 21, 24, and 27 cm were placed in the center of the RSE and ignited. A fuel leveling system was used to feed the pools and allowed experiments lasting up to 20 minutes.

Unlike the earlier natural-gas burns where the gas flow corresponding to a given fire size was simply initiated, the liquid-fueled fires required a finite period to grow to their final size. Crude control of the ultimate fire size was achieved by varying the burner size and the flow of cooling water to the burner.

The general behaviors observed for the fires were similar to those for the natural-gas burns. Lean conditions (low heat-release-rate fires) generated low levels of CO. As the fires began to become underventilated, the CO concentration began to increase. Observed concentrations of CO in the front and rear of the RSE were quite different with dry concentrations of 5-6% measured in the front of the enclosure and 2% in the rear. These levels can be compared with typical values of 3% in the front and 2% in the rear for underventilated natural-gas fires. CO<sub>2</sub> measurements gave the opposite behavior with the higher concentrations being in the rear. Figure 1 shows time plots of CO and CO<sub>2</sub> concentrations in the front and rear for a heptane fire using the 24 cm burner.

Upper-layer temperatures in the lower-heat-release rate fires were cooler in the rear than in the front as observed during the natural-gas fires. As the fires became highly underventilated, the temperatures in the front and rear of the enclosure became more similar. Maximum upper-layer temperatures approached 1500 K which are considerably higher than observed during the natural-gas



burns. Both the increased temperature uniformity and higher temperatures can be attributed to increased radiation trapping due to the much higher soot levels expected for heptane fires.

The higher temperatures observed in the heptane fires also provide an explanation for the high CO levels observed in the front of the upper layer. These high temperatures are sufficient to cause the rich mixtures to begin to approach thermodynamic equilibrium. For such temperatures the formation of CO becomes highly favored.

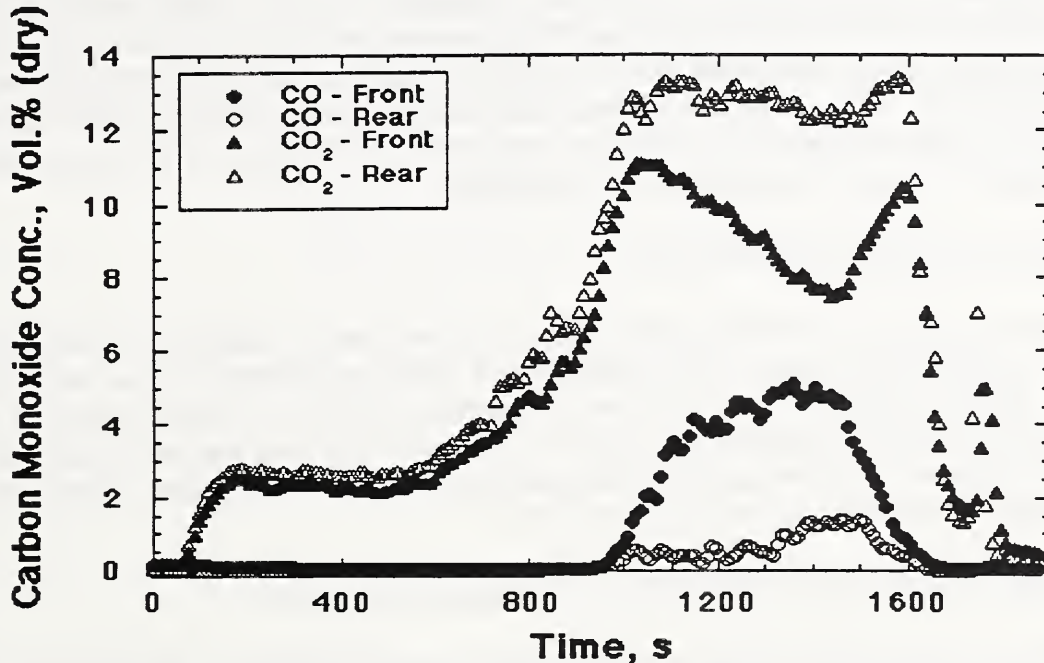


Figure 1. CO and CO<sub>2</sub> concentrations as a function of time in the front and rear of the upper layer for an underventilated heptane fire in the FSE.

Even though the behaviors of fires using the two fuels are somewhat different, the results for heptane-fueled fires are consistent with the mechanisms of CO formation previously determined.

## 2. Full-Scale Fire Tests (Bryner)

An important question to ask is whether results of measurements in the RSE can be scaled to make predictions for a full-scale enclosure (FSE). In order to answer this question a limited series of natural-gas fires was burned in the standard ASTM/ISO configuration (dimensions of 2.44 m x 2.44 m x 3.66 m with a single doorway). The fire was fueled by natural gas with a burner configuration (diameter 35.6 cm) similar to that for the RSE studies. Temperature and concentration measurements were performed at locations based on linear scaling from those used in the RSE.

Fire sizes ranged from 450 kW to 3.5 MW. The fire size was estimated using a standard doorway flow scaling law ( $s^2Ah^{1/2}$ , where  $s$  is the scaling factor,  $A$  is the area of the doorway, and  $h$  the doorway height). The full-scale fire size for which the fire just became underventilated was in good agreement with the prediction based on the RSE results.

The gross temperature and concentration behaviors for the FSE were similar to those observed in the RSE. For overventilated conditions the concentration of CO remained low. As the fire size was increased and the fires became underventilated, the CO increased dramatically and

reached levels exceeding 6% for the largest fires. Unlike the RSE results, concentrations in the front and rear were similar. Note that the concentrations of CO in the front of the enclosure are roughly a factor of two higher than observed in the RSE.

Temperatures in the upper layer were 100-200 K higher than observed in the RSE, but showed the same trend with the front of the upper layer being considerably hotter than the rear. The increased temperatures can be understood in terms of heat loss mechanisms within the enclosure. The larger enclosure has a smaller wall surface area to volume ratio than the RSE with the result that wall heat losses are relatively reduced. The larger volumes of the FSE should also trap radiative energy more efficiently, thus raising the temperature. Radiation is also trapped more efficiently in the full-scale enclosure due to the reduced area of the doorway relative to the total wall surface.

Maximum upper-layer temperatures in the FSE for highly underventilated conditions were on the order of 1550 K. The observation of these high temperatures provides a likely explanation for the higher CO levels observed in the FSE as compared to the RSE since the rich upper-layer mixtures will begin to approach thermodynamic equilibrium.

### 3. Phi-Meter Development (Mulholland)

Earlier work had led to the development of an instrument capable of measuring local equivalence ratio ( $\phi$ ) in flame gases. This instrument is based on conversion of all excess fuel to water and CO<sub>2</sub> using a catalysis in a high temperature furnace (1300 K). Measurements of oxygen in the resulting flow allow the determination of  $\phi$ . During the past year this instrument has been reconfigured and improved to allow easier operation and to provide a direct readout. This instrument was used for measurements in both the RSE and FSE.

### 4. Algorithm for Predicting CO Formation in Enclosure Fires (Pitts)

The findings during the past few years have been used as the basis for the development of an algorithm designed to provide engineering guidance for predicting CO in enclosure fires. This algorithm appears in the abstract for the 1994 Fire Conference. [W. M. Pitts, "An Engineering Algorithm For The Estimation of Carbon Monoxide Generation In Enclosure Fires"]

### Reports and Publications

"The Phi-Meter: A Simple, Fuel-Independent Instrument for Monitoring Combustion Equivalence Ratio," V. Babrauskas, W. J. Parker, G. Mulholland, and W. H. Twilley, *Reviews of Scientific Instruments*, to appear.

"Carbon Monoxide Formation in Fires by High-Temperature Anaerobic Wood Pyrolysis," *Twenty-Fifth Symposium (International) on Combustion*, to appear.

"Application of Thermodynamic and Detailed Chemical Kinetic Modeling to Understanding Combustion Product Generation in Enclosure Fires," W. M. Pitts, *Fire Safety Journal*, to appear.

"Carbon Monoxide Production in Compartment Fires--Reduced-Scale Enclosure Test Facility," N. P. Bryner, E. L. Johnsson, and W. M. Pitts, *NISTIR (1994)* to appear.

"The Global Equivalence Ratio Concept and the Prediction of Carbon Monoxide Formation in Enclosure Fires," W. M. Pitts, *NIST Monograph 179* (July, 1994).

"Fire-Induced Mass Flow into a Reduced-Scale Enclosure," E. L. Johnsson, N. P. Bryner, and W. M. Pitts, to be submitted.

### Related Grants

"Compartment Fire Combustion Dynamics," U. Vandsburger, Virginia Polytechnic Institute and State University and R. J. Roby, Hughes Associates.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

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NIST Scientific Officer Dr. W. M. Pitts

Technical Abstract:

Introduction

Exhaust gas inhalation accounts for approximately two-thirds of all deaths in fires [1]. Many of these fatalities occur at enclosed locations which are remote from the burning compartment [2]. Carbon monoxide (CO), an odorless and colorless gas, is a major component within the exhaust gases which are transported through burning buildings and into locations remote from the actual fire. Studies have also indicated that (CO) is the most significant toxic exhaust gas for a wide range of fuels [3].

The purpose of the present study is to investigate the oxidation of exhaust gases from a burning compartment as they are transported down an adjacent hallway. Concentrations of CO within the burning compartment have experimentally measured to reach up to 6% in a non-flammable compartment and up to 14% inside a wood lined compartment ceiling [4]. Sustained external burning, the oxidation of fuel rich gases as they exhaust from a burning compartment into ambient air, has been found to reduce CO levels within the exhaust gases vented from the burning compartment into the atmosphere [5].

The focus of the experiments reported herein was to determine the phenomena which control the oxidation of the exhaust gases during sustained external burning within a hallway. This was done by varying the global equivalence ratio (GER, defined as the mass ratio of fuel to air inside the compartment nondimensionalized by the stoichiometric mass fuel to air ratio) and the fluid dynamics within the hallway. With knowledge of the gas concentrations inside the compartment [5], the degree of oxidation of the exhaust gases from the burning compartment was determined at different points along the hallway. In addition, the overall oxidation efficiency was determined through measurements at a location downstream of the hallway. These efficiencies were then compared to those obtained from the experiments of the burning compartment which exhausted directly into the atmosphere [5].

## Experimental

The experiments were performed at the VPI&SU Compartment Fire Dynamics facility which is discussed in detail elsewhere [6]. Liquid hexane fires were burned in 20 cm and 23 cm diameter, 6.4 cm deep steel fuel pans located in the center of the floor inside the compartment. Air was supplied to the fires via natural draft from a circular duct connected to a plenum below the burning compartment. By measuring the fuel vaporization rate and the air into the fire, the GER was experimentally determined.

Exhaust gases escape the compartment from a window style vent 20 cm below the ceiling of the compartment on the side opposite the air inlet duct. The exhaust vent was adjusted from 25 x 16 cm to 51 x 24 cm. Global equivalence ratios ranging from 1.5 to 3.5 were obtained using different combinations of the exhaust vent sizes and fuel pan diameters.

Once the combustion gases exited the burning compartment through the exhaust vent, they were transported down a hallway 3.66 m long, 1.14 m wide and 1.47 m tall. The fluid dynamics inside the hallway were varied by adjusting the soffit heights from 0 to 20 cm at both the entrance and the exit of the hallway.

The exhaust gases were sampled at different locations along the length of the hallway and in the fume hood duct which was downstream of the hallway. The concentrations of CO, CO<sub>2</sub>, O<sub>2</sub> and total unburned hydrocarbons (THC) within the exhaust gases was determined for each test at the sampled location. The vertical temperature profile at the sampled locations within the hallway was determined using a rake of nine aspirated thermocouples spaced 6.4 cm apart.

Data was averaged over a two second period and recorded. Each test was video taped to provide permanent visual record of the experiment. The recorded data was then averaged over the “quasi” steady state period which was during sustained external burning.

## Results and Discussion

Two types of experiments were performed. In the first type combustion gases were sampled downstream of the hallway in the exhaust duct while in the second type gases were sampled at different locations within the hallway. The post-hallway sampled data provided information on the overall oxidation efficiency of the exhaust gases while the in-hallway experiments showed the evolution of the exhaust gases as they were transported and oxidized down the hallway. Species yields were only calculated when sampling within the exhaust duct since the air entrainment into the flame during sustained external burning was not determined experimentally. The post-hallway experiments were averaged over a 30 second period during sustained external burning, and the in-hallway experiments were averaged for a 20 second period during sustained external burning. All compartment fires were sufficiently underventilated to ensure sustained external burning within the hallway.

Gottuk et al. [5] performed hood experiments where exhaust gases eventually ignited external of the compartment forming an unconstrained jet of fire in the open atmosphere. The most efficient oxidation of the compartment exhaust gases occurred in these experiments, as shown in Table I. The overall oxidation efficiency of the combustion gases which were transported from a burning compartment and down a hallway which contained different soffit combinations are also documented in Table I for a GER ranging from 1.5 to 3.5.

Figure 1 shows a detailed mapping of the normalized species concentrations along the length of the hallway which was generated from the results of the in-hallway experiments with no soffits at the inlet and exit of the hallway. The poor oxidation of the CO within the hallway was attributed to the inefficient mixing of the exhaust gases with the air in the hallway, the presence of the hydrocarbons and the thermal quenching of the exhaust gases. The exhaust gases were at the ceiling of the hallway when they escaped from the compartment thus permitting mixing to primarily occur at the interface of the hot upper layer of gases flowing over cool air which was already a thermally stable environment. The presence of the hydrocarbons in the hallway, where temperatures in some areas exceeded 1100°K, inhibited the overall reduction in CO yields because hydrocarbons oxidized faster than CO in addition to



forming CO when they did oxidize. By the time most of the hydrocarbons oxidized, the exhaust gases had cooled down sufficiently for the CO reactions to be frozen. This usually begins to occur as the gas temperature drops below 950°K [7].

With no soffit at the inlet of the hallway and a 20 cm soffit attached at the exit of the hallway, the oxidation of CO, THC's and soot became even less efficient, as seen in Table I. These reductions in oxidation were attributed to the upper layer becoming much thicker which further decreased the mixing of ambient air into the layer.

The next set of experiments had a 20 cm inlet soffit with no soffit at the exit of the hallway. The soffit at the inlet of the hallway made the constrained fire plume exiting the compartment during sustained external burning more jet like in structure. Thus, the turbulent, buoyant jet entering the hallway enhanced the mixing and increased the interfacial area between the cool air and the hot exhaust gases. For fuel vaporization rates less than 0.010 kg/s, the oxidation of CO was as efficient as an unconstrained jet of fire. When it was greater than 0.010 kg/s, the oxidation of CO was reduced. The THC reduction levels were only slightly dependent on the fuel vaporization. The efficiency of reducing the soot levels was in between the CO and THC oxidation. A detailed mapping of the normalized species of the exhaust gases as they are transported down the length of the hallway for these soffit conditions is shown in Figure 2.

When 20 cm soffits were placed at both the entrance and the exit of the hallway, the reduction in species yields was still as efficient as the unconstrained jet experiments when fuel vaporization rates were less than 0.009 kg/s. Increasing the fuel vaporization rate above 0.009 kg/s gave rise to less oxidation of species within the hallway. This was again attributed to the thicker layer forming in the hallway.

## Conclusions

Table I. summarizes the results of the oxidation efficiencies of the exhaust gases being transported and oxidized down a hallway with different soffit sizes at both the beginning and the end of the hallway. Poor oxidation of the exhaust gases was present when there was no soffit at the hallway inlet. The addition of a 20 cm soffit at the hallway exit decreased the oxidation of the exhaust gases when no soffit was present at the hallway entrance. With a 20 cm soffit at the inlet of the hallway, the oxidation of the exhaust gases was as efficient as the unconstrained jet experiments when the fuel vaporization rate is less than 0.010 kg/s with no exit soffit. When a 20 cm soffit is present at the hallway inlet and exit, the fuel vaporization rate must be above 0.009 kg/s for the oxidation of the exhaust gases to become less efficient than the unconstrained fire jet experiments. In the period between the writing of this report and the presentation, the effect of the hallway-to-compartment orientation on the exhaust gas history will be examined.

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Table I. Post-compartment exhaust gas oxidation with the GER ranging from 1.5-3.5.

Species	Free Jet Experiments [5]	Soffits: 0 cm inlet 0 cm exit	Soffits: 0 cm inlet 20 cm exit	Soffits: 20 cm inlet 0 cm exit <sup>1</sup>	Soffit: 20 cm inlet 20 cm exit <sup>2</sup>
CO	75-90%	54-68%	22-42%	78-89% (45-55%)	71-91% (39-51%)
THC	N/A	83-93%	75-89%	92-97% (88-91%)	91-98% (86-93%)
Soot	50-100%	48-86%	22-57%	61-92% (42-56%)	56-88% (28-46%)

1 values in parenthesis are for fuel rates > 0.0010 kg/s

2 values in parenthesis are for fuel rates > 0.009 kg/s

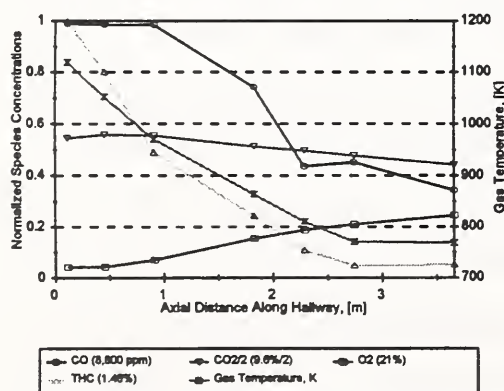


Fig. 1 0 cm inlet and 0 cm exit soffits.

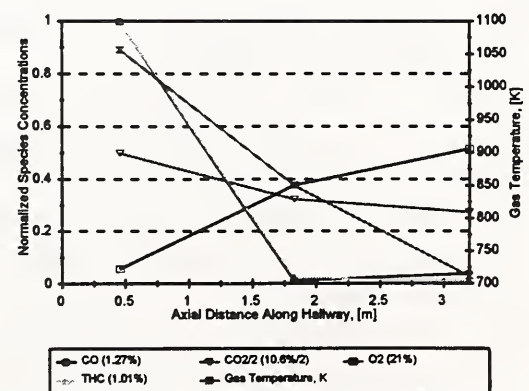


Fig. 2 20 cm inlet and 0 cm exit soffits.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

EVACUATION MANUAL FOR DISABLED OFFICE OCCUPANTS

Funding Agency

US Fire Administration

Professional Staff

Richard W. Bukowski, Project Leader

Edwina Julliet, contractor

Project Objective

To produce a manual which can be utilized both by building managers and the disabled to establish procedures for emergency evacuation of office occupancies.

Scope

The manual is to present information on extant equipment and procedures with both positive and negative aspects clearly discussed, from which the parties can assess needs and establish effective procedures.

Technical Accomplishments

The effort has involved a range of advocates representing various disabled groups to provide feedback and advice on what is needed. The resulting manual should then be readily accepted by these parties as addressing their special needs. Coordination has also been worked with federal agencies (GSA) and private groups (BOMA) for similar purposes from the facilities managers perspective. The plan is to make the manual available in english, spanish, braille, and audio tape.

Reports and Publications

None: new project

Related Grants

None





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

FIRE SAFETY OF AIR TRAFFIC CONTROL TOWERS

Funding Agency

Federal Aviation Administration

Professional Staff

Richard W. Bukowski, Project Leader

John H. Klote, Mechanical Engineer

Project Objective

To address deficiencies in the emergency egress capabilities of ATCT's related to the provision of a second means of egress.

Scope

Solve code compliance problems with ATCT's and the Life Safety Code's current requirements and develop an approach to protected elevators which solve longer term issues of disabled access.

Technical Accomplishments

The project involved two related efforts. First, avenues for changing the Life Safety Code were pursued; changes needed to correct compliance problems with OSHA. These efforts culminated in a request for a TIA which is still in process. As a backup, a negotiated settlement between FAA and OSHA was also arranged.

In parallel, the technical basis for a code change proposal to add protected elevators as a second means of egress was developed and a code change proposal prepared. Several ATCT's were visited with a view to retrofit -- an option which was found to be impractical. This option will however be exercised for all new tower designs.

Reports and Publications

Klote, John H., Levin, B.M., and Groner, N.E., Feasibility of Fire Evacuation by Elevators at FAA Control Towers, NISTIR 5445, Nat. Inst. Stand. Tech., 1994.

Related Grants

Human Behavior Considerations for Fire Evacuation Using Elevators, George Mason University.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROGRAM - FY94

Institution George Mason University

Contract No. 50SBNBIC6527

Contract Title Human Behavior Considerations for Fire Evacuation

Principal Investigator Dr. Carl Harris, Chairman  
Operations Research and Engineering  
George Mason University  
Fairfax, VA 22030-4444

Other Personnel Dr. Bernard M. Levin and Dr. Norman E. Groner

NIST Scientific Officer Dr. John Klote

Technical Abstract The Federal Aviation Administration (FAA) is interested in the possibility of using elevators for evacuation of air traffic control towers during fire emergencies. Assuming that the FAA could design, install and maintain elevators that could safely be used by tower occupants during fire evaluations, it would be important to study a number of human factors considerations. This report, which is partly based on interviews of occupants in thirteen FAA towers, discusses these issues. Given the fact that there has been a 20 year campaign to discourage elevator use during fire emergencies, most interviewees indicated a willingness to use such elevators as a backup mode of escape with some reluctance. The controls in the elevator would not need any major modification but a special communication system would be needed. Fire emergency plans and training are important to assure proper use of the proposed system and confidence in the safety it provides.

Introduction This is phase two of the contract. Phase 2 is entitled Human Factors Considerations in the Potential for Using Elevators for Fire Evacuation of FAA Air Traffic Control Towers.

This study is part of a wider investigation of the feasibility of using elevators for emergency egress in Federal Aviation Administration (FAA) air traffic control towers. This study is also part of an ongoing effort to examine those factors that will allow the design, installation and maintenance of elevators that can be safely used to evacuate occupants during fire emergencies from all types of occupancies.

Air traffic control towers are tall and narrow. The limited area on each floor discourages installing two stairways and precludes installing two stairways that are remote from the standpoint of providing independent access to the exit stairways. (Once in the stairways the routes could be adequately independent.)

Most current air traffic control towers contain both a single stairs and a single elevator serving the upper portion of the tower. The elevator is used to avoid using a long stairway to travel to and from a location below the work site in the cab. (The elevator does not serve the cab itself. The cab can be reached only by a single stairway.) The stairs are needed for emergency egress and as a backup when the elevator is not in operation due to routine maintenance or unanticipated problems.

The presently installed elevators in the towers, as well as current elevators in other buildings, are unacceptable as a means of leaving the building during a fire emergency. The towers are left, therefore, with only a single means of emergency egress. Towers with 25 or more occupants fail to meet the OSHA requirement for two means of egress.

The authors visited representative air traffic control towers. Thirteen towers were visited by one or more members of the project team. These towers were selected to provide examples of all the principal architectural designs used by the Federal Aviation Administration, as well as some "non-standard" types which are not replicated elsewhere.

Written fire safety plans are generally created to serve two, often incompatible, goals. First, they provide information to building occupants about the appropriate procedures to be followed during an emergency, that is, an "action document." Second, they provide evidence to organizational and regulatory authorities that an appropriate plan has in fact been developed, that is, a "compliance document." The two goals tend to be incompatible: the first goal encourages brevity, clarity, and the absence of information that is non-essential to the reader; the second emphasizes comprehensiveness to ensure that all the elements of the plan have been incorporated. One approach to resolving the conflict would be to prepare two documents, one directed at each goal.

A fire evacuation system using fire safe elevators would be useful only if the building occupants believe in the safety of the system and were willing to use it. Factors that would influence the acceptance of and compliance with the emergency plan include:

Simulated or real fire drills, training programs, and useful fire safety plans will improve performance, confidence, and compliance with the fire plan.

There is a need for a program to convince the occupants that this elevator system is safe, despite 20 years of advice to avoid elevators in fires.

People have a strong psychological need to exert some control over their own fate and they have less control when they use elevators rather than stairs.

Users need confidence that the elevators system is very well maintained since they recognize that a malfunction could have disastrous consequences.

Occupants should be aware of the nature of fire growth and smoke spread. People may attempt to use unsafe escape routes in preference to elevators if they incorrectly evaluate the safety of the alternative routes.

Occupants may become anxious if there is a long wait for the elevator.



The use of elevators for fire evacuation of air traffic control towers would be similar to using elevators to evacuate occupants with disabilities in larger buildings with two major exceptions.

There would be a delay in initiating the evacuation in air traffic control towers because of the need to transfer control of aircraft to another facility.

There is a lower probability that there will be a central control center to control the evacuation in the air traffic control towers. A good telephone system with phones in elevators and elevator lobbies as well as work spaces would facilitate the necessary communications.

Current standards for controlling elevators in fire emergencies would need one important modification. The criterion for taking elevators out of routine service would need to be changed so that insignificant amounts of smoke would be ignored.

No human factors related problems were uncovered that would preclude the use of fire safe elevators in air traffic control towers.

Acknowledgements Dr John Klote, project officer, made significant technical contributions to this project in addition to technical and administrative guidance.

#### Reports and Papers

Groner, Norman E., and Levin, Bernard M., (1992). Human Factors Considerations in the Potential for Using Elevators in Building Emergency Evacuation Plans, NIST-GCR-92-615, National Institute of Standards and Technology, Gaithersburg, MD.

Klote, John H. et al. (1992). Feasibility and Design Considerations of Emergency Evacuation by Elevators, NISTIR 4870, National Institute of Standards and Technology, Gaithersburg, MD.

Klote, John H., Levin, Bernard M., and Groner, Norman, E. (1994). Feasibility of Fire Evacuation by Elevators at FAA Control Towers, NISTIR 5445, National Institute of Standards and Technology, Gaithersburg, MD.

Levin, Bernard M. and Groner, Norman, E. (1994). Human Factors Considerations for the Potential Use of Elevators for Fire Evacuation of FAA Air Traffic Control Towers, National Institute of Standards and Technology, Gaithersburg, MD. (In Press)



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY 94

HAZARD DEVELOPMENT

Professional Personnel

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Objective

To produce a fundamental capability to analyze the hazards associated with a specified fire scenario.

Scope

Each year, billions of dollars are spent to protect occupants and equipment against fire and fire related damage and loss. Yet in spite of the increased spending many people continue to die annually and there is still a large dollar loss. To ease these problems, a systematic approach to understanding the effect of fires in buildings is necessary. The fundamental capability has been provided as a fully-supported software package for personal computers. The software design is aimed at a broad range of applications from fire safety education to fire reconstruction.

Technical Accomplishments

BFRL developed the software HAZARD I, which predicts the hazard to a building and to occupants any where within the building. The fire hazard assessment methodology embodied in the HAZARD I software provides a vehicle by which fire science can be applied to improve fire safety. Continued enhancement of its capabilities and validity is a primary aspect to the mission of BFRL's fire program. Version 1.0 was released in summer of 1989, version 1.1 was released in the fall of 1991, and version 1.2 was released in the spring of 1994. This latter version includes new phenomenon and features to continue providing a state-of-the-art tool for hazard analysis for use by fire protection professionals. We have also improved the documentation by providing a step-by-step learning guide and integrating the example cases in the technical reference.

The research this year includes a most important missing pieces in most fire models: "prediction of the growth of the fire." Single-surface pyrolysis, and fire suppression algorithms are being incorporated in the fire model. We continued the unification of the user interface with a new-generation input editor and hazard shell. The internal structure of the core model of HAZARD, CFAST, has been addressed by redefining the internal data structures to be consistent with the streamlining of the solver routines completed last year. The benefits of this year's research are twofold: The pyrolysis and fire detection/suppression algorithms will allow the user to study fire scenarios without costly full-scale testing to develop input data for the model. Improving the internal structure will allow easier



inclusion of algorithms in the future and allow more researchers, both within NIST and elsewhere to contribute to the development of the model. The resulting model will provide a predictive tool for manufacturers, purchasers, architects, FPE's, code officials, and practitioners to evaluate safety performance, code equivalency, and code change proposal issues.

**Pyrolysis model:** Several single-surface pyrolysis models that predict real-scale fire growth from bench-scale test data are being evaluated to find the one most appropriate for inclusion into the CFAST model. Beyond wall flame spread models developed in BFRL, we have also concentrated on simplifications to the existing furniture model by Dietenberger. This flame spread model described in this paper is a new algorithm which provides the capability to calculate a self-consistent fire based on bench scale fire data. The flame spread model simulates object fire growth and burnout of a slab in a room and produces acceptable predictions of the spread of fire, smoke and production of both toxic and non toxic gases. The purpose of the flame spread model is to allow a fire to grow realistically, possibly making a hole in the material surface. This is one mechanism for barrier penetration. The algorithm is based on empirical data, gathered from standard tests, including the Cone Calorimeter and the LIFT (lateral ignition flame spread test method). An objective of including the flame spread model is to predict the accelerative growth of a fire from ignition to a peak value and then the gradual termination normally seen in a fire. The three-dimensional aspects of the flame spread model include: first, panels made of combustibile materials with different thicknesses and at various orientations; second, flames of two basic types, pool fire and purely wall fire; third, radiation heat exchange between objects, flames, and gases. The pool fire has a flame spreading polygon on a horizontal panel and the wall fire is used either for inclined or vertical panels.

The dynamic features of the model include: (a) flame spreading in any (and all) direction(s) on a panel, (b) the varying mass and heat release rates in multiple flames because of the scaled burning history of surface elements on the panels, (c) the temperature changes of surface elements, walls, and gas layers, and (d) the growth of the upper gas layer with combustion products. The reliance of the model on effective scaling of the Cone Calorimeter data and of the flame spreading data, and its validation with the full scale fire tests is an important feature. Use of these test results allows us to avoid some theoretical difficulties associated with radiation blocking and charring. This also allows us to make a firm connection between bench scale tests and full scale predictions. This will be important for establishing the usefulness of bench scale testing as a substitute for full scale tests.

**User interface:** A new user interface to replace the existing CEDIT and HAZARD Shell has been developed. The interface, which will run on multiple computing platforms, allows the user to develop input for the model with a state-of-the art graphical interface. Significant features include:

Structure overview that allows a user to know at a glance the number of compartments, number of horizontal and vertical flow openings in each compartment, number of HVAC openings in each compartment, and "main" fire compartment and "other" objects compartments.

Horizontal and vertical flow selection screens allow a user to know at a glance all compartments with flow from current compartment, and the number of vents for each compartment pair, compartments that cannot be connected because of positioning, compartments that could be connected but are not currently.

HVAC system overview allows user to see graphically which compartments are connected by HVAC ducts and fans, and the topology of the connection path, direction of flow through fans, which nodes are "external" and which are "internal."

### **Internal model improvements:**

In the past year, new physical routines were added to the model: flow through holes in ceilings and floors; another zone for each compartment that contains a fire (ceiling jet). The latter makes the estimate of heat loss from and to the ceiling much more realistic; finally, new radiation and conduction models are now used which solves the boundary discrepancy between convection/conduction and radiation and incorporates the conduction calculation directly into the differential equation set solved by CFAST. A detection/suppression capability has been added, though the suppression is a simple correlation to heat reduction versus applied water, and the detection is based on the standard temperature correlation. The latter will be fixed to incorporate detection based on smoke mass density (photo), smoke particle density (ionization) and temperature for heat detectors.

All of these were documented in two new comprehensive reports on the model - a Technical Note on the model and an IR as a User's Guide. The model (source as well as executables) is now being distributed to outside agencies: The Departments of Energy and Defense (Navy). In addition, we are developing cooperative agreements with universities and other governments to continue the effort to standardize on CFAST as the preferred fire model. We are in the process of developing CRDA's to use the fire model CFAST as the engine in at least two fire related real time applications.

This fiscal year has seen a minor update of the methodology including the combined EXITT/TENAB models as well as the initial testing of the next major release, including a new graphical user interface.

### Reports and Publications

"Verification of a Model of Fire and Smoke Transport." Peacock, R. D., Jones, W. W., and Bukowski, R. W., Fire Safety Journal 21 89-129, 1993.

"Calculating Flame Spread on Horizontal and Vertical Surfaces." Ahmed, G. N., Dietenberger, M. A., and Jones, W. W., NIST Internal Report 5392 (1994).

"Analyzing and Exploiting Numerical Characteristics of Zone Fire Models." Forney, G. P. and Moss, W. F., NISTIR 4763, 1992.

"Modeling Smoke Movement through Compartmented Structures." Jones, W. W. and Forney, G. P., NISTIR 4872, 1992.

### Related Grants

"Expansion of the Applicability of EXIT89." R. F. Fahy, National Fire Protection Association

"Development of a Graphical Interface for Post-Processing the Results of a CFAST Simulation." J. Barnett, Worcester Polytechnic Institute

"Computational Heat Transfer for Zone Fire Modeling," W. F. Moss, Clemson University.

"Sensitivity for Mathematical Modeling," M. Kostreva, Clemson University.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

<u>Institution</u>	Clemson University
<u>Grant No.</u>	60NANB2D1281
<u>Grant Title</u>	Computational Heat Conduction for Zone Fire Modeling
<u>Principal Investigator</u>	Professor William F. Moss Department of Mathematical Sciences Clemson University Clemson, SC 29634-1907
<u>NIST Scientific Officer</u>	Dr. Glenn P. Forney

Technical Abstract

Introduction The topic of this grant is computational heat transfer applied to zone fire modeling. Heat conduction through the ceilings, walls, and floors of the rooms in a zone fire model can be modeled by an initial-boundary value problem for the 1-D or 2-D heat equation. Using the method of lines (MOL), this problem can be reduced to a differential-algebraic equation (DAE) system. This DAE system, together with the ordinary differential equations for pressure, layer height, and upper and lower layer masses in a room, make up the full model. A domain decomposition method has been developed for splitting the full model DAE system into a main system and a secondary one. The main system is solved for pressure, layer height, upper layer mass, lower layer mass, and the temperatures at ceiling, wall, and floor surfaces. The secondary system is used to model heat conduction.

A number of experimental computer codes have been produced for this grant and previous grants. These codes are designated by names of the form CONRADx. A brief description of the principle codes follows.

**CONRAD1** Full DAE system, benchmark code.

**CONRAD2** Domain decomposition using the centered finite differences.

**CONRAD2.2** Domain decomposition using the cubic Hermite MOL.

**CONRAD2.3** A linearization for the exterior radiation boundary condition.

**CONRAD2.35** Linearization for the exterior radiation boundary condition by polynomial prediction.

**CONRAD2.42** CONRAD2.2 plus a Quasi-Newton method.

**CONRAD3** Bi-cubic Hermite MOL for the 2-D heat equation.

**CONRAD4** CONRAD2.35 with improved organization, comments, and data structures.

**CONRAD4.2** CONRAD2.35 with 2-D heat conduction in walls.

## CONRAD5.1 and 5.2 Moving meshes.

The current grant has created a code for 2-D modeling of walls in an attempt to more accurately approximate the vertical temperature gradient in the walls. For this purpose, the bi-cubic Hermite MOL has been used. Experimentation has also continued on the use of moving spatial meshes or grids to capture rapid changes in temperature profiles.

Moving Meshes All CONRAD codes prior to CONRAD5.1 used a fixed, material dependent, breakpoint mesh in ceiling, wall, and floor heat conduction nodes. Except for CONRAD2, these codes used the cubic Hermite MOL to solve the heat conduction problem. Here, 5 breakpoints were found to provide sufficient accuracy. The first and fifth breakpoints are at the endpoints. The second breakpoint is dependent on the time interval for output, TPRINT, while the fourth breakpoint is dependent on the total simulation time TFINAL. The third breakpoint is midway between the second and fourth (see [1]). The second breakpoint is positioned to guarantee sufficient accuracy for times near TPRINT and the fourth is positioned to guarantee accuracy for times near the end of the simulation. The third breakpoint takes care of the in-between times. This approach is surprisingly robust even though the breakpoint mesh is far from optimal at times much shorter than TPRINT. We have, however, observed that the error in the temperature profiles decays as the time approaches TPRINT and that these early errors do not have any long term consequences.

A second consequence of this approach, is a slight inconsistency in outputs from overlapping simulations. Consider two simulations, one with TPRINT = 1, TFINAL = 20, and a second one with TPRINT = 20, TFINAL = 600. The affect of using TPRINT and TFINAL dependent breakpoint meshes is that the output at time 20 will not be exactly the same for these two simulations although the difference is small.

Even though a fixed breakpoint strategy may not cause large errors, it seems possible that it could slow down the rate of convergence of the DAE solver at each step. With CONRAD5.1 and CONRAD5.2, we explored dynamic breakpoint mesh updating to see the effects on accuracy and CPU time.

We assume that one side of a heat conduction node experiences a sudden increase in heat flux at time  $t = 0$ , and that a heat “wave” moves through the node. This assumption can breakdown if the fire power output is oscillatory. This sudden increase in heat flux clearly occurs in rooms of fire origin, but in other rooms there is typically a delay between the time the fire starts and the time that hot gases begin to enter the room.

The general qualitative features of the temperature profiles in heat conduction nodes are exhibited by the semi-infinite ( $0 < x < \infty$ ) rod solution to the heat equation

$$u(x, t) = T_{\text{amb}} + (u_1 - T_{\text{amb}})\text{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right), \quad (1)$$

where  $u(0, t) = u_1$ , a constant, the initial temperature is  $T_{\text{amb}}$ ,  $\alpha = \frac{K}{\rho c}$ , and  $\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$  denotes the complementary error function. We found through experimentation that this function is uniformly approximated for  $x$  in  $[0, W]$  and  $t$  in  $[10^{-12}, 600]$  using a cubic Hermite interpolant based on the dynamic mesh

$$\begin{aligned} x1(t) &= 0 \\ x2(t) &= \text{MIN}\left(2\sqrt{\alpha t}0.6, \frac{W}{4}\right) \end{aligned}$$



$$\begin{aligned}
x3(t) &= \text{MIN} \left( 2\sqrt{\alpha t}2.1, \frac{W}{2} \right) \\
x4(t) &= \text{MIN} \left( 2\sqrt{\alpha t}5.0, \frac{3W}{4} \right) \\
x5(t) &= W
\end{aligned}$$

where  $W$  denotes the thickness of the heat conduction node. The maximum absolute error is  $3.8 \times 10^{-3}$ . We note that for  $t$  sufficiently large this mesh becomes uniform. In CONRAD5.1 we update after each DAE solver step. In CONRAD5.2, an update is done if  $t - t_u > rt$  where  $0 < r < 1$  and  $t_u$  denotes the time of the previous update. Experiments were done with  $r = .02, .05, .1, .2, .4, .8$ . The value  $r = .05$  produced accurate results with minimum execution time.

The comparison between CONRAD1 and CONRAD5.1 indicates that the choice of mesh in CONRAD1 was a good one. Note that this is the mesh used in all fixed mesh codes that use the cubic Hermite MOL. We assumed that the results of CONRAD5.1 are more accurate than those of CONRAD1 because of the mesh updating scheme. Consequently, we measured the error in CONRAD5.2 using CONRAD5.1 as a benchmark.

The execution times for CONRAD5.2 are comparable to those of CONRAD3.5. These codes are the same except for the mesh updating scheme. Apparently, the added cost of mesh updating is offset by faster DAE solver convergence. While CONRAD5.2 appears to be slightly more accurate than CONRAD2.35, both these codes are very accurate on the fire scenarios explored to date.

CONRAD4 and 4.2 CONRAD4 is a rewrite of CONRAD2.35 with improved organization, comments, and data structures. In CONRAD4, all material specifications were collected into subroutine MATERL. Subroutine INIT computes the normalizations and initializes the solution variables. Subroutine INITYP initializes the time derivatives of the solution variables. INITYP is called by INIT.

Our DAE solver DASSL is quite sensitive to having good initial values for  $Y$  and  $YP$ , the solution variable array and its time derivative. Previously, the CONRAD codes let DASSL compute initial values for  $YP$  and initially set the pressure relative to the ambient pressure, to a quasi steady-state value. This was an attempt to avoid integrating the initial pressure transient and to decrease execution time. Recent experiments have shown that comparable execution times can be obtained by starting the relative pressure at zero and using the initial values of  $YP$  computed by INITYP. The CONRAD codes have always used a rapid but not instantaneous turn-on of the fire. The fire output is ramped up using the function  $1 - e^{-t}$ .

Following the guidelines in [2], we modified the error tolerances for temperatures. We changed the relative error tolerance from 1.D-2 to 1.D-4 and the absolute error tolerance from 0.D0 to 0.5D0.

The effect of these two changes can be seen in the following results. For our standard one room, 10 minute simulation, CONRAD2.35a requires 5.2 seconds, while CONRAD4 requires 2.6 seconds. For our standard four room, 10 minute simulation, CONRAD2.35a requires 29.6 seconds, while CONRAD4 requires 29.4 seconds.

We also created subroutine RCOPY to copy the solution variable array into physical variable arrays for relative pressure, layer height, upper layer mass, density, and temperature, lower layer mass, density, and temperature, and ceiling, floor, and wall temperatures. In CONRAD4, the data structure used in array  $Y$ , is only encountered in subroutines INIT, INITYP, and RCOPY.

In CONRAD4 we have introduced the concept of a panel. A panel is defined as a union of rectangular slabs made of the same material and for which a single heat conduction model can be

used. This is an important but confusing concept. In CONRAD4, we have three panels per room. The ceiling panel is a single rectangular slab consisting of a single material. The floor panel is a single rectangular slab consisting of a single material. The wall panel consist of four rectangular slabs made up of a single material. In CONRAD4, we apply our 1-D model to these three panels. In CONRAD4.2, we apply our 1-D model to the ceiling and floor panels and our 2-D heat conduction model to the wall panel. In future codes, we will consider up to four wall panels per room. Each of these can be made of a different material and each can transfer heat to an adjoining room. To illustrate this point consider a room with two walls of concrete with exterior transfer of heat to ambient, one wall of gypsum with exterior transfer of heat to ambient, and one wall of gypsum with exterior transfer of heat to an adjoining room. We would count this as three wall panels. The two concrete walls would be lumped into one panel and considered together. The gypsum walls cannot be lumped together, because they have different exterior boundary conditions.

To add the 2-D wall model of CONRAD3 to CONTAD4, we first changed the data structure in array Y to handle NY2D temperature solution variables per wall panel. NY2D is currently set to 5.

CONRAD4.2 models a wall that is insulated at top and bottom and held at ambient on its outside surface. Consider simulations with CONRAD4 and CONRAD4.2 for a one room model which has a kaowool ceiling, a concrete floor, and gypsum walls. Ten minutes of real time is simulated with a 500,000 watt fire. There are qualitative similarities between these two runs, but also some differences, the most striking of which is that at 600 seconds the 1-D model predicts a lower layer temperature of 379, while the 2-D model predicts 349. This difference is large enough to be significant and suggests that the 2-D model is needed in the room of fire origin. We conjecture that the 2-D wall model is only needed in rooms of fire origin and possibly in adjoining rooms if heat is transferred into them by conduction. The computational cost of the 2-D wall model using NY2D = 5 is surprising low. We expect that it could be improved by using a radiation routine set up for NY2D wall temperatures. Because the upper and lower wall areas change with time, the configuration matrix for a room must be recomputed at each call to RAD4. However, in our 2-D model, the wall is divided into NY2D - 1 horizontal subpanels whose areas do not change with time. Thus the configuration matrix for a room with 2-D walls need only be computed once.

### References

- [1] Moss, W. F. and Forney, G. P., Implicitly coupling heat conduction into a zone fire model, Internal Report 4886, NIST, 1992.
- [2] Brenan, K. E., Campbell, S. L., and Petzold, L. R., *Numerical Solution of Initial-Value Problems in Differential- Algebraic Equations*, North-Holland, New York, 1989.

### Reports and Papers

Moss, W. F., Computational Heat Transfer for Zone Fire Modeling, Progress Report: NIST Grant No. 60NANB2D1281, Clemson University, March 1994.

Forney, G. P. and Moss, W. F., Numerical characteristics of zone fire models, to appear in the Fire Science and Technology.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

**Institution:**

Center for Firesafety Studies  
Worcester Polytechnic Institute  
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**Grant No.:** Cooperative Agreement 70NANB3H1406

**Grant Title:**

Development of a Graphical User Interface for Post-Processing the Results of a CFAST Simulation.

**Principal Investigator:**

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**Other Personnel:**

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**NIST Scientific Officer:**

Rebecca Portier

**Technical Abstract:**

This project develops a software package consisting of a Graphical User Interface (GUI) for the analysis of compartment fire simulations using the computer program CFAST.

The purpose of the software is to enhance a user's ability to analyze simulations consisting of multi-variable time variant data generated by CFAST. To this end, the software will be developed with the end user in mind, using on-line help and a mouse driven interface. The software provides an improvement over the previous CFAST post-processor, CPLOT.

Care has been taken to ensure compatibility with current plans for the future development of CFAST. The program has been designed to run on multiple hardware platforms, and may be used in a X-Window, Microsoft Windows, and MS-DOS operating systems.

**Introduction:**

The current post-processor, CPLOT, is limited to simple Cartesian plots of user specified variables. In order to use CPLOT, the user specifies variables of interest using key words. Variables thus selected may then be plotted using additional commands. Only four plots may be viewed at once on the same screen. There is no user interaction with these plots, once the variables have been selected and the graphs drawn, the user must start over in order to view additional variable sets or alter graph bounds. CPLOT is capable, however, of exporting its graph-data for use by other programs.

The only other mechanism currently available for viewing the results of CFAST consists of run-time graphics. In this mode, the user specifies in the CFAST input file, graphs or tables of variables that will be displayed on the screen during program execution. In addition, the user can select pre-drawn screen diagrams on which CFAST displays information such as hot gas layer height and temperature.

This project's GUI software will replace both of these mechanisms with one program. This new program will display floor diagrams obtained from information contained in the CFAST input data file, display the fire's progress on these diagrams, enable the user to interact with these diagrams using pop-up menus and a mouse interface, and draw graphs of the various CFAST variables.

This project greatly enhances the CFAST user's ability to analyze program results and therefore improve the engineering utility of the CFAST software.

**Accomplishments:**

As described above, work progressed in two main areas of the program, a Graphing utility, and a Floorplan generation utility. Presently, both utilities are near completion, with primarily cosmetic alterations remaining before progress begins in new directions.

The following are some pictures of the program in action. Due to the limitations of this paper, colors cannot be displayed. Color plays a large part in the postprocessor, as it is used to depict room temperature and as one way (of many) to differentiate between displayed graphs.

Figure 1 illustrates graphs of hotlayer heights for three rooms. These can be extracted from a pre-existing CFAST history file without touching the keyboard, in about 1 minute. To make the display as simple as possible, additional information is available on a context-sensitive basis-- for instance, clicking on the vertical axis at the left of the graph informs the user that the graphs are of Hotlayer Height, for rooms 1,2, and 3 of a certain history file.

Figure 2 shows a depiction of a CFAST room, including vents, objects, and a layer interface. This display can be directly created from a normal CFAST history file. Using the history file as input, CVIEW can provide the user with a movie-like replay of the simulation that produced the history-file. The user may proceed forward and backwards frame by frame or playback the whole simulation in either direction, at any desired playback speed. This way the results of the simulation may be quickly examined with a minimum of effort and time.



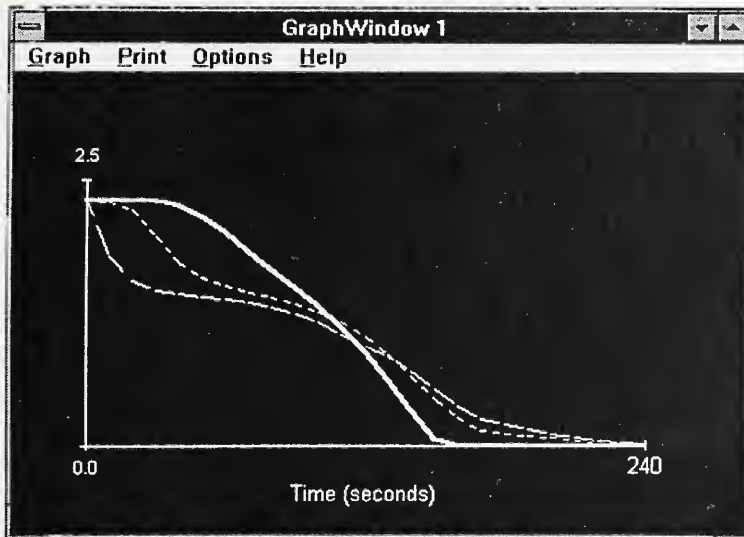


Figure 1: Graphs of layer heights for three rooms.

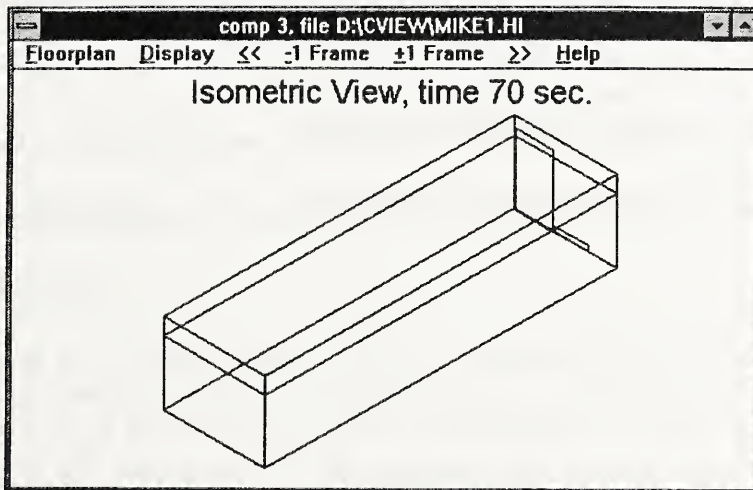


Figure 2: Three dimensional wire-frame of a CFAST room.



Figure 3: Plan view of a CFAST room.

Figure 3 shows a normal plan-view of the room depicted in Figure 2. For instance views of the XY- YZ- or XZ-plane in two dimensions, are of course available, with context-sensitive information available to the user by clicking on the depicted objects in the displayed floorplans.

**Future Work:**

There are many possibilities for further visualization work with CFAST. Future work might include improvements to the program's current 3D rendering procedure, including shading (the routine currently produces a wire-frame rendition) perspective projection, or texture-mapping.

Additionally, room for progress also exists in the area of compartment inter-connectivity, individual object ignition, and vent location, items that are determined ambiguously at the current time.

More accurate depiction of object ignition, vent locations, and room connectivity, together with expansion of the 3D engine will allow for more powerful presentations of the CFAST output to non-engineers, allowing 'walk through' tours of simulated burning structures.

**References:**

Peacock, Richard D., et.al. *CFAST, the Consolidated Model of Fire Growth and Smoke Transport*. NIST Technical Note 1299, National Institute of Standards and Technology, U.S. Department of Commerce.

Russo, J. K., 1991. *Fire Simulation*. MQP 91B005M, Worcester Polytechnic Institute.

Voorhis, M., 1992. *Enhanced Fire Graphics*. MQP 92E021M, Worcester Polytechnic Institute.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

INSTITUTION: California Institute of Technology

GRANT NO.: 60NANB3D1444

GRANT TITLE: Experimental Study of Heat Transfer and the Environment  
in a Room Fire

PRINCIPAL INVESTIGATOR: Edward E. Zukoski  
Jet Propulsion Center, 301-46  
California Institute of Technology  
Pasadena, CA 91109

OTHER PERSONNEL: T. Kubota, Professor Emeritus  
S. Palm, Master's Student  
L. Benedict, Graduate Student

NIST SCIENTIFIC OFFICER: Dr. Leonard Y. Cooper

TECHNICAL ABSTRACT:

Transient Development of a Ceiling Layer We have completed the investigation of the transient development of ceiling layer in a hood that is closed except at the bottom and that is 2.44 m square and 1.22 m deep. A 1.36 g/s flow of natural gas, corresponding to a heat-release rate for complete combustion of about 67 kW, was ignited at the beginning of the experiments and was held constant thereafter. The flame was stabilized on a 19-cm diameter glass bead burner that was placed 10 cm below the bottom edge of the hood and in the center of the lower surface. Transient measurements of the concentrations of O<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub>, and CO, and the gas and wall temperatures were obtained several times per second for about 2000 seconds. A simple mass balance allowed the concentrations of N<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> to be determined. Gas chromatograph measurements indicated that these were the primary species in the gas.

These measurements are available for use in checking models for the production of CO in fires when temperatures in the ceiling layer are less than 500 degrees Kelvin in Report 1994-2 by Palm and Zukoski. Some interesting results are presented in the following paragraphs.

The data indicated that for this hood the distribution of chemical species is almost independent of position; that is, the volume within the hood can usefully be treated as a homogeneous region after the first 20 seconds.



With a height-to-width ratio of 1.5 for the hood, the entire volume becomes filled with recirculating products within the first 15 seconds of the test. This is in agreement with earlier salt-water modeling results.

For these conditions, CO is observed near the bottom of the shaft at concentrations of 0.1 mole % within the first minute and rises to 1.6 mole % after about 1000 seconds. The rate of increase in the concentration of CO changes abruptly at about 70 seconds when the equivalence ratio of the gas within the hood increases past 0.50. At this same time, the concentration of CH<sub>4</sub> becomes measurable at about 0.1 mole % and increases rapidly thereafter to reach peak values greater than 8 mole % at about 800 seconds.

Buoyant Flows in Shafts Buoyant flows in vertical shafts are being investigated in an experimental program that will elucidate the influence of heat transfer from the buoyant fluid to the walls of the shaft on the penetration of the hot buoyant gas up the shaft from a source of light, hot gas at the bottom of the shaft.

The sketch below shows the apparatus that is being used to study flow in a vertical shaft. The shaft is a rectangular box constructed of 1.3-cm thick aluminum plates with a length of 2.5 m, and a width and breadth of 25 cm. The thickness of the aluminum side walls is large enough to assure that the walls will appear to be infinitely thick during the course of the experiments. The hot box at the bottom of the shaft is a circular chamber with internal baffles as suggested in the sketch, and the box is 1.22 m in diameter and 0.62 m in height.

During the hot gas experiments the temperature of gas within the "hot box" is maintained at temperatures between 350 and 500 degrees Kelvin by recirculating a flow of hot gas that is heated to the desired temperature with electric heaters. For room-temperature experiments, density differences between the gas inside the shaft and hot box can be produced by supplying a variety of gases with different densities to the shaft and hot box regions. Gases such as CO<sub>2</sub>, He or SF<sub>6</sub> will be used.

Three sections of the side wall, 0.62 m in height, are instrumented with 13-micron-diameter thermocouples at 10 positions across a horizontal plane that allow the arrival of the hot gas front and the time history of the gas to be monitored as the front moves up the duct. One of these sections also is instrumented with surface heat-transfer and temperature gauges. These sections can be moved to any position on the side wall; by performing experiments with identical system parameters and with these instrumented sections in different positions, a complete time history of events for a given set of initial conditions can be obtained.

The apparatus described in the previous paragraphs has been substantially completed and the following experiments begun in the current grant year which ends September 30, will be completed in the next grant period.

The main focus of this work will be a study of heat transfer to the walls of the shaft and the effects of this heat transfer on the gas temperature and location of the front of the heated gas. The bottom of the shaft, initially filled with air at an ambient temperature 300 degrees Kelvin, is suddenly exposed to hot gas by opening the bottom. The effect of changing the hot-gas temperature through a range from 350 to 500 degrees Kelvin will be studied.



The influence of heat transfer will also be illuminated by examining a flow in which no heat transfer will be present: with the entire system at room temperature, the shaft is initially filled with a gas that is heavier than air, say, carbon dioxide and perhaps sulfur hexafluoride, and the motion of air into the shaft will be examined.

Because the mixing process being studied here is slow, the flow of air through leaks in the shaft can produce flows of gas from the upper part of the shaft that may be more important than the effect under study here. Hence, the influence of openings at the top of the shaft on the temperature distribution of the gas and the heat transfer to the walls of the shaft will also be studied by varying the size of the leaks from none to areas comparable to the cross section area of the shaft. Both heated and room temperature gas will be used in these experiments.

Fire-Plume Models We have also completed a review of all the Caltech data regarding entrainment into the near and far fields of fire plumes obtained over the past 12 years. The data are discussed in Zukoski 1994. A correlation was developed for the mass flux in both the far-field adiabatic plume and the near-field (or flaming region) of the fire.

#### REPORTS AND PAPERS:

Palm, S. and Zukoski, E. E., "Measurement of the Transient Development of a Ceiling Layer," Fourth International Symposium on Fire Safety Science, Ottawa, June 1994.

Palm, S. and Zukoski, E. E., *Evolution of chemical species in a transient ceiling layer with a steady state equivalence ratio of 2.3*, Jet Propulsion Center Report, October 1994, California Institute of Technology, Pasadena CA, 91125.

Zukoski, E. E., "Mass Flux in Fire Plumes," Fourth International Symposium on Fire Safety Science, Ottawa, June 1994.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution: Rutgers, The State University of New Jersey  
New Brunswick, New Jersey

Grant No.: 60NANB1H1171

Grant Title: Flow Through Vents in Compartment Fire

Principal Investigator: Professor Yogesh Jaluria  
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Telephone: (908)445-3652

Other Professional Personnel: G.P. Mercier (M.S. Student)  
Glenn Wu (Research Assistant)

NIST Scientific Officer: Dr. Leonard Y. Cooper

Technical Abstract:

Introduction. This project has been directed at two experimental studies concerning transport processes in compartment fires. The first phase of the effort concentrated on flow through horizontal vents with nonzero pressure and density differences across these. Recently, most of the effort has been focused on the movement of smoke and hot gases in open vertical shafts. The experimental findings of this research project have application in the prediction of fire spread and growth in enclosed spaces with vents, such as ships, nuclear containment buildings and multi-room compartments, and in multi-leveled buildings with vertical shafts, such as elevator shafts or staircases.

The flow in vertical shafts is very important in the accurate modeling of fire growth in multi-leveled buildings since a considerable amount of flow and thermal transport occurs in the shaft. This transport mechanism must be included for predicting the spread of smoke, hot gases and other combustion products, particularly toxic ingredients. Despite the importance of vertical shafts in the spread of fire in multi-leveled buildings, not much work has been directed at this problem. Some experimental work has been done on stairwells and vertical shafts using a relatively short shaft which gave rise to a wall plume. The natural convective flow pattern in vertical shafts has also been analytically modeled and brine solution and dense gas-air experiments have been carried out to validate the models. The present effort was undertaken to provide both a better understanding of the flow in vertical shafts as well as to obtain quantitative inputs which may be used in the modeling of building fires.

Experimental Arrangement and Results. Substantial work has been done so far on the flow in vertical shafts with natural ventilation. A fairly versatile experimental system has been designed and fabricated. A sketch of the experimental arrangement is shown in Fig. 1, along with a few photographs of the system. Smoke or hot gases are injected into the shaft at the upper opening and the downstream flow is monitored by means of thermocouples, hot-wire anemometers, visualization and optical sensors. The inlet temperature of the hot gases can be varied up to around 80 °C. Both natural and forced ventilation can be investigated in the shaft. The opening dimensions can be varied up to around 0.2 m. The shaft is about 2.0 m in height and has an aspect (height/width) ratio  $A$  of about 3.0. The conditions at the outlet



are also monitored to determine the effects of entrainment into the flow and heat transfer to the walls. Wide ranges of all the physical variables in the problem are obtainable, allowing the simulation of flow due to fire in multi-leveled buildings with vertical open shafts. Typical values of the operating conditions have been investigated, ranging from high buoyancy levels, for which the flow stays close to the vertical wall of the shaft, to much lower levels, at which the flow enters the shaft with a significant flow velocity and spreads outward very quickly.

Experimental results on the velocity and temperature distributions in the shaft have been obtained using a naturally vented, relatively short, vertical shaft. Figure 2 shows typical isotherms obtained for a range of Reynolds and Grashof numbers,  $Re$  and  $Gr$ , respectively, where these parameters are based on the conditions at the inlet. The measured velocity  $V$  and temperature  $T$  in the shaft are also nondimensionalized by the values at the inlet. The vertical distance  $x$  and horizontal distance  $y$  are measured from the inlet and are normalized by the inlet channel height  $D$  or the width of the shaft  $W$ . It is seen that the temperature is not uniform across a horizontal plane in the shaft. A wall plume is generated which conveys the hot fluid rapidly along the shaft wall from the inlet to the outlet. A recirculating flow arises away from this wall due to the wall plume and affects the transport in the wall plume. This leads to effects on the entrainment into the flow, decay of the temperature field and downstream movement of the hot gases. Horizontal uniformity can not be assumed here, as employed in previous studies. The wall plume has to be modeled in this case, considering the entrainment into the boundary layer flow and the effect of the recirculating flow on the temperature field. For tall shafts, horizontally uniform conditions are expected to arise. Therefore, the conditions under which the model has to be based on wall plume analysis and under which horizontally uniform conditions can be assumed need to be determined from such measurements of the thermal field, using different inlet conditions and shaft aspect ratio. This result will be an important input for the modeling of flow in vertical shafts. Figure 3 shows the nature of flow for the two extreme circumstances, as well as the inclusion of forced ventilation.

Shadowgraph pictures of the thermal field in the neighborhood of the inlet channel were also obtained. This visualization allowed the study of the different flow patterns and regimes that arise in the shaft. The time taken for smoke injected at the lower opening to reach the top opening as a function of the inlet temperature was determined. With increasing temperature at the inlet, the buoyancy effect becomes larger resulting in higher velocities and shorter time to reach the top. This time is an important quantity since it indicates the speed with which smoke and other combustion products reach into the higher levels of the building. The effect of the inlet mass flow rate was found to be smaller, with a larger flow rate resulting in smaller time. The temperature at the outlet depends on heat transfer to the walls as well as on the flow velocity and was measured. Some of these results have been reported earlier and additional results are to be presented at the conference.

Acknowledgments: The several discussions with Dr. Leonard Y. Cooper on this problems are acknowledged.

#### Reports and Papers:

1. Y. Jaluria, S.H.-K. Lee, G.P. Mercier and Q. Tan, "Visualization of Transport Across a Horizontal Vent due to Density and Pressure Differences," in Visualization of Heat Transfer Processes, ASME Heat Transfer Div., Vol. 252, pp. 65-81, 1993.
2. S.H.-K. Lee, W.K.-S. Chiu and Y. Jaluria, "Experimental Study of Enclosure Fires with Horizontal Vents," Proc. Fall Tech. Meeting, Eastern Sect. Combust. Inst., Princeton, NJ, pp. 327-330, 1993.
3. Abib, A. and Jaluria, Y., "Generation of Stable Thermal Stratification by Turbulent Flows in a Partially Open Enclosure," in Fundamentals of Natural Convection, ASME Heat Transfer Div., Vol. 264, pp. 127-140, 1993.
4. Jaluria, Y., Lee, S.H.-K. and Mercier, G.P., "Flow of Fire-Induced Buoyant Gases Across Horizontal Vents and in Open Vertical Shafts," Ann. Conf. Fire Res., Rockville, MD, 1993.
5. Jaluria, Y., Chiu, W.K.-S. and Lee, S.H.-K., "Flow of Smoke and Hot Gases Across Horizontal Vents in Room Fires," submitted, 1994.



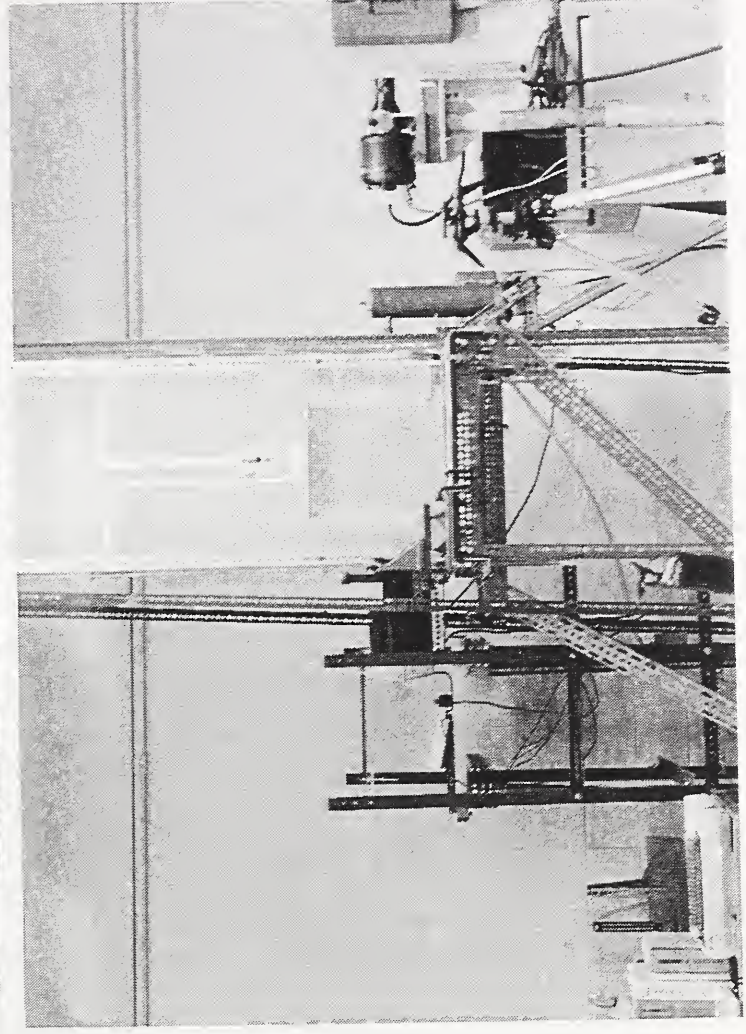
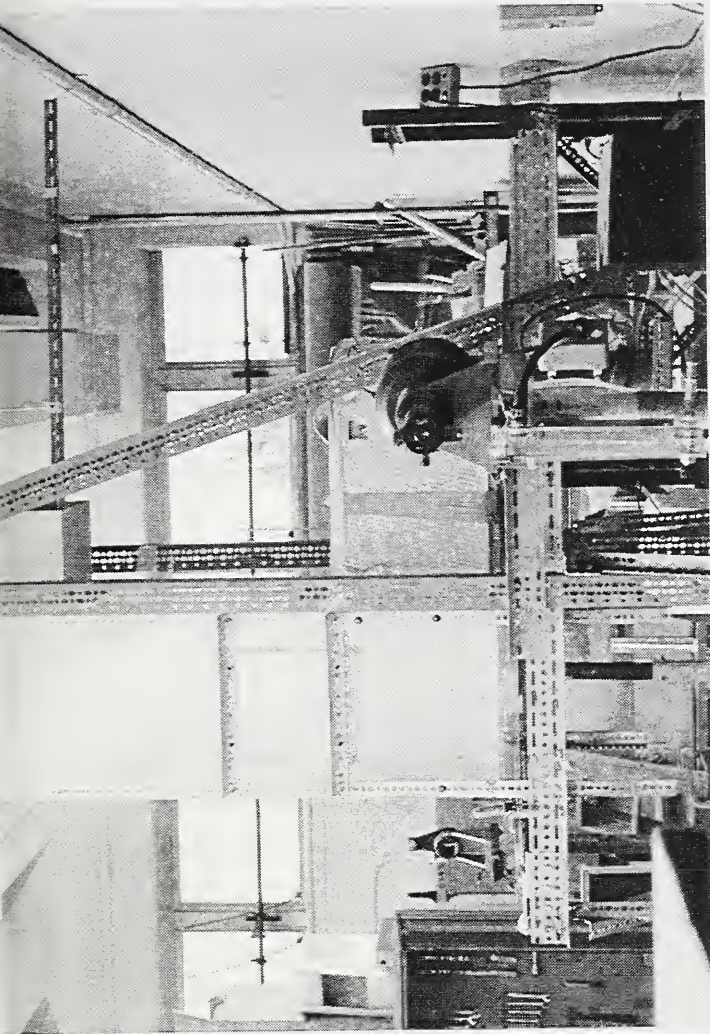
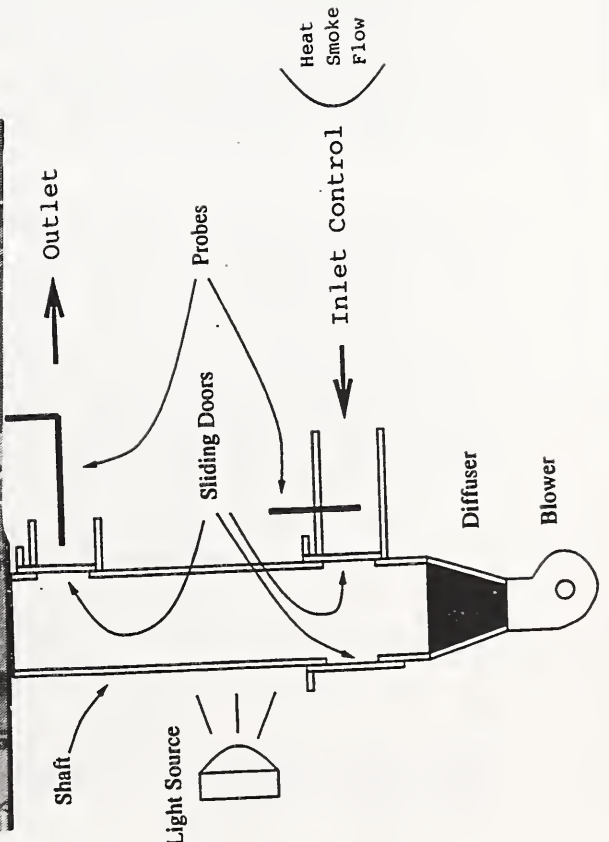
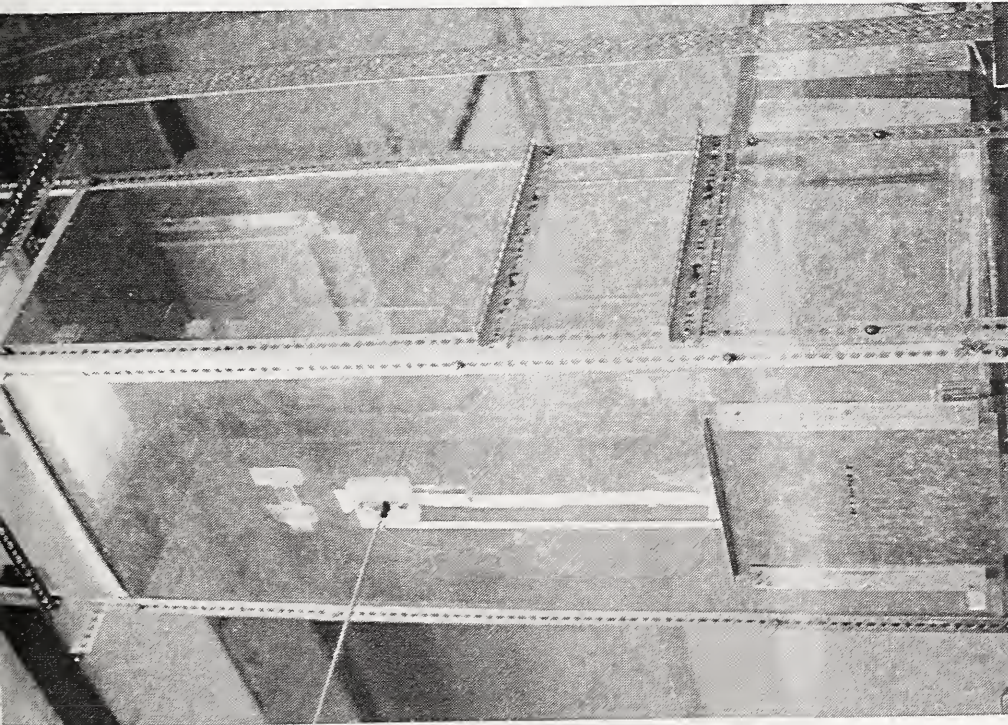


Fig. 1. Experimental arrangement for studying flow in a vertical shaft due to a fire.





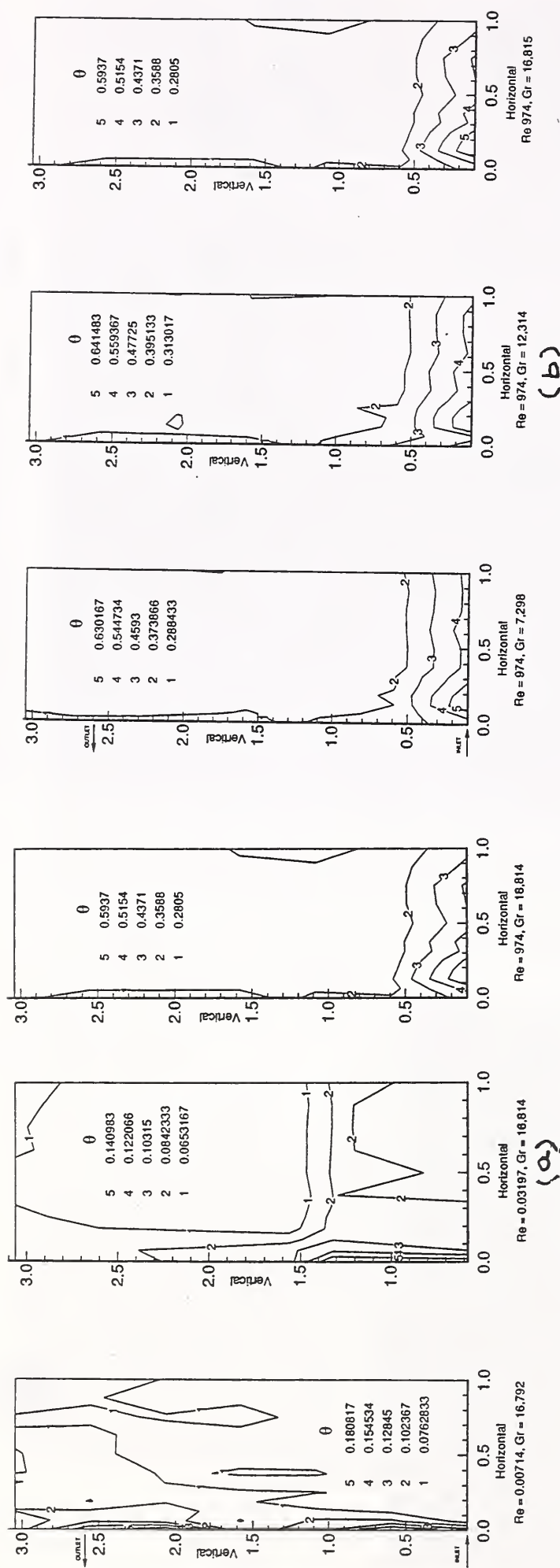


Fig. 2. Temperature field in the vertical shaft in terms of isotherms, at fixed Grashof number Gr with varying Reynolds number Re, and at fixed Re with varying Gr.

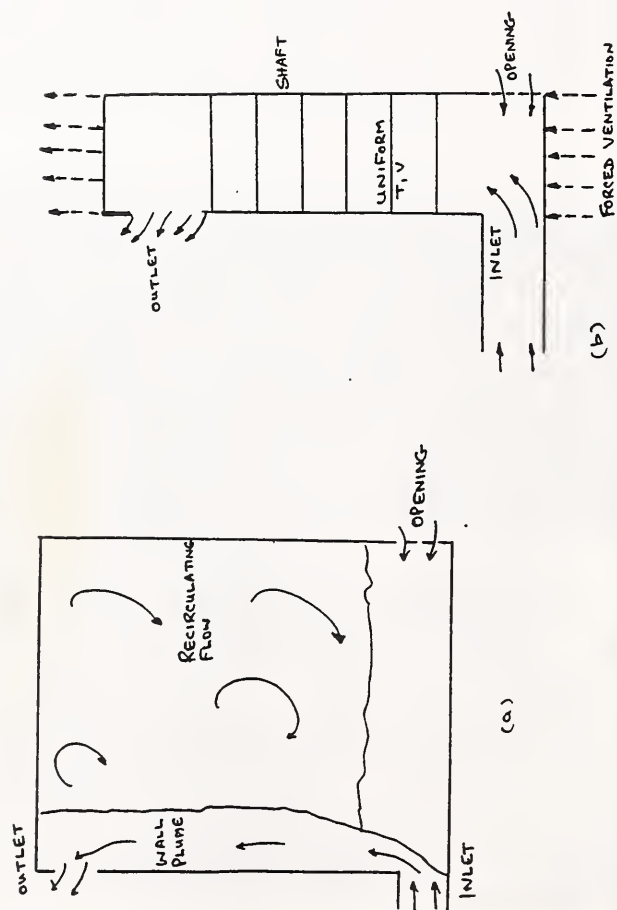


Fig. 3. Different flow patterns in a vertical shaft. (a) Wall plume in a small aspect ratio, large Froude number ( $Gr/Re^2$ ), case; (b) Horizontally isothermal flow in a large aspect ratio, small Froude number, case.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

LARGE SCALE SMOKE MOVEMENT

Professional Staff

John H. Klote, Project Leader  
Leonard Y. Cooper

Project Objective

Develop and verify algorithms for modeling large scale smoke movement in buildings.

Scope

The simulation of smoke movement in HAZARD has limited applicability to large spaces such as atria and shafts. The algorithms developed by this project will allow realistic simulation of smoke transport in these spaces. The applicability of the HAZARD methodology will be extended to large scale smoke flow including office buildings, apartment buildings, homes for the elderly, and Navy and merchant ships.

Technical Accomplishments

An algorithm and associated FORTRAN 77 subroutine, called *VENTCF2*, was developed for calculating the effects on two-layer compartment fire environments of the quasi-steady flow through a circular, shallow (i.e., small ratio of depth to diameter), horizontal vent connecting two spaces. The two spaces can be either two inside rooms of a multi-room facility or one inside room and the outside ambient environment local to the vent. The description of the flow through the vent is determined by combining considerations of the uni-directional-type of flow driven by a cross-vent pressure difference and, when appropriate, the combined pressure- and buoyancy-driven flows which occur when the density configuration across the vent is unstable, i.e., a relatively cool, dense gas in the upper space overlays a less dense gas in the lower space.

In another effort, a conceptual approach to modeling smoke flow in shafts was developed. Traditional zone fire modeling is inadequate to simulate the fire-generated environment in room configurations with large height-to-span ratios, e.g., elevator shafts and long, vertical, ventilation shafts and ducts. A means of removing this limitation is developed. This involves a method of analysis and associated model equations that can be implemented and used to advance zone fire models. The model equations simulate time-dependent flows in a long, ventilated, vertical shaft/duct with an arbitrary vertical density distributions, including one or more intervals along the shaft/duct length where the vertical distribution of the average cross-section density may be unstably stratified, i.e., density increasing with increasing elevation. The model equations are partially validated by favorable comparisons between solutions and previously published data from unsteady experiments.

Work is ongoing to develop information about the design application of various techniques of fire modeling to analysis of smoke movement in a stratified environment in atria. Modeling techniques include zone fire modeling and computational fluid dynamics (CFD). The final paper will explain the physical concepts behind conventional atrium smoke exhaust design approaches. When conventional approaches are inappropriate, CFD can be used for design analysis.

### Reports and Publications

Combined Buoyancy- and Pressure-Driven Flow Through a Horizontal Vent: Theoretical Considerations, Cooper, L.Y., presented at the 1993 Fall Technical Meeting of Eastern Section of the Combustion Institute, Oct. 25-27, 1993, Princeton NJ and published in the Proceedings of the Meeting; submitted for publication in the Journal of Heat Transfer.

Combined Buoyancy- and Pressure-Driven Flow Through a Horizontal, Circular Vent, Cooper, L.Y., NISTIR 5384, National Institute of Standards and Technology, Gaithersburg MD, April 1994; (first part of NISTIR 5384); accepted for presentation at the 1994 ASME Winter Annual Meeting in session on Fundamentals of Combined Modes in Heat Transfer, Chicago, Nov. 13-18, 1994 and for publication in the Meeting Proceedings; submitted for publication in the Journal of Heat Transfer.

Calculating Combined Buoyancy- and Pressure-Driven Flow Through a Horizontal, Circular Vent: Application to a Problem of Steady Burning in a Ceiling-Vented Enclosure, Cooper, L.Y., (second part of NISTIR 5384) to be submitted to Fire Safety Journal.

Simulating Smoke Movement Through Long Vertical Shafts in Zone-Type Fire Models, Cooper, L.Y., in review, to appear as a NISTIR, National Institute of Standards and Technology, Gaithersburg MD; also to be submitted for publication in Fire Safety Journal.

*VENTCF2*: An Algorithm and Associated Computer Software for Calculating Flow Through a Horizontal Ceiling/Floor Vent in a Zone-Type Compartment Fire Model, Cooper, L.Y., in review, to appear as a NISTIR, National Institute of Standards and Technology, Gaithersburg MD; also to be submitted for publication in the Journal of Fire Protection Engineering.

Overview of a Theory for Simulating Smoke Movement Through Long Vertical Shafts in Zone-Type Fire Models, Cooper, L.Y., submitted for presentation at the 1993 Annual Fire Research Conference, Oct. 17-20, 1994, and for publication in the Proceedings of the Conference; to be submitted for presentation at the 1994 Fall Technical Meeting of the Eastern Section of the Combustion Institute and for publication in the Proceedings of the Meeting.

### Related Grants:

Flow Through Horizontal Vents as Related to Compartment Fire Environments, Rutgers - State University of New Jersey.

Experimental Study of Environmental and Heat Transfer in a Room Fire, CALTECH.



**BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94**

Institution: Clemson University

Grant No.: 60NANB0D1023

Grant Title: Mathematical Modeling of Human Egress from Fires in Residential Buildings

Principal Investigator: Michael M. Kostreva, Professor  
Department of Mathematical Sciences  
Clemson University  
Clemson, SC 29634-1907  
Telephone: (803) 656-2616

NIST Scientific Officer: Richard Peacock

Technical Abstract: In recent years, this research project has produced some significant findings and discovered that there are some areas of research left to investigate. Mathematical modeling of egress of individual occupants from residential buildings remains the focus. The basic mathematical framework for all the fire egress models is a network superimposed on a geometric model of a residential building. Nodes in the network represent locations within and around the building, while links comprise potential egress routes. Each link carries several cost functions, possibly dependent on time, to be minimized by occupants in egress. Assignments of nodes, links and costs are made to closely reflect an actual scenario. Each occupant in the building is initially located at a unique node of the network, an origin node. The problem is to find, for each occupant, all nondominated paths (those minimizing all costs) leading from his/her origin node to a single destination node, representing safety outside the building.

In our research, we have derived several approaches which can solve the path planning problem in networks with multiple time varying objective functions. Applying dynamic programming to fire egress modeling allows for generalization of the network assumptions made in the current version of HAZARD I and development of a unified framework for handling a new more complex model based on a multiple objective dynamic network in which links and nodes may be removed, and in which link weights are multi-dimensional and changeable in time. Such assumptions provide the network model a perspective not previously considered in the literature. Although they increase the

mathematical complexity of the problem, the network model becomes a more realistic representation of the highly variable environment. The network evacuation model is, in fact, strongly multiple objective in nature. There are various performance measures of a physical nature and of a behavioral nature inherent to the problem. Any meaningful model possesses dynamics due to an expanding and evolving fire and its changing parameters. An approach through time dependent multiple-objective dynamic programming, such as what we have developed, has the required capabilities for fire egress modelling and has great potential for application to fire safety planning and building design.

The results we have obtained so far are significant contributions to scientific knowledge and literature. Recently some Graduate Students in the Department of Mathematical Sciences have participated in the research activity of this project at no cost to NIST. As trainees, they acted as technical resources provided by the Department of Mathematical Sciences. They were under the direction of the senior researchers, and they provided computer programming assistance. Some of the newer results were documented in the work of Emsermann (1993), Newton (1993) and Wilson (1992). These results also documented that the results could be implemented into usable FORTRAN programs. After testing at Clemson, programs were transferred to NIST and tested there. In addition, a comparison with existing EXITT methodology was carried out this year and reported in Lancaster (1994). It seems that the methodology created by this research can be made understandable to graduate level students, who can then be assigned to implement the algorithms into FORTRAN programs with some consultation from those responsible for creating and proving the validity of the mathematics.

The final integration of the methodology into HAZARD packages remains to be performed. It will likely be accomplished at NIST, where the research programs are centered and where all production computer codes reside.

#### Reports and Papers:

Emsermann, Markus, "Time Dependency in Multiple Objective Dynamic Programming: The General Monotone Increasing Case", Department of Mathematical Sciences, Clemson University, April 1993.

Lancaster, Laura, "A Comparison of Two Methodologies for Fire Egress Analysis", Department of Mathematical Sciences, Clemson University, April 1994.

Newton, Jennifer, "An Approximate Algorithm for the Time Dependent Multiple Objective Routing Problem", Department of Mathematical Sciences, Clemson University, May 1993.

Wilson, Michael, "A Time Dependent Vector Dynamic Programming Algorithm for the Path Planning Problem", Department of Mathematical Sciences, Clemson University, May 1992.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

BALANCED DESIGN

Professional Personnel

Richard W. Bukowski, Project Leader

John Gross

Walter Jones

Gamal Ahmed

Project Objective

To quantify the reliability of detection systems, suppression systems, and compartmentation, and to conduct a comparative analysis of compartmentation using fire resistive and noncombustible construction.

Scope

Trade-offs between active and passive fire protection strategies are often made without technical foundation. As legislation mandates sprinklers and detectors in specified occupancies the role of compartmentation must be understood so that overall safety is not compromised. Thus, *PL102-522* tasked NIST to conduct this study as a joint effort of the public and private sectors. As required in the legislation, the scope of the project has been reduced to reflect the actual private sector funding level. This has limited the scope of the study to the quantification of reliability; performance prediction is being addressed

Technical Accomplishments

During FY94 project planning was carried out for both the technical approach and identification of resources -- both financial and informational. Committees for technical and financial planning were established and the private sector funding required in the legislation was secured. A general consensus was reached as to timing and direction and a program start date of August 1, 1994 was agreed.

Reports and Publications

None: new project

Related Grants

None





**BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94**

**Institution** Hughes Associates, Inc.

**Grant No.** 60NANBAD1531

**Grant Title** Enhanced PC-based Building Fire Assessment System

**Principal Investigator** Edward K. Budnick, P.E.  
Hughes Associates, Inc.  
6770 Oak Hall Lane, Suite 125  
Columbia, MD 21045-4731

**Other Personnel** Harold E. Nelson, P.E.  
Sean P. Hunt, E.I.T.

**NIST Scientific Officer** Richard W. Bukowski

**Technical Abstract**

**Introduction** The objective of this effort is to develop an engineering based method for fire hazard/risk analysis of existing and planned buildings. Recent progress and ongoing efforts to develop and validate analytical methods for predicting fire hazards and the impact of various fire protection features provide at least an initial basis for introduction of quantitative methods for fire hazard analysis and code compliance. This investigation involves development of a PC-based version of the existing Fire Safety Evaluation System for office buildings and integration of quantitative methods and fire models to enable engineers to perform detailed fire hazard, risk equivalency, and cost optimization analyses.

**Status** A draft version of the basic PC-based Enhanced Fire Assessment System (EFAS) has been developed. The program is written in Microsoft Visual C/C++, designed to run in the Microsoft Windows Version 3.1 or higher environment and is a literal translation of the NFPA 101M FSES for Business Occupancies. The program includes extensive explanatory text to assist the user in selection appropriate conditions, simplification of exceptions in order to minimize inconsistency in output among different users, and a number of visual cues to indicate the status of the evaluation. The current version of the program provides the user with building scores relative to fire control, egress capability, and general fire safety. In addition, the program can perform limited fire safety equivalency evaluations.

The current version of the program contains four modules of encapsulated code, each with specific tasks. The Applications Module is the main program. This module controls the individual performance elements, including calculations, output, and interface parameters. The FSES has been encoded as a single document application, allowing the user to address one building at a time. A future consideration will be expansion of the program to multiple document (building) applications.

The Main Window Module is the outer framework of the Windows based program. It is analogous to the Program Manager in Microsoft Windows and allows the user access to file input/output features, print features, window controls, and program help.

The Document Module is the storage medium for user input. This module is invisible to the user. The document module is used to store the individual scores for each parameter, the column that was selected for each parameter, the row that the user selects for each parameter screen, building height, number of stories, whether the building is new or existing, and a number of flags that are used to determine if a parameter screen has been altered and/or corrected. The document module also contains all of the scoring functions, filters that check if data are complete and accurate, and all of the code for storing data to a file.

The View Module is the interface, used for entering data and selecting score categories. Currently, there are 15 elements in the view module, including a general building data screen, a general building characteristics screen, the parameter access screen, and an element for each fire safety parameter. None of the viewing elements are erased when not in use unless user specified.

Future Work The baseline program will undergo field testing to verify program output on a limited scale and identify critical factors needing experimental verification. In addition, the feasibility of integrating specific analytical methods will be determined in order to provide the user with quantitatively based output and the ability to assess different fire protection features or strategies in terms of overall building fire protection objectives. This effort will include an attempt to integrate the necessary predictive methods to evaluate fire protection designs on the basis of time to hazard, escape time, or a similar quantitative basis.

### Acknowledgements

BFRL currently has a major initiative in development of quantitatively based methods for building fire risk analysis. This effort involves enhancement of available predictive methods, development and verification of new methods to calculate fire hazards in generic building environments, and introduction of these methods into the mainstream engineering and building communities under the umbrellas of risk-based engineering methods. Several researchers in BFRL are actively involved in these efforts. Our discussions with Mr. Richard Bukowski, the scientific officer for this grant, and Mr. Dan Madrzykowski have helped to formulate the framework of the program such that verified enhancements can be incorporated and the resulting method will be integratable into broader scope initiatives under development at NIST.

### Reports and Papers

This is a new initiative. A technical report outlining the progress to date will be completed by the end of 1994.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

COMPREHENSIVE FIRE RISK ASSESSMENT METHOD

Professional Personnel

Richard W. Bukowski, Project Leader

Project Objective

To develop an internationally accepted fire risk calculation method that is suitable as the foundation for a performance fire code by 2000.

Scope

This project is intended to develop a harmonized process for conducting fire safety engineering calculations on buildings to assess their fire safety performance. Such calculations could be utilized to demonstrate compliance with any performance-based code in the world.

Technical Accomplishments

The first step was to establish an international, cooperative effort under CIB W14 and in direct support of ISO TC92/SC4. We volunteered to chair the activity, but the arrangements took a long time due to a change in the W14 leadership. This has now been accomplished. A working group has been established where participants are funded by their own organizations, and task groups formed to address an initial set of crucial issues.

The group needs to review the existing body of work and identify the elements which should form the final methodology, including optional components. Three methods (Japan, Australia, and US) are ostensibly complete, although some portions of each contain only place holders due to limitations in the technology. A major expense this year was the translation of the Japanese method (\$50,000). Additionally, a new UK methodology was released this year. These all need to be studied and the research needed to fill gaps needs to be done.

Several initial project collaborations have been identified and the working relationships are being worked out. A joint effort on structural performance prediction has been established between US and Canada with interest expressed by Australia and Japan. A project on uncertainty assessment of models and data has been outlined. This would provide a mechanism for qualifying calculational techniques on the basis of computational uncertainty related to design safety factors. Sven-Erik Magnussen of Lund Univ. in Sweden has agreed to chair this effort. Other collaborations on verifying zone models and adding phenomena to CFAST have been discussed.

Reports and Publications

Bukowski, Richard W. and Babrauskas, V., Developing Rational, Performance-based Fire Safety Requirements in Model Building Codes, *Fire and Materials*, in press.

Related Grants

A Risk Assessment Methodology for Fire Safety Factors in Performance-based Design of Buildings, Factory Mutual Research Corporation





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY 94

FIRE MODEL EVALUATION

Professional Personnel

Richard D. Peacock, Project Leader  
Paul A. Reneke, Computer Scientist  
Henri Mitler, Physicist  
Emil Braun, Physicist  
Walter W. Jones, Leader, Fire Modeling Group

Objective

To develop protocols to quantify the level of accuracy of computer-based predictive fire models and the experimental, statistical, and analytical techniques to support this method by 2002.

Scope

Fire models have progressed to the point of providing good predictions for some parameters of fire behavior. However, users and authorities are often asked to accept building fire safety design based on fire models without accepted statements of their predictive accuracy. Key to the increased use of models in performance based standards and elsewhere is the ability to state with confidence how close actual conditions are to those predicted by the model. There is no domestic or international agreement on a procedure for quantifying fire model accuracy and demonstrating suitability for a particular application.

In order to check that such a computer model satisfactorily represents physical reality a process of validation is necessary to test the adequacy of a model's theoretical basis and its implementation. The project must address multiple areas to address evaluation of fire models: model documentation and useability, review of the theoretical basis and implementation of models, sensitivity analysis, techniques for obtaining and comparing experimental data and model results, and documentation requirements for the comparisons. In addition, a sufficient base of experimental data must exist over a wide range of test conditions to compare with fire models. What constitutes a "sufficient base" must be determined.

Technical Accomplishments

Analytical models have progressed to the point of providing predictions of fire behavior with an accuracy suitable for most engineering applications. Two obvious questions arise concerning the use of these models for engineering calculations:

- How good is the output of model (How close are the actual conditions to those predicted by the model)?
- How good do the inputs to the model need to be (How do changes in the model inputs effect the model outputs)?

These questions are the subject of this project. This year's effort has developed a procedure for quantifying the accuracy and acceptability of these models. Computational tools and experimental techniques are required to support the procedure. Two areas were identified for application this year: development of temperature measurement techniques and examination of their variability to help determine the quality of future real-scale experiments designed for model evaluation, and examination of techniques for sensitivity analysis of complex fire models using the CFAST model to provide input data for the analysis.

**Sensitivity Analysis:** A sensitivity analysis of a model is a study of how changes in model parameters affect the results generated by the model. Model predictions may be sensitive to uncertainties in input data, to the level of rigor employed in modeling the relevant physics and chemistry, and to use of inadequate numerical treatments. The purpose of conducting a sensitivity analysis is to determine:

- the dominant variables in the models,
- the acceptable range of values for each input variable, and
- the sensitivity of output variables to variations in input data.

Conducting a sensitivity analysis of a complex fire model is not a simple task. Many models require extensive input data and generate predictions for numerous output variables over an extended period of time. Several methods of sensitivity analysis have been applied to fire models, but most have had little utility. These range from explicit evaluation of the equations used in simple models such as ASET to pointwise evaluation of complex models from numerous computer runs of the model. The technique chosen for use will be dependent on the resources available and the model being analyzed.

For the simple ASET-B model, a factorial design was applied for the sensitivity analysis to study the effect of changes in the input parameters for floor area, heat loss fraction, and room height. Floor area took on the values 8.919 and 26.756 m<sup>2</sup> (96 and 288 ft<sup>2</sup>),  $\lambda_c$  took on the values .6, .7, .8, and .9 and the height above the burner took on the values 2.134 and 4.267 m (7 and 14 ft). The height of the burner measured from the floor was set at .305 m (1 ft) and  $\lambda_r$  was fixed at .35. The energy release rate was 1 kW for the time period [0,180) and 25 kW [180,1200). All other parameters were held

**Table 1.** Relative range of change in outputs for a 10% change in inputs to the ASET-B model.

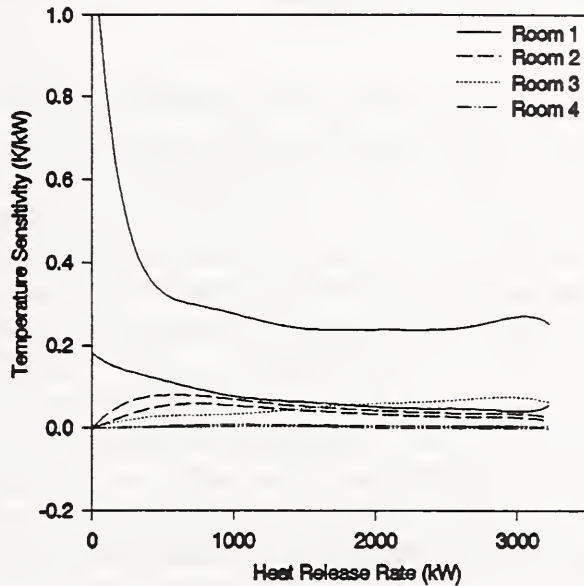
↓ Inputs / Outputs→	Interface Height	Upper Layer Temperature
Room Area	+2 - +5%	+10%
Height Above the Burner	0 - +10%	-10 - -8%
$\lambda_c$	+2 - +5%	-12 - -75%

at their nominal levels. When each run was made, the sensitivity measures were computed assuming a 10% perturbation in each of the following parameters: area,  $\lambda_c$ , and height above the burner. Each run was terminated when the interface height had reached the floor and the upper layer temperature had reached 100°C. From numerous plots made to study the effects of perturbations in the inputs on the interface height, upper layer temperature and time to reach a particular height or temperature,



an overall picture of the sensitivity of the ASET model can be obtained (table 1). ASET-B is fairly insensitive to the uncertainty in the room area and height above the burner, but can be quite sensitive to the uncertainty in the value of  $\lambda_c$ . Since the objective of ASET is to be able to determine available safe egress time,  $\lambda_c$  can be selected according to whether time to detection or time to hazardous conditions is desired.

For more complex fire models, obtaining an overall assessment of model sensitivity may become extremely complex, with numerous model inputs and outputs. Thus, more narrowly focused local sensitivity investigations are appropriate. With numerous model simulations, however, an overall picture of model performance can be obtained. Figure 1 shows this sensitivity for the four-room scenario studied. Except for relatively low HRR, the upper layer temperature sensitivity is less than 1 K/kW and usually below 0.2 K/kW. Not surprisingly, the layer that the fire feeds directly is most sensitive to changes. The lower layer in the fire room and all layers in other rooms have sensitivities less than 0.2 K/kW. This implies, for example, that if the HRR for a 1 MW fire is known to within 100 kW, the resulting uncertainty in the calculation of upper layer temperature in the fire room is about  $\pm 30$  K.



. Sensitivity of temperature to heat release rate for a four-room growing fire scenario

**Measurement Techniques:** Experimental results from fire tests have historically been made without estimates of uncertainty. This, at best, permits only a qualitative judgement of the "goodness" of the comparison. In order to *quantitatively* compare the experimental results of a fire with the predictions of a model, the accuracy of the test results must be known. Thus, we must have a thorough understanding of the measurements and of the uncertainties in those measurements in the experiments performed. One of the important tasks, therefore, is to have or develop appropriate measurement techniques.

We must first establish just how accurately needed measurements must be made. For example, it would make no sense to try to measure something more accurately than the fluctuations in the given variable, in a given experiment. On the other hand, it is necessary to make measurements accurate enough to permit quantification of the degree of replication possible for any given experiment. A number of considerations shows that the accuracy to which gas temperatures should be made is to within a few degrees Celsius. For example, consider flux measurements. Suppose we want to calculate radiation fluxes to within 1%. Since the radiation flux from the hot layer is proportional to  $T^4$ , it is clear that the absolute temperature must be known to within 0.25%. For  $T = 1000$  K, therefore, to within 2.5 K.

The premier device used is the thermocouple. We therefore examined its adequacy for the measurements. The thermocouple type most commonly used in our work is the type K Chromel/Alumel thermocouple, good from 270 K to 1640 K; when properly calibrated, it yields measurements good to within 0.7 K. The response is reasonably sensitive and linear. Thus the *nominal* accuracy of the

thermocouples is more than adequate. There is an extensive literature on the problems attendant on the measurement of temperature with thermocouples. The principal *instrumental* sources of error can all be substantially reduced by appropriate techniques. A second class of errors arises if one naively assumes that the thermocouple reading is the gas temperature. In fact, radiation and conduction corrections need to be made. For a large-diameter thermocouple, the radiation correction can be 100 K or more. Analysis of the radiation correction shows that the results from using a set of thermocouples with different sizes of beads can be used to extrapolate to a zero-sized bead, which has no radiation correction.

When the gas is laden with particulates, such as soot, some deposition onto the thermocouple will take place. Some questions then arise, such as: what does the deposit do? what are the magnitudes of these effects? what, if anything, do we need to do to correct for these effects? Some experiments were carried out in a reduced-scale apparatus, at a low power level. In these experiments, the temperature in the box only rose to about 340 K. It was found that, apart from the expected excursions at the times the thermocouples were removed for cleaning and replacement, the traces appear to be nearly identical. Examination of the temperature **differences** among the thermocouples shows that the largest difference occurs during the initial pulse, and is less than 1 K. This is well within the accuracy of the thermocouples, particularly since the locations were not identical. The first conclusion is that scraping the thermocouple clean of soot appears to have no adverse effect on its subsequent performance. Secondly, even though there was about 1 mm of soot on the bead which was exposed for 30 min, the readings appeared unaffected, at these low temperatures. Clearly, further experiments are needed to quantify the effects of sooting, especially at higher temperatures.

#### Reports and Publications

"The Use of Thermocouples in Reference Fire Tests." Mitler, H. E., NISTIR to be published.

"Understanding Sensitivity Analysis for Complex Fire Models." Peacock, R. D., Reneke, P. A., Forney, C. L., and Kostreva, M. M., journal article to be published.

"Verification of a Model of Fire and Smoke Transport." Peacock, R. D., Jones, W. W., and Bukowski, R. W., Fire Safety Journal 21 89-129, 1993.

"Comparison of Full Scale Fire Tests and a Computer Fire Model of Several Smoke Ejection Experiments," Braun, E., Lowe, D. L., Jones, W. W., Tatem, P., Bailey, J., and Carey, R., NISTIR 4961 (1992).

"Field Modeling of Room Fires," Davis, W. D., Forney, G. P., and Klote, J. H., NISTIR 4673 (1991)

#### Related Grants

"Sensitivity Analysis for Mathematical Modeling," M. Kostreva, Clemson University.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY 94

DEVELOPMENT OF THE FDMS DATABASE SYSTEM FOR FIRE RELATED DATA

Professional Personnel

Rebecca W. Portier, Project Leader

Objective

Develop a centralized database of test values generated from a variety of sources within the fire community accessible through communications networks. Provide a platform-independent user interface to the database to support importing new data, editing existing data, querying and selecting specific test values, and interfacing to existing fire models.

Scope

A unified method of accessing data is crucial to both experimental and modeling efforts in the development of the science of fire. FDMS, the Fire Data Management System, is a computer database for organizing and presenting fire data obtained from bench-scale and real-scale tests as well as fire simulation programs. By storing available fire test values in a common format, this data is readily available to computer models, plotting programs, and report generators.

Technical Accomplishments

File formats proposed in "Fire Data Management System, FDMS 2.0, Technical Documentation," have been implemented on IBM-PC and Unix platforms with refinements to improve data access speed. A text-based user interface to provide querying capability of available data has been completed for both platforms. Export functionality exists to generate an FDMS import format file with additional export formats in development including Lotus 123 and ASCII comma-delimited. Once the import functionality is completed, available test results will be loaded into the database with an anticipated beta test beginning in FY-95.

Reports and Publications

"Fire Data Management System, FDMS 2.0, Technical Documentation," Portier, R.W., NIST Technical Note 1407, 1994.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - 1994

SUPPORT OF THE NAVY FIRE MODELING PROGRAM

Funding Agency

Naval Research Laboratory

Professional Staff

Walter W. Jones, Project Leader

Glenn P. Forney

Paul A. Reneke

Project Objective

Develop algorithms to enhance the predictive capabilities of CFAST in handling semi-confined fire development as applicable to Navy ships.

Technical Accomplishments

The zone model CFAST has been developed to predict fire growth and smoke spread in any compartmented structure. Several phenomena of particular interest to the US Navy have been incorporated. These include conductive heat transfer through barriers, such as ship decks. The Navy is particularly interested in the ceiling/floor aspect in solving the problems encountered in the STARK (ISCS) fire in the Persian Gulf. We will also begin planning for incorporating horizontal flow into CFAST. This is the hybrid extension which is important for detector siting and for testing smoke mitigation efforts with pressurization. A concept for a hybrid model has been developed. This would introduce the horizontal momentum equation into the zone model framework. Finally, a flame spread algorithm is under development.

Reports and Publications

"Calculating Flame Spread on Horizontal and Vertical Surfaces," G.A. Ahmed, M.A. Dietenberger, and W.W. Jones, NISTIR 5392 (1994).





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

SMART ELEVATORS

Professional Staff

John H. Klote, Project Leader

Project Objective

Study the feasibility of using developing smart elevators for fire evacuation.

Scope

In many tall buildings, fire evacuation by stairs can be very time consuming. Further, there are people who cannot use stairs because of physical disabilities. The adaptation of elevators for general fire evacuation is a potential solution to these problems. This project will study the feasibility of developing smart elevators for general fire evacuation based on inputs from its own sensors and other building systems (fire suppression, fire alarm, firefighters command center, HVAC etc.).

Technical Accomplishments

None: New Project.

Reports and Publications

None: New Project.

Related Grants:

None





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

CEILING FIRES

Professional Personnel

H.E. Mitler, Project Leader  
P. Reneke, Computer Scientist

Project Objective

To develop an understanding of the effects of the presence of a ceiling on the evolution of a wall, corner, or other room fire, followed by the spread of the fire across the ceiling. This should be at a level sufficient to produce a preliminary (engineering-level) algorithm by September 1993, a much superior one by September 1994, and which can be incorporated into HAZARD.N by September 1995.

Scope

This project addresses the problem of fire growth on walls and ceilings in enclosures, and particularly on their mutual interactions. The effects of the ceiling on room fires is one of the most notable lacunae in our ability to predict the development of room fires. The wall-fire project (as well as other studies) have yielded reasonably successful models which predict wall fires. Most of these studies, however, neglect the effect of the ceiling; this is the case, in particular, for SPREAD, the BFRL model which is being prepared for insertion into HAZARD. That is, most extant models assume (in effect) that the wall is infinitely high. In fact, the presence of a ceiling has several important effects. Studying and modeling these phenomena is a natural -- indeed, a necessary -- sequel to the Wall Fire project. There are a number of other areas where having such a model will be important.

Technical Approach

The work is being done in three phases. In the first year, a literature survey of fires impinging on ceilings, including axisymmetric fires, wall fires, and corner fires, was carried out. Flame extensions, fluxes and their position dependence, entrainment rates, effect on combustion rates, and ignition of flammable ceilings were all looked at. As a result of the survey, it was determined what areas need to be studied further, and it was established how much time and other resources are needed. It was also determined what experimental work we can carry out at BFRL. A detailed work plan was developed. The theoretical understanding of flows and combustion under ceilings was tied together with empirical observations, and a preliminary algorithm put together. This includes a preliminary plan for writing a stand-alone ceiling fire computer program, to be incorporated into the wall-fire computer program SPREAD.

In the second year, experimental data will be obtained and used to improve the algorithm, and plans for its insertion into CFAST will be formulated. We will also plan and carry out new experiments. Based on the new data, we will devise a much better algorithm, and write a NISTIR on the work.

In the third year we will calculate effects of ceiling ignition when the ceiling is flammable, program the algorithm, merge it with SPREAD, and harmonize it with CFAST. Finally, we will validate the new program, write documentation, and help the group to insert the program into CFAST.

### Technical Accomplishments

Documentation for SPREAD was completed, and went to WERB review.

A literature survey on studies of fires on ceilings was carried out. A definitive Project Plan, based on analysis and the literature survey, was completed (in the form of a memo). Discussions were held with the University of Kentucky regarding possible cooperative work on the project.

An algorithm predicting the behavior of a wall fire which impinges on the ceiling was devised. Several reports were completed.

### Reports and Publications

H.E. Mitler and K.D. Steckler: Memo outlining detailed three-year project plan, March 1993.

Mitler, H.E., and Steckler, K.D. (1993) "Comparison of Wall-Fire Behavior With and Without a Ceiling," NISTIR 5380, National Institute of Standards and Technology, Gaithersburg, MD, 20899

H.E. Mitler and K.D. Steckler (1994) Wall Fires and the Approach to Flashover in an Enclosure, to be published in the Safety Journal

Mitler, H.E. (1994) "An Algorithm to Describe the Spread of a Wall Fire Under a Ceiling," to be published as a NISTIR; in review

### Related Grants

"Prediction of Fire Dynamics," R. Alpert and J. deRis, Factory Mutual Research Corp.

"Upward Flame Spread on a Vertical Wall," A. Kulkarni, Pennsylvania State University.

"A Study of Fire-Induced Flow Along the Vertical Corner Wall," K. Saito, University of Kentucky.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution: Factory Mutual Research Corporation

Grant No: 60NANB1D1177

Grant Title: Prediction of Fire Dynamics

Principal Investigator: J. de Ris

Other Professional Personnel: H.W. Emmons  
L. Orloff  
D.M. Karydas

NIST Scientific Officer: W.W. Jones/H. Mitler

Technical Abstract:

This report summarizes accomplishments of a Factory Mutual Research Corporation (FMRC) project on the Prediction of Fire Dynamics for the NIST grant period indicated. Work performed under a subcontract by Professor H.W. Emmons on Ceiling-Jet Dynamics is described under Task 1. The accomplishments of three tasks performed at FMRC are then presented in summaries of Tasks 2, 4, and 5. All of this work is aimed at the development of submodels or algorithms that can be used in NIST/BFRL comprehensive computer fire models. The FMRC tasks have previously led to the development of practical smoke-point measurement techniques for solid combustible materials, as described in a paper presented at the 4th International Symposium on Fire Safety Science, Ottawa, June 1994. More recently, the FMRC tasks have led to the development of important similarity relationships for flames on vertical surfaces.

Task 1: Prediction of Fire in Buildings (H.W. Emmons)

During the past year, the ceiling jet equations with y momentum pressure correction were solved assuming the equations held everywhere even ahead of the advancing front where the velocity is zero. It was assumed that the Froude number equals 1 at the open end and that the layer started at  $x = 0$  with zero slope and at the specified inlet temperature. There was no requirement on the ceiling jet at its leading edge as it advanced.

Completed results show that the front moves at about  $Fr = 1$  as it advances. The solutions are oscillatory as expected when the y momentum is included. However, after about 10 seconds an instability develops at  $x = 2(m)$ . The cause has not yet been found. Is it a basic instability or a coding error? It may be because there is too rapid a drop in the jet depth where a large heat loss begins. Several solutions to this unexpected problem are being tried.

Task 2: Models for Turbulent Flame Chemistry and Radiation (J. de Ris) and

Task 4: Soot and CO Oxidation in Buoyant Turbulent Diffusion Flames (L. Orloff)



The objective of Task 2 is to develop models for predicting 1) wall fire radiative feedback to the fuel surface, which controls wall fire burning rates, and 2) the combined soot and CO oxidation which controls the release of incomplete (toxic) products of combustion (soot, CO, etc.) and radiation from buoyant turbulent diffusion flames. Task 4 has the objective of providing experimental data for the development of these models.

Considerable progress has been achieved during the past year towards the formation of similarity relationships that may be very encouraging to fire modelers. Analysis of temperature and soot layer thickness profiles together with Markstein's<sup>1,2</sup> radiant extinction measurements show that the profiles remain geometrically similar for a fixed overall fuel to entrained air equivalence ratio corresponding to a fuel mass transfer rate,  $\dot{m}''$ , which increases with the square root of height,  $Z$ .

Various pyrolysis zone heights were simulated by supplying propylene to up to ten 132 mm high and 320 mm wide water-cooled sintered-metal gas burners. The forward heat transfer zone was simulated by a 660 mm high water-cooled heat transfer plate mounted above the gas burners. The flow was maintained two-dimensional by 150 mm deep water-cooled side walls attached to the burner apparatus over its entire height.

The thickness of the soot layer,  $\delta_s$ , was measured by inserting arrays of 5 mm glass rods into the flames perpendicular to the wall surface and rapidly withdrawing them after a two second exposure to the flames. The soot layer thickness was determined from the average length of soot deposit on ten rods.

Figure 1 shows the length ratio,  $Z/\delta_s$ , correlated against the inverse modified equivalence ratio  $\rho_A(2gZ)^{1/2}/(\dot{m}''-\dot{m}_o'')$ . The modification of the equivalence ratio is required because the soot vanishes and the flames become blue for mass transfer rates less than  $\dot{m}_o''=4 \text{ g/m}^2\text{s}$ . As a result of wall cooling and dilution by the products of combustion at low mass transfer rates, the data show that the cut-off,  $\dot{m}_o''$ , is independent of  $Z$ . The turbulent motion typically transports the luminous soot (e.g. visible flames) out into the incoming air all the way to where the mean gas temperature drops to around 1000K. The correlation says that the soot layer thickness is proportional to  $Z$  for a given ratio of entrained air,  $\rho_A(2gZ^3)^{1/2}$  to supplied fuel  $\dot{m}''Z$  above its blue flame value  $\dot{m}_o''Z$ . The correlation extends over a very wide range of flame equivalence ratios.

Temperature profiles across the flame boundary layer were measured by a thermocouple rake consisting of 15 insulated Chromel-Alumel thermocouples inside 1.6 mm diameter Inconel sheaths spaced 12.6 mm on center and protruding 1 cm downward into the rising flow. The measured temperatures inside the flame were significantly depressed by radiation heat loss. On the other hand, the thermocouple temperatures outside the flame were significantly increased by radiant heat transfer from the flame. We corrected for both these effects with a simple heat transfer model to obtain the correlations shown in Figure 2. The vertical dashed line at  $y/\delta=1$  shows the boundary of the soot layer occurring at temperatures near  $T=1000\text{K}$ . Inside the soot layer, the presence of cold fuel is seen by the temperature drop near the wall. Outside the soot layer, the mixing of combustion products with the entrained air causes the corrected temperatures to asymptotically approach the ambient temperature as  $y/\delta$  increases. These outer temperature profiles correlate reasonably well when plotted against  $(y-\delta)/Z$ .

Markstein<sup>2</sup> reports measurements of the extinction of infrared radiation,  $\epsilon_o$ , by soot (at wavelengths  $\lambda_o = 0.9 \mu\text{m}$  and  $1.0 \mu\text{m}$ ) across the flame boundary layer. These measurements immediately provide

the integral of the soot volume fraction,  $f_v \delta_s$ , across the flame,  $f_v \delta_s = -\lambda_o \ln(1-\epsilon_o)/7$ , which is replotted here in Figure 3 using coordinates similar to those in Figure 1. The factor of 7 in the above expression is recommended by Hottel and Sarofim<sup>3</sup> for soot. The correlation is not as good as for the soot standoff distance (Figure 2), apparently because the soot volume fraction,  $f_v$ , depends weakly on the flow time.

The faired curves in Figure 3 indicate that the fractional conversion of fuel carbon to soot,  $\chi_s$ , at a fixed mass transfer rate (1) initially increases proportional to the flow time up to a height  $Z=0.75$  m for the  $C_3H_6$  flames, and then (2) becomes constant at greater heights.

Figure 4 shows the measured transverse temperature profiles for four  $C_3H_6$  flames at two heights and two equivalence ratios,  $\dot{m}/Z^{1/2}$  near 11 and 26  $g/m^{5/2}s$  respectively. Notice the dependence of profile-shape on equivalence ratio, but almost perfect similarity at fixed equivalence ratios. Theory suggests that the heat release by combustion per unit wall height increases with  $Z^{1/2}$  at fixed equivalence ratio. The present data suggest that the soot and gas radiation initially increase almost linearly with height for small  $Z$  where radiation is unimportant, but convective heat loss is important. At somewhat greater heights the radiation increases more nearly with  $Z^{1/2}$  due to radiant heat loss. Ultimately the radiation will level off at very large  $Z$  after the flames become optically thick.

The similarity of combustion observed in this study greatly eases the task of analyzing experimental data and will make it much easier to tailor future detailed semi-empirical turbulent combustion models, so that their predictions exactly agree with experiment (at least for situations having  $\dot{m} \sim Z^{1/2}$ ). One rarely finds such true similarity (i.e. reducible to one-dimensional behavior) in combustion, especially turbulent buoyant combustion.

We believe that these similarity relationships can be exploited to describe turbulent buoyant fires, with the radiative and completeness of combustion properties of the fuel characterized by the smoke point. A series of radiant and total heat feedback measurements in turbulent wall fires are planned in which the use of binary  $C_2H_6/C_3H_6$  fuel mixtures will provide comparisons of these measurements with predictions based on the smoke point of the fuel mixture. Markstein's<sup>2</sup> measurements on  $C_3H_6$  wall fires have shown that the overall heat transfer back to the surface is only about 70% of the outward heat transfer. This important effect of radiant blockage due to cold sooty gases near the wall will be studied in the planned series of  $C_2H_6/C_3H_6$  fires.

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3. Hottel, H.C., and Sarofim, A.F. (1962), *Radiative transfer*, McGraw-Hill, New York, p. 199,

## Task 5: Methods for Developing Probability Estimates in Fire Risk Analyses (D.M. Karydas)

The Fire Risk Analysis approach establishes a performance based methodology where the performance parameter is quantified risk associated with fire hazard. The general framework of the approach includes the deterministic models of fire spread and smoke movement, the probabilistic models of the safety and control systems, and the event tree models with fire initiating event and engineered safety system functions. The associated concepts of accident prevention, consequence mitigation and hazard elimination are established. Inputs to the event tree models are provided by the deterministic models of fire spread and growth, smoke movement and deposition, and the

detection/protection actuation. Additionally, the frequency of fire initiating and the success/failure probabilities of the fire safety and control systems (such as detection systems, protection systems, etc.) are provided by the probabilistic models. Adjustment to site specific fire risk assessment that deviate from the generic models are introduced at the level of accident initiation or consequence mitigation by using Bayesian inference theory. Based on this fire risk framework, a computer program is under development that can demonstrate the functional relationships of the elements of the methodology outlined and provide on-line explanation of the basic fire risk assessment terminology.



Correlation of Soot Stand-Off Distance  
 $C_3H_6$  Wall Fires

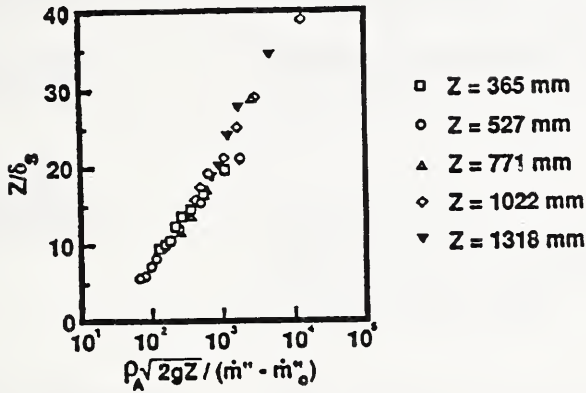


Figure 1. Height to soot layer thickness ratio correlated against inverse modified equivalence ratio.

Corrected Temperature Map  
 $C_3H_6$  8 Burners  $Z = 1.022$  m

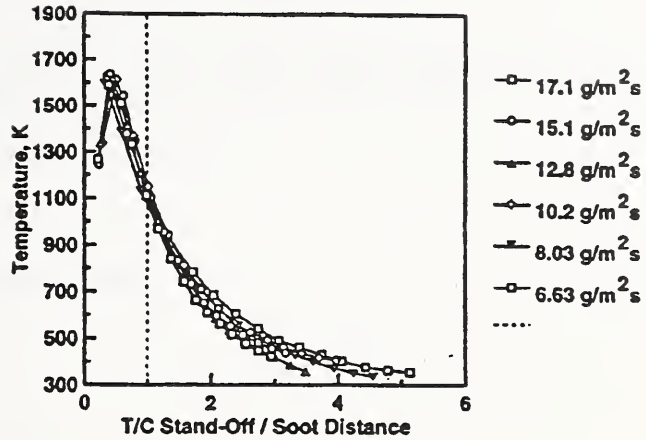


Figure 2. Thermocouple temperatures at height  $Z = 1022$  mm for a range of fuel mass transfer rates corrected for radiation heat loss by thermocouples inside the flames and radiative heat flux to thermocouples outside the flames. Vertical dashed line shows boundary of soot layer.

$C_3H_6$  Wall Fires

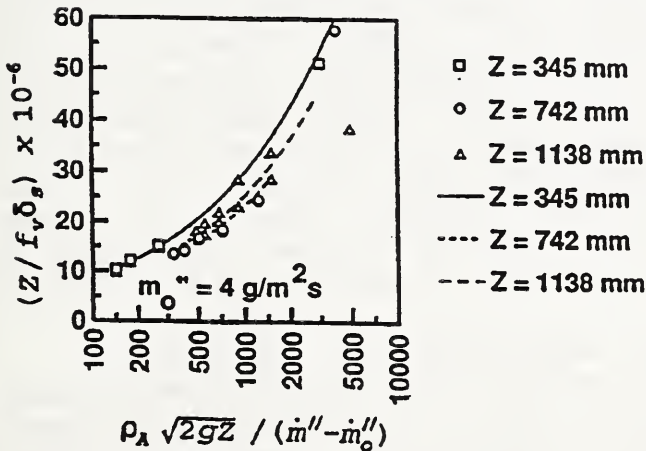


Figure 3. Ratio of height to integral of soot volume fraction across the flame correlated against inverse modified equivalence ratio.

Similarity of Temperature Profiles

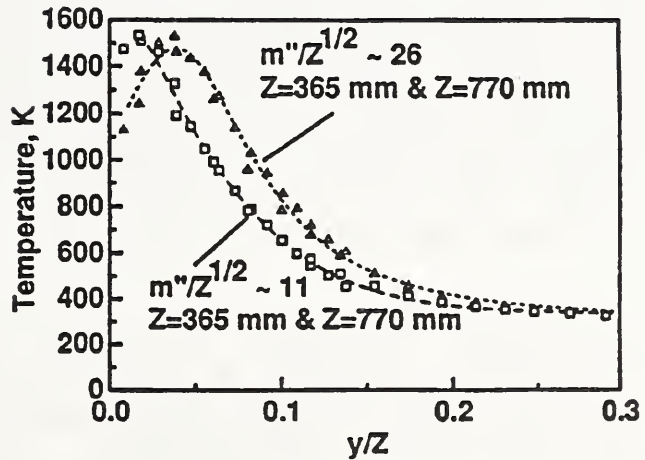


Figure 4. Temperature profile vs. normalized distance from wall.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution           The University of Kentucky

Grant No.            61NANB3D1443

Grant Title         Upward Flame Spread Along The Vertical Corner Walls: Effects of Ceiling  
on Spread Behavior

Principal Investigator   Professor K. Saito  
Department of Mechanical Engineering  
The University of Kentucky  
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Other Personnel       Qian, Cheng, Doctoral Student  
Ishida, Hiroki, Visiting Scholar

NiST Scientific Officer        Dr. Walter Jones  
Dr. Henry Mitler

Technical Abstract

Most rapid flame spread occurs along the vertically oriented corner walls where both the radiative and convective heat transfer effects are enhanced due to the right angle geometrical structure of the corner. From a fire safety point of view, therefore, the prediction of fire spread rate along vertical corner walls is a very important task. Initial attempts to develop prediction models have been successful for upward flame spread over a single vertical wall. By contrast, the development of prediction models for corner walls has been hindered due to the difficulty of the three-dimensional nature of the fire induced flow and the lack of reliable experimental data.

Recently, we developed an infrared imaging temperature measurement system, and for the first time, we obtained a series of transient temperature maps on vertical inert corner walls with and without an inert (Marinite) ceiling. Interestingly, the experimental data showed unexpected results indicating that both the heat flux and the temperature distributions on the wall with a ceiling are somewhat lower than those without ceiling. Figures 1 and 2 respectively show the temperature and the heat flux distributions on the Marinite corner wall. To attempt to explain the heat transfer mechanism associated with the presence of a ceiling, we



are initially conducting simple convective heat transfer calculations assuming the walls have no heat loss (adiabatic), and without accounting for radiative heat transfer.

Temperature and velocity distributions were calculated with and without a ceiling. To understand the convective heat transfer along the corner walls, velocity profiles of the fire-induced flow were also calculated. The flow field results by the computation is very useful, because quantitative measurements of three dimensional velocity profiles are extremely difficult.

In summary, comparison of the experiments with the convective heat transfer calculations are made and followings were found:

(1) The calculations show higher temperature and faster flow field with ceiling in disagreement with the experiments. The disagreement is likely due to the adiabatic wall and no-radiant heat transfer assumptions. However, it is not clear which effect is more important on the actual heat transfer process. Therefore, further work is needed.

(2) Closed loop isotherms shown in the experiments are qualitatively simulated by the calculations for at least the without-ceiling case, but the model failed for the with-ceiling case possibly due to the non-adiabatic wall assumption which resulted in the hottest spot in the upper corner of the wall. However, our experiments indicated that large heat loss occurred at the upper corner wall causing flow stagnation rather than flow acceleration due to the existence of the ceiling. Therefore, the transient heat transfer process through the corner wall needs to be implemented into the model.

#### Acknowledgement

We would like to thank Drs. Walter Jones and Henry Mitler for their instruction in this research program.

#### Reports and Papers

1. Saito, K., Fire Spread Along the Vertical Corner Wall, Part I, Final Report submitted to National Institute of Standards and Technology, Gaithersburg, MD 20899, 1993.
2. Arakawa, A., Saito, K., and Gruver, W.A., Combust. Flame 92:222 (1992).
3. Qian, C., Ishida, H., and Saito, K., Upward Flame Spread Along PMMA Vertical Corner Walls, Part II: Mechanism of "M" Shape Pyrolysis Front Formation, Combustion and Flame, 1994, to appear.

4. Hirano, T., and Saito, K., Fire Spread Phenomena: The Role of Observation in Experiment, Progress in Energy and Combustion Science, 1994, to appear.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT-FY94

Institution: The Pennsylvania State University

Grant No: 60 NANB8D0849

Grant Title: Upward Flame Spread on a Vertical Wall  
Under External Radiation

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Amy Norton, Graduate Student

NIST Scientific Officer: Dr. Walter Jones

Technical Abstract:

Introduction: This is the final year of the project on upward flame spread on vertical walls under external radiation. The overall objective of the present project was to understand the upward flame spread phenomenon under simulated surrounding fire conditions. It was achieved by conducting experiments on upward flame spread under external radiation, developing a mathematical model, measuring relevant material properties needed, and checking validity of the model by comparing predictions with data. Emphasis was placed on studying and predicting the behavior of practical wall materials used in building interiors and textiles. Comparison of data and model predictions for several wall samples were made. Presented below is a concise description of progress made in the past year and a wrap-up of the three-year project.

Technical Accomplishments:

Flame spread tests were conducted on several materials and a numerical model of the upward flame spread process was developed. In order to predict the flame tip and pyrolysis front advancement, a set of coupled equations was developed to model heat conduction into the wall, flame heat feedback, flame size, and transient local heat release rate,. The theoretical development of the upward flame spread model prescribed the necessary parameters to permit closure of the system of equations. The model required material thermal property data and relevant material "fire properties", which could be measured in small scale tests. One important "fire property" was the local transient mass loss rate. The mass loss for each test sample was measured as a function of time for various levels of external radiation. An analytical expression to model the mass loss was derived to conveniently input this information to the flame spread model.

An experimental test facility was designed and fabricated to measure flame spread under various external radiation levels. An upward flame spread test facility was designed which could burn 1.2 m high by 0.3 m wide samples at moderate levels of external radiation (0-15 kW/m<sup>2</sup>). Measurements of flame height as a function of time were made on vertical samples of wall material.



The materials tested were typical wall materials or wall coverings such as pine plywood, solid poplar, cotton textile, cardboard, hardboard, and Douglas Fir particle board. In addition to flame spread measurements, thermocouples were used to measure surface temperature and heat flux gages were used to measure total heat feedback to the sample surface. The experimental measurement of total heat feedback was used to model forward heat feedback, an important parameter in predicting upward flame spread rates and necessary input for some upward flame models. Flame tip and temperature histories were used to validate the numerical model.

As an example, results for 3.2 mm hardboard burning under three different levels of external heat flux are shown in Fig. 1. The symbols denote experimental data with circles, triangles, and squares being used for data taken at external radiation levels of 0, 7.6, and 13.5 kW/m<sup>2</sup>. For the two higher levels of external radiation, the numerical model underpredicted the flame height. The difference between the prediction and data can be generally attributed to the lack of accurately known material property data. This was confirmed by studying the sensitivity of the results to the uncertainty in the material property data.

The numerical model was used by researchers at NIST to predict flame spread on a vinyl ester and woven roving glass composite material. The material properties required for the model were measured at NIST and the experiments to obtain flame spread were also conducted at NIST. Energy release rate for the sample was measured in the Cone Calorimeter and also was an input to the model. Results comparing the numerical and experimental flame heights are shown in Figure 2. The agreement was very good.

The upward flame spread process depends strongly on the flame heat feedback, and consequently, on the local energy release rate (or mass loss rate) of the pyrolyzing area. At a given location, the mass loss rate is highly transient, going through a peak (occasionally two peaks) during the period between ignition and extinction. The peak mass loss rate and time to peak are two of the parameters commonly used to describe the flammability of a material. These values were obtained from the mass loss rate experiments as a part of the present investigation. Table 1 lists the peak mass loss rates and time to peak as determined by the current set of tests. Also included in the table are values obtained from previous researchers' work. The peak mass loss rates increase with increasing levels of external radiation. Comparison with other works showed peak mass loss rates that were on the same order of magnitude, but were not directly comparable due to differences in testing (heat fluxes, sample thicknesses, and ignition methods differ).

Overall, the upward flame spread results confirmed that above a certain critical flux level, many materials do exhibit sustained upward flame spread, and these critical levels were determined for the materials tested. With higher flux levels, flame spread rates were enhanced, and quantitative flame spread information for several materials was measured which demonstrated this trend. Comparison of the numerical predictions with the experimental results were in reasonable agreement, and the model predicted the correct trends. Appropriate thermal property data for the model was found to play a significant role in obtaining good predictions. The model is intended to be used for the prediction of flame spread on practical (charring) materials.

#### Selected Reports and Papers :

Brehob, E. and Kulkarni, A. K. 1993. Time-dependent Mass Loss Rate Behavior of Wall Materials Under External Radiation, *Fire and Materials*, vol. 17, no. 5, pp. 249-254.

Brehob, E. G. and Kulkarni, A. K. 1993. A Numerical Model for Upward Flame Spread Under External Radiation, *Annual Conference on Fire Research*, Rockville, MD.

Costa, J. T., and Kulkarni, A. K. 1993. A Numerical Model of Buoyant Plumes in Room Fires with Two-Layer Stratified Atmosphere, *Annual Conference on Fire Research*, Rockville, MD.

Nair, R. B., Kulkarni, A. K., and Thynell, S. T. 1993. Measurement of Spectral Hemispherical Reflectance of Materials, *Annual Conference on Fire Research*, Rockville, MD.

Brehob, E., 1994. Upward Flame Spread on Vertical Walls with External Radiation, Ph.D. Thesis, The Pennsylvania State University, University Park, PA.

Brehob, E. G. and Kulkarni, A. K. 1994. Experimental Measurements of Upward Flame Spread with External Radiation, Proceedings of the *First ISHMT/ASME (US-India) Joint Heat and Mass Transfer Conference*, pp 756-764, Tata McGraw-Hill.

Brehob, E. G., and Kulkarni, A. K. Experiments for Upward Flame Spread Under External Radiation *Experimental Thermal and Fluid Science* (accepted for publication)

Manohar, S. S., A. K. Kulkarni, and S. T. Thynell. In-Depth Absorption of Externally Incident Radiation in Nongray Media, *Journal Heat Transfer* (to be published)

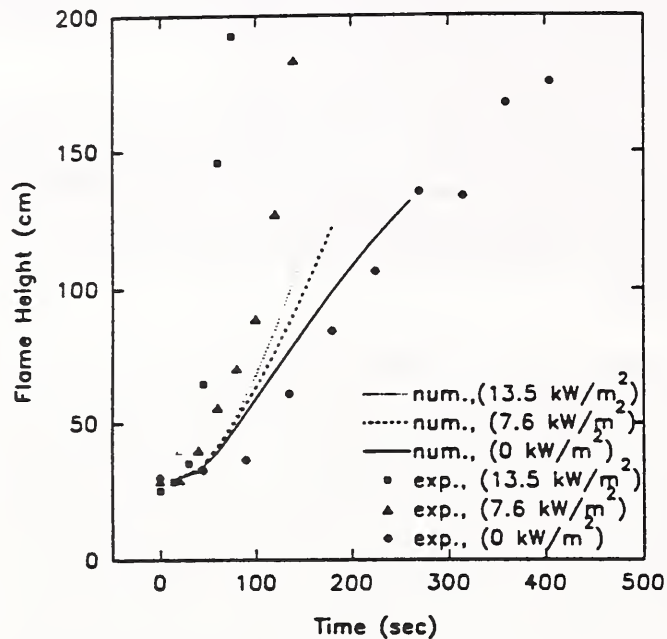


Figure 1 Numerically predicted and experimental flame heights for hardboard

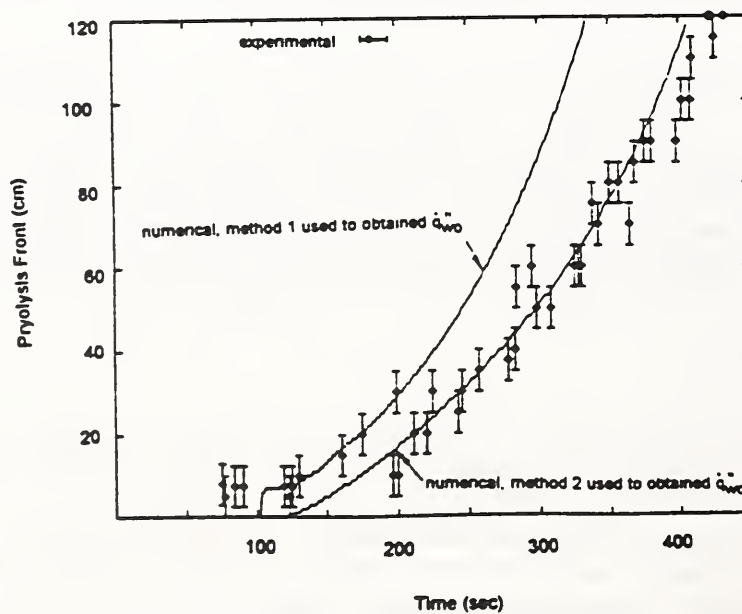


Figure 2 Numerically predicted and experimentally determined pyrolysis front locations for material tested at NIST

Table 1 Peak mass loss rates

material	source	thickness (mm)	t <sub>peak</sub> (sec)	$\dot{m}''_{peak}$ (kg/m <sup>2</sup> s)	sample mass (g)	$\dot{q}''_{cr}$ (kW/m <sup>2</sup> )
hardboard		3.2	250	10.7x10 <sup>-3</sup>	53.6	0.0
hardboard		3.2	260	16.4x10 <sup>-3</sup>	53.6	7.0
hardboard		3.2	245	19.2x10 <sup>-3</sup>	53.6	9.2
hardboard		3.2	195	18.4x10 <sup>-3</sup>	53.6	12.3
hardboard	16 <sup>#</sup>	-	-	11.1x10 <sup>-3</sup>	-	25.0
hardboard	16*	-	-	25.7x10 <sup>-3</sup>	-	20.0
hardboard	16*	-	-	24.5x10 <sup>-3</sup>	-	25.0
PMMA		3.2	322	10.3x10 <sup>-3</sup>	50.6	0.0
PMMA		3.2	216	16.7x10 <sup>-3</sup>	50.6	7.0
PMMA		3.2	190	16.4x10 <sup>-3</sup>	50.6	9.2
PMMA		3.2	170	19.8x10 <sup>-3</sup>	50.6	12.3
PMMA	1	25.0	-	14.6x10 <sup>-3</sup>	-	35.0
PMMA	1	25.0	810	41.4x10 <sup>-3</sup>	-	75.0
cardboard		5.6	240	5.4x10 <sup>-3</sup>	61.7	0.0
cardboard		5.6	166	8.5x10 <sup>-3</sup>	61.7	7.0
cardboard		5.6	146	8.9x10 <sup>-3</sup>	61.7	9.2
cardboard		5.6	148	9.9x10 <sup>-3</sup>	61.7	12.3
particle bd.		15.9	622	6.8x10 <sup>-3</sup>	171.5	0.0
particle bd.		15.9	230	9.1x10 <sup>-3</sup>	171.5	7.0
particle bd.		15.9	208	9.9x10 <sup>-3</sup>	171.5	9.2
particle bd.		15.9	230	10.5x10 <sup>-3</sup>	171.5	12.3
particle bd.	4	-	--	9.9x10 <sup>-3</sup>	-	20.0
particle bd.	14	12.7	50	15.8x10 <sup>-3</sup>	-	50.0
particle bd.	15 <sup>#</sup>	13.0	120	14.2x10 <sup>-3</sup>	-	35.0
particle bd.	15 <sup>^</sup>	13.0	120	16.7x10 <sup>-3</sup>	-	35.0
particle bd.	17	-	--	13.5x10 <sup>-3</sup>	5100	25.0
particle bd.		9.5	120	8.8x10 <sup>-3</sup>	102.3	0.0
particle bd.		9.5	112	10.7x10 <sup>-3</sup>	102.3	1.9
particle bd.		9.5	136	10.2x10 <sup>-3</sup>	102.3	7.0
particle bd.		9.5	100	14.4x10 <sup>-3</sup>	102.3	12.3
particle bd.		25.4	340	6.1x10 <sup>-3</sup>	255.5	0.0
particle bd.		25.4	352	7.4x10 <sup>-3</sup>	255.5	1.9
particle bd.		25.4	300	9.9x10 <sup>-3</sup>	255.5	7.0
particle bd.		25.4	304	11.1x10 <sup>-3</sup>	255.5	12.3
poplar		19.0	224	6.3x10 <sup>-3</sup>	140.7	0.0
poplar		19.0	208	6.5x10 <sup>-3</sup>	140.7	1.9
poplar		19.0	208	10.0x10 <sup>-3</sup>	140.7	7.0
poplar		19.0	180	14.0x10 <sup>-3</sup>	140.7	12.3
plywood		12.7	212	6.1x10 <sup>-3</sup>	93.0	0.0
plywood		12.7	120	10.0x10 <sup>-3</sup>	93.0	1.9
plywood		12.7	116	8.2x10 <sup>-3</sup>	93.0	7.0
plywood		12.7	116	8.8x10 <sup>-3</sup>	93.0	12.3

Please refer to Brehob (1994) Ph. D. thesis for details and sources.

\*data obtained using the Cone Calorimeter, O<sub>2</sub> consumption method

#data obtained using the thermopile method, OSU apparatus

^data obtained using the O<sub>2</sub> consumption method, OSU apparatus





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
STRS PROJECT - FY94

ADVANCEMENT OF FPEtool

Professional Personnel

Richard W. Bukowski, Project Leader  
Scot Deal  
Charles Arnold

Project Objective

Provide a improved user interface to FPEtool.

Scope

Move FPEtool into a windowing environment and integrate its use with HAZARD I.

Technical Accomplishments

Last year a new version of FPEtool was produced which incorporates new capabilities, including corridor flows, flows into areas of refuge, and suppression. The documentation for the code was brought up to date, and the package was prepared for distribution through the HAZARD I distributors to relieve the need for staff to duplicate and distribute it.

As part of the impending release of HAZARD I v2,0, FPEtool has been incorporated into the user interface. Specifically, the FIREFORM routines have been integrated as a "pop-up" calculator in CEDIT to facilitate off line calculations needed to make decisions about inputs to CFAST. This should provide enhanced user capabilities while demonstrating the utility of both products.

The user interface of FPEtool is being written into the windowing system utilized in CEDIT, retaining the features asked for by current users. Further, FIRE SIMULATOR is being replaced by a two-room version of CFAST which will facilitate future expansion, improve the technical basis of the code, and provide a more seamless link to HAZARD I.

Reports and Publications

Deal, Scot, A Technical Users Guide to FPEtool, NISTIR in press.





## **B. FIRE SAFE MATERIALS AND PRODUCTS**



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

BURNING RATE OF MATERIALS

Professional Personnel

Takashi Kashiwagi, Group Leader  
Kenneth Steckler, Physicist  
Anthony Hamins, Mechanical Engineer  
Philip Austin, Post-Doctoral Associate  
Katsuyuki Konishi, Guest Researcher  
Mun Choi, Post-Doctoral Associate

Project Objective

To develop the capability to predict the burning rates of thermoplastic and char-forming polymers based on improved understanding of the physics and chemistry of gasification and the energy feedback from a pool flame to the fuel surface by September, 1995.

Scope

In order to accurately model the burning rates of polymers, both gasification rates and heat feedback rates from a flame to the fuel surface must be understood. Polymer gasification consists of three parts: thermal degradation chemistry, heat transfer, and mass transfer processes in the polymer. Through a detailed study of each major component in the gasification process, a global model consisting of simplified sub-models will be developed. Flame transport processes including heat feedback to the fuel surface are studied in a pool fire configuration. Pure liquid fuels are used to simulate the burning of polymer degradation products.

Technical Accomplishments

I. Solid Phase Measurements

An experimental apparatus for studying transient gasification of materials exposed to radiant heating in a nitrogen atmosphere has been completed. The apparatus includes a stainless steel water cooled chamber (0.6 m diameter and 1.5 m tall), a pneumatic lift for inserting the sample assembly into the chamber, precision mass balance, radiant heater, and a water-cooled shutter located between the sample and the heater. Incident flux levels in the range 28 to 73 kW/m<sup>2</sup> are achieved by changing the distance between the sample and the 800°C heater. Nitrogen purging can reduce the oxygen concentration in the chamber to 0.2 percent. Shakedown experiments on thermoplastics, charring materials, and liquids have produced encouraging results.

Techniques for preparing samples for gasification experiments are being developed. Some of these samples must be instrumented with thermocouples to measure the transient temperature gradient within the gasifying solid. Thermoplastic samples have been formed from layers of 6 mm thick sheets, with fine-wire thermocouples between layers, by heating a stack of sheets in a vacuum oven under a small mechanical load.

Molding techniques to produce char-forming polymer samples with imbedded thermocouples are being tested. Techniques for characterizing various thermo-physical properties of the char layer are being developed. An experiment to determine the suitability of using the flash method for measuring the thermal diffusivity of char



samples is being conducted. For these tests, a method of dissecting the char layer to produce "uniform" samples has been developed.

## II. Gas Phase Measurements

Emission measurements (200 Hz) at 900, 1000 and 4350 nm taken at two locations using a probe technique (1 cm path, separated by 1 cm vertically) were used to determine the local temperature, soot volume fraction, CO<sub>2</sub> concentration, and vertical velocity in 10 and 30 cm heptane pool fires. Mixture fraction correlations were used to estimate the H<sub>2</sub>O and CO concentrations. The data were used to calculate the radiative heat feedback to the fuel surface. The importance of simultaneously taking data at multiple flame locations was tested in heat transfer calculations and found to be not significant when average heat fluxes were considered.

A technique to determine the refractive index of soot was developed using a combination of iso-kinetic sampling and laser transmission.

FTIR measurements are underway to quantify the impact of fuel absorption on radiative heat feedback. This information will be used to improve the simple global model discussed below.

## III. Burning-Rate Model

The development of a burning-rate model for char-forming materials was begun. The combustion of a horizontal slab of wood, exposed to an external radiant source, is being modeled in terms of two coupled sub-models which simulate gas and solid (condensed) phase processes.

*Gas Phase Model:* The algorithm which was used to model the gas phase phenomena has been described previously (Hamins et al., 1992). It is a simple global model which predicts the mass burning flux for pool fires burning in a quiescent environment. The model assumes constant bulk properties such as flame temperature, soot volume fraction, and species concentrations. The computational procedure requires knowledge of the combustion properties of a fuel (the radiative heat loss fraction, the combustion efficiency, and a characteristic soot volume fraction in the flame) and fuel properties such as the stoichiometry, heat of vaporization, heat capacity, and boiling point. The combustion properties can be characterized by a single variable, the smoke point height of the fuel (Tewarson, 1988). The shorter the smoke point the more sooty the fuel. The smoke point can also be correlated to a characteristic soot volume fraction for a pool fire.

For simplification, this model treats wood as a single component fuel, with the gas phase combustion properties invariant as a function of time after ignition.

An average component-weighted heat of combustion for Douglas Fir was found to be 12.6 kJ/g. This is in contrast to the bomb calorimeter results which yield values from 17 to 22 kJ/g for air-dried soft woods (Domalski et al., 1978). The bomb calorimeter heat of combustion results vary strongly with water content and can be as low as 5 kJ/g (Domalski et al., 1978). Cone calorimeter measurements (described below) gave a 12 kJ/g heat of combustion for the conditioned Douglas Fir sample. Thus, the combustion efficiency  $\chi_a$  can be estimated as  $\chi_a \approx 12/12.6 = 0.95$ .

The radiative heat loss fraction  $\chi_r$  and  $f_v$  were estimated using the relationship between the combustion properties and the smoke point (Tewarson, 1988). The smoke point height of wood (estimated as 16 cm) and  $\chi_r$  were determined using Tewarson's correlations (1988) and  $f_v$  was estimated from pool fire results (Bard and Pagni, 1981).<sup>81</sup> as a function of the fuel smoke point height. For simplicity and because few data exist regarding the effect of scale, the current gas phase model assumes that the combustion properties are invariant with scale over the range of interest.

*Solid Phase Model:* The model we are using currently (Atreya, 1983) treats the solid as an opaque, one-dimensional, locally reacting body, with finite thickness and density-dependent thermal properties. The local density is determined by a first order Arrhenius reaction. Gasification products from any location within the solid are assumed to be transported instantaneously to the exterior of the solid.

The governing equation is basically the heat conduction equation with the addition of the following source/sink term:

$$\frac{\partial \rho_s}{\partial t} [\Delta H_v - C(T - T_0)] \quad (1)$$

where  $\rho_s$  is the density of the solid,  $t$  is time,  $\Delta H_v$  is the heat of pyrolysis,  $C$  is a constant comprising the specific heats and densities of the virgin, char, and volatile materials,  $T$  is the temperature of the solid, and  $T_0$  is the initial temperature of the solid. Note that the heat of pyrolysis term (the first term) in the bracket is an energy sink, whereas the second term is an energy source. Consequently, a net exothermic condition occurs when  $T$  reaches a certain level (about 400°C for the current calculations in which the heat of pyrolysis was 125 kJ/kg).

Figure 1 shows the results of gasification calculations made with this model. The solid curve was generated using a value of  $C = 0.37$ , which was determined from typical values of wood, char, and volatile properties. The second peak on this curve is larger and the time scale is shorter than expected from experiment. The dotted curve in the figure is closer to what is observed experimentally. The latter curve was generated by setting  $C = 0$ , which is equivalent to assuming that the enthalpy carried away by the volatiles is equal to that gained as a result of change from the solid to the char material. Although this is not a valid assumption, the results illustrate that the second peak is very sensitive to the physical properties of the components. Other calculations have shown that the second peak is sensitive to the rear-face boundary condition.

Research continues to resolve the discrepancy between calculated and expected results. We suspect that important factors include a) the uncertainties associated with the material properties and b) finite heat loss from the rear face of specimens during experiments.

### References

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"Simultaneous Optical Measurement of Soot Volume Fraction and Temperature", Choi, M.Y., Hamins, A., and Kashiwagi, T., to appear *Combust. and Flame* (1994).

"Simultaneous Optical Measurement of Soot Volume Fraction, Temperature, and CO<sub>2</sub> in Heptane Pool Fires", Choi, M.Y., Hamins, A., Mulholland, G., and Kashiwagi, T., to appear in the *Twenty-Fifth Sym. on Combust.* (1994).

"Comparisons of the Soot Volume Fraction Using Gravimetric and Optical Techniques", Choi, M.Y., Mulholland, G., Hamins, A., and Kashiwagi, T., submitted to *Combust. and Flame* (1994).

"Volume Rendering of Pool Fire Data", Rushmeier, H., Hamins, A., and Choi, M., submitted to 1994 Conference on Volume Visualization.

## Related Grants

"A Study of Entrainment and Flow Patterns in Pool Fires using Particle Imaging Velocimetry", J.P. Gore, Purdue University.

"Modeling of Combustion, Fluid Mechanics, and Radiation in Buoyant Turbulent Fires", O.A. Ezekoye, University of Texas at Austin.

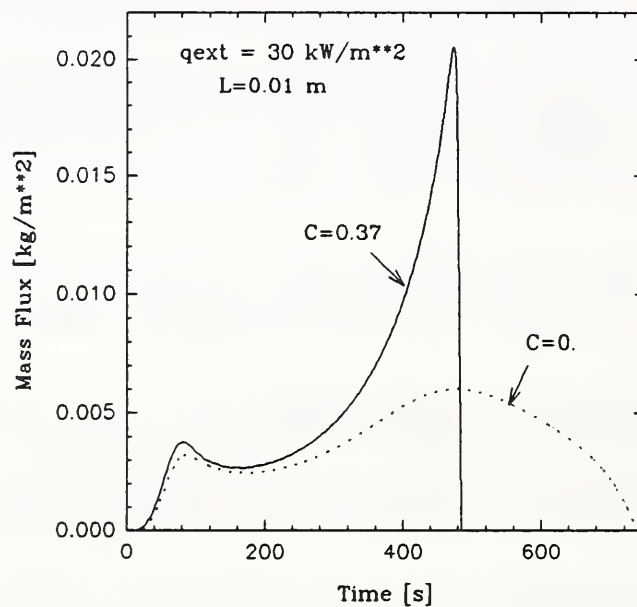


Figure 7. Calculated gasification rates.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT-FY 94

Institution: Brown University

Grant Number: 60NANB0D1042

Grant Title: The Behavior of Charring Materials in Simulated Fire Environments

Principal Investigator: Prof. Eric M. Suuberg  
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NIST Scientific Officer: Dr. Thomas Ohlemiller

Technical Abstract:

Introduction. The complicated interplay of chemistry, heat and mass transfer serves to make the study of combustion phenomena generally quite difficult, particularly when a solid phase is also involved. The general topic of concern in this project is the adequacy of current models of charring solids pyrolysis. Detailed kinetic models will not be soon developed for most cases of practical interest, so there is a question as to whether approximate methods can capture the essence of the processes. In particular, there is concern about whether small scale laboratory pyrolysis data can be reliably used to model fire situations. To address this question, it was necessary to compare the pyrolysis behavior on both a laboratory scale and on a scale that is relevant to fire situations. Techniques have been developed for performing well-controlled experiments on both scales, using the same material.

Any study of fire phenomena that involves the study of chemistry in an environment that is removed from that encountered in actual fire situations runs a significant risk of producing results that do not accurately model actual fire behavior. The concern is with our ability to predict *a priori* the key variables that must be controlled in order to accurately simulate conditions of relevance. The role of a char layer in complicating the analysis of the combustion process must also be recognized. The main factor that very strongly determines the release of combustible volatiles is the temperature history of the solid. Thus the laboratory scale experiments must be guided by a knowledge of the heat transfer situation in real fires, or in our case, a knowledge of the heat transfer situation in our fire simulation device. This determined the temperatures and heating rates for study on the laboratory scale.

Further, it is not sufficient to be merely concerned with the rates of volatile release from a small isothermal sample, if it is the prediction of the burning behavior of a thick sample that is of interest. The thermal and mass transport properties of the char layer will strongly influence the course of pyrolysis of subsurface layers. It turned out to be difficult to reliably utilize literature values for estimating the temperature histories of subsurface layers, because many parameters were only very crudely known. Thus these parameters also had to be measured in the context of the fire simulations (and the properties were functions of the extent of pyrolysis).

Experimental Approach There is a need to tie the impressive progress that has been made

in measuring and predicting char yields from pyrolyzing organic solids under laboratory conditions to predicting the yield under actual fire conditions. The particular approach employed here involves the use of equipment that has been developed to simulate the environment of real wall fires. The device was earlier extensively utilized in Center for Fire Research supported work on the combustion properties and behavior of pure and fire retarded cellulose, under the direction of Professor M. Sibulkin of Brown University, and has some similarity to apparatus used by workers at Factory Mutual Research Corporation for studies on flammability of plastics (Tewarson and Pion, Comb. and Flame, 26, 85 [1976]), except that the present device is intended mainly for studies on the pyrolytic behavior of the solid samples, rather than for studies on flaming combustion.

Briefly, the equipment allows bulk samples of several centimeter diameter and length to be held in an insulating ceramic holder atop an electronic balance. The assembly is held in a controlled gas environment, which can be purged with either nitrogen or nitrogen containing some low levels of oxygen. The sample surface is heated by radiant quartz heaters which can provide a flux of up to about  $100\text{kW/m}^2$ , which covers the range of relevance in fire situations (somewhere around  $40\text{kW/m}^2$  is a "standard" condition). The sample itself is instrumented within its interior with thermocouples, to provide a temperature profile. The yield of volatiles is provided by the data on mass loss of the sample. The analysis of the volatiles is provided by gas chromatography and mass spectrometry. The analysis by GC provides information only on the gaseous species, and the tars must be separately collected by condensation, or determined by difference.

To simulate wood or other bulk cellulosic building materials, high purity alpha cellulose powder (Whatman CF-11) was dry-pressed in an ordinary laboratory press into pellets whose bulk densities bracketed those of real woods (0.4-1.0 g/cc). The intent here was *not* to simulate the full complexity of wood, but rather to obtain detailed data on a model charring material that is very wood-like in its behavior. The densities were reproducible from sample-to-sample to about 5%. An advantage of these samples is that they are relatively pure (0.009% ash) and contain none of the heterogeneity of real wood (i.e. no hemicellulose or lignin). This is important insofar as establishing the kinetics of pyrolysis is greatly simplified when potentially catalytic impurities are absent, and when there are not several distinct organic phases present. This allowed comparison with the large amount of data in the literature on cellulose decomposition, and also offered the possibility of reliable experimentation, on several scales, using several analytical techniques, to establish key properties.

Results Obtained The results of experiments on simulated woods and real woods are shown in Figure 1. The experiments were simulated fire experiments in which samples of 3.8 cm diameter and 1 cm thickness were irradiated on their front faces by a quartz lamp delivering  $40\text{ kW/m}^2$ . The irradiation was chosen to simulate a fire level heat flux, but in this case the experiment was performed under inert gas, to avoid the further complexities introduced by actual combustion. Clearly the results show the ability to simulate wood behavior, as far as combustibles release rates are concerned. The relatively constant pyrolysis front propagation velocity, implied by the nearly linear decrease in mass with time, is a consequence of the constant heat flux surface condition. A relatively constant temperature gradient between surface and pyrolysis front is maintained.

The residual "char" yields from such experiments were in the neighborhood 20%, by mass. The term char is operationally defined as what is left behind as solid, following about one half to one hour of heating. In thin samples (a few mm thickness), the char was rather uniform in nature, and was quite black. In thicker samples, the char at the rear of the sample was brown, and obviously not as severely pyrolyzed; the char layer ahead of it had effectively insulated this material, so that even at final steady state, it was not fully pyrolyzed. This shows the danger in simply reporting "char" yields in fire situations. The chars may in fact be quite different in character (e.g. different in potential for further pyrolysis if conditions change; different in reactivities in smolder situations).



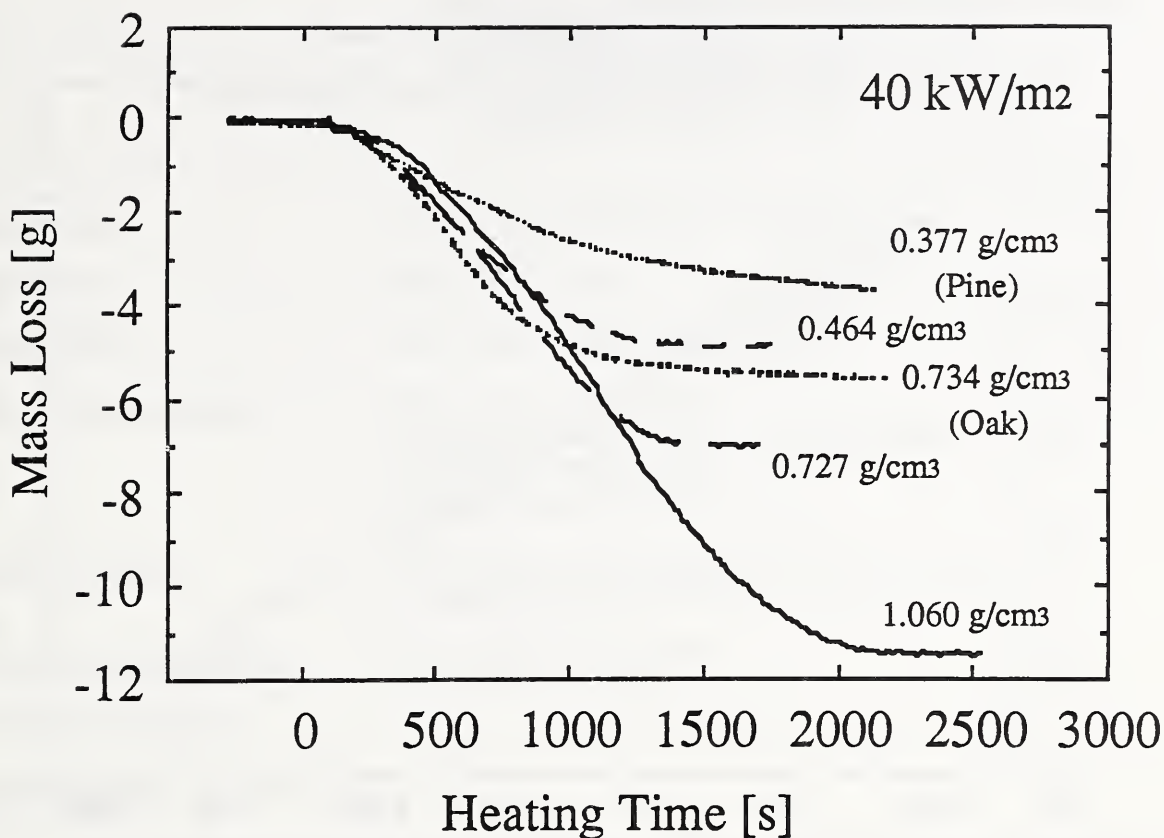


Figure 1. Mass loss as a function of time under simulated fire conditions for three different density cellulose samples and for two wood samples.

It was noted in this work that the “alligating” behavior commonly seen in wood could be observed or suppressed, depending upon sample preparation. Alligating involves the macroscopic cracking of the sample, due to shrinkage during pyrolysis. Allowing small samples to shrink inward during pyrolysis largely prevents alligating, whereas confining the edges of a sample to prevent inward shrinkage, causes cracking failure in the middle of the sample. It was observed in the process of studying this phenomenon that the effective flux of volatiles in the high density samples was parallel to the surface of the sample, in a direction normal to the incident radiative flux. The volatiles would often apparently flow a much longer distance in the direction parallel to the face of the sample than flowing a short distance through the front face. Thus alligating cracks potentially serve as important conduits of volatiles, and an assumption of uniform surface flux of volatiles may be rather poor in some situations.

It was in attempts to model the data that several deficiencies in understanding were noted. First, it was found that the common assumption of a char surface emissivity near unity was a poor assumption in the energy balance part of the model; subsequently, values near 0.7 were directly measured *for the relevant range of wavelengths*. There were also few studies that considered the temperature dependence of thermal transport properties. These were also directly measured, in response to the identified need (heat capacity by DSC and thermal diffusivity by a transient forcing function method). Finally, reported global kinetics did a poor job of fitting the mass loss behavior of the model - it was as though two different sets of kinetic parameters were needed to describe the surface and interior of the char. This led to a more complete examination of the kinetics of cellulose pyrolysis on the laboratory scale. An interesting feature of that work is shown in Figure 2. The kinetic examination resulted in the conclusion that in the rapidly heated surface layers, different decomposition kinetics are followed than in the slowly heated interior of the sample. It is not heating rate *per se* that matters; the heating rate only determines at what temperature most decomposition occurs. As



Figure 2 suggests, there is a transition in kinetics at near 600 K.

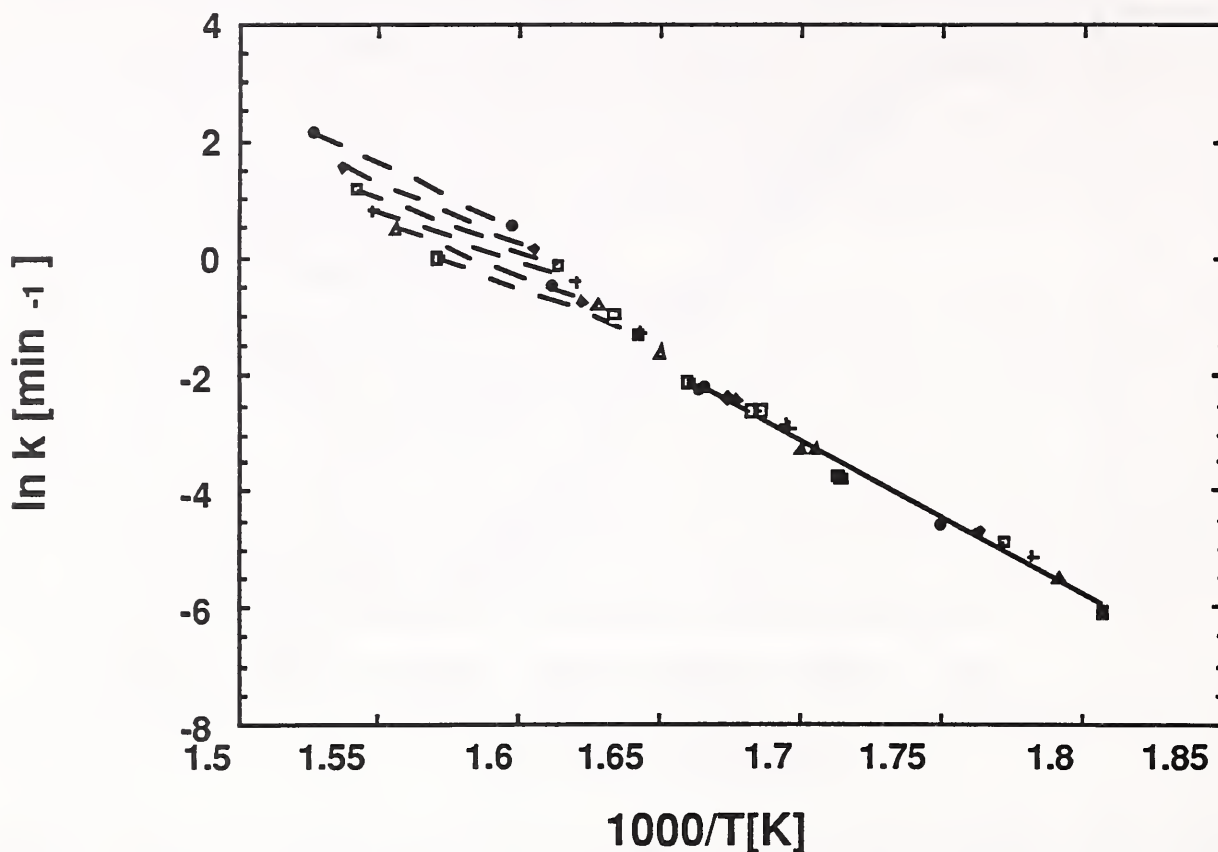


Figure 2. The results of the TGA examination of cellulose kinetics using heating rates of 0.1, 1, 6, 15 and 60 K/min. Each point is for a different conversion.

It has been shown in connection with data such as these that the regime above 600 K is characterized by an activation energy of about 140 kJ/mol, whereas the regime below 600 K is characterized by an activation energy of around 218 kJ/mol (for this particular cellulose). Thus it was concluded that great care must be exercised in applying kinetics from laboratory scale testing, if there is a failure to recognize a difference in conditions from the practical application.

Acknowledgements We acknowledge many useful discussions, over the course of this project, with Drs. Thomas Ohlemiller and Takashi Kashiwagi of NIST.

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Plus three other papers in preparation.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT-FY94

Institution University of Maryland, College Park

Grant No. 60NANB2D1266

Grant Title Fire Growth models for Materials

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Other Personnel B. Rhodes, MS (currently with Hughes Assoc.)  
D. Hopkins, MS candidate

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Technical Abstract

Introduction

The proposed research seeks to determine a transient burning rate model that can be used to generalize data from the Cone Calorimeter. This will involve several models built upon a consistent framework. Each model will be appropriate to a specific *Class of Materials* as described below. It will apply to materials where one dimensional burning rate is approximated. It will therefore apply to materials where regression is not excessive. Also the horizontal orientation will be considered in the Cone Calorimeter to avoid the effects of melting and dripping. The current work is completing its study of thermoplastics (materials with surface vaporization) and is beginning its study of charring materials (solid vaporization and surface char development).

Background and Approach

The Cone Calorimeter is a widely used device to measure the mass loss ( $\dot{m}''$ ) and energy release ( $\dot{Q}''$ ) rates per unit area under a specified external radiative heat flux. The ratio of these two quantities gives the instantaneous heat of combustion ( $\Delta H_c$ ) relative to the gaseous fuel produced during flaming combustion. Generally, during flaming combustion, it has been shown that this heat of combustion is approximately constant for the material. In the least, it can be measured, and is not expected to be scale dependent, i. e. change as a larger area of fuel is burned. Also, except for multi-dimensional effects involving seams, joints, edges, etc, the thermal and chemical properties of the decomposing material would also be independent of scale. In contrast, the heat flux ( $\dot{q}''$ ) to the material's surface would depend on scale and on test conditions in the Cone Calorimeter. Hence, it follows that under these one dimensional burning conditions

$$\dot{m}'' = f(\dot{q}'', \text{thermo-chemical properties}) \quad (1)$$

$$\text{and } \dot{Q}'' = \dot{m}'' \Delta H_c \quad (2)$$

Equation (1) symbolically represents a model involving the surface heat flux and the needed properties. The objective is to develop the model in sufficient detail to describe the transient

burning behavior. Since materials decompose in different ways, and may differ also in their construction, a different model will be needed for each class of material.

Based on previously published work [1,2], an approximate model was developed for a thermoplastic material. This is presented below:

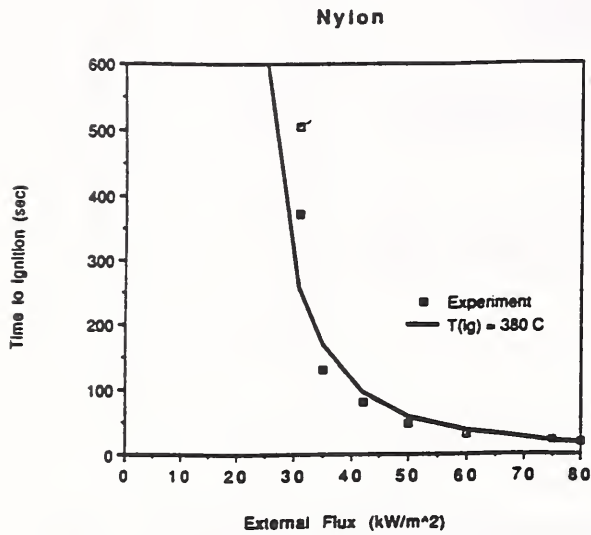


Figure 1: Calculated and measured ignition time of Nylon 6/6 as a function of external heat flux.

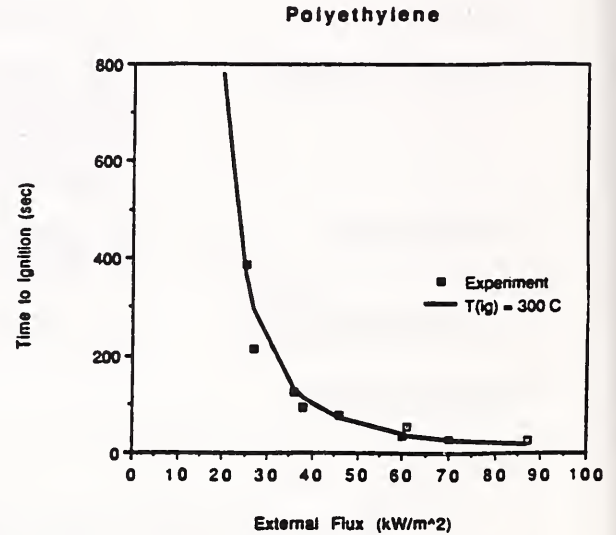


Figure 2: Calculated and measured ignition time of Polyethylene as a function of external heat flux.

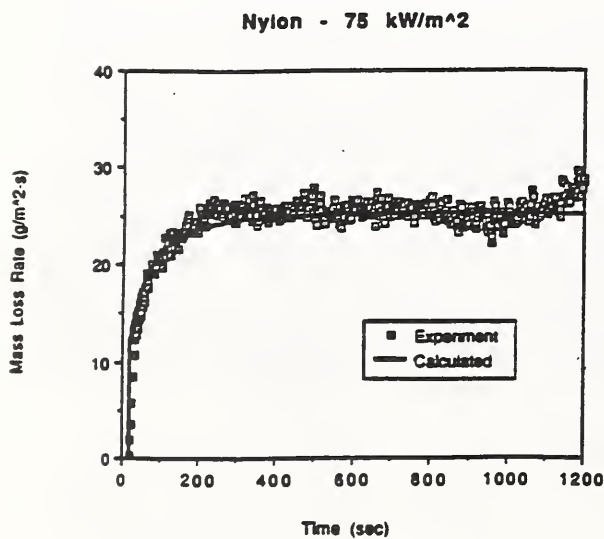


Figure 3: Calculated transient mass loss rate of Nylon with a 75 kW/m<sup>2</sup> external heat flux.

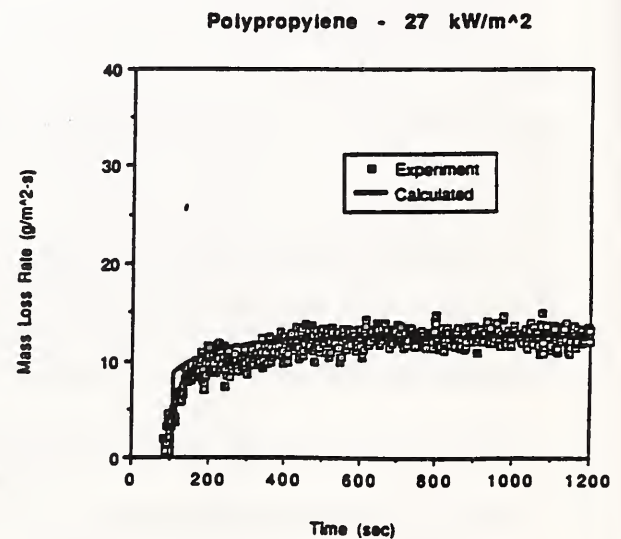


Figure 4: Calculated transient mass loss rate of Polypropylene with a 27 kW/m<sup>2</sup> external heat flux.



The burning rate per unit area,  $\dot{m}''$ , is given as

$$\frac{\dot{m}''L}{\dot{q}''} = 1 - \left( \frac{L}{\Delta H_v} - 1 \right) \left( \frac{\delta_s}{\delta} - 1 \right) \quad (1)$$

where the dimensionless time after ignition is

$$\tau - \tau_{ig} = \frac{2}{3} \left( \frac{\Delta H_v}{L} \right) \left\{ \left( \frac{\delta_{ig} - \delta}{\delta_s} \right) - \ln \left( \frac{\delta_s - \delta}{\delta_s - \delta_{ig}} \right) \right\} \quad (2)$$

$\delta$  is a parameter that physically represents the thermal penetration into a semi-infinite solid. It varies as:

$$\delta_{ig} \leq \delta \leq \delta_s.$$

The steady state value for  $\delta$  is given as :

$$\delta_s = \frac{2kL}{c\dot{q}''}. \quad (3)$$

The  $\delta$  at ignition is given as:

$$\delta_{ig} = \sqrt{6\alpha t_{ig}}. \quad (4)$$

The time for ignition is approximately given by

$$t_{ig} = \frac{2}{3} k\rho c \frac{(T_{ig} - T_i)^2}{\dot{q}''(t_{ig})^2}. \quad (5)$$

Dimensionless time is given as:

$$\tau = \frac{4\alpha t}{\delta_s^2}. \quad (6)$$

The net surface heat flux,  $\dot{q}''$ , changes at ignition to account for the flame heat flux which includes both radiative and convective fluxes to the surface. Moreover, it has been shown that this net flame flux is constant for each thermoplastic regardless of the time and irradiance.

$$\dot{q}''(t) = \dot{q}''_{ext} - h_c(T_s - T_i) - \sigma T_s^4 \text{ for } t \leq t_{ig}, \quad (7)$$

and

$$\dot{q}''(t) = \dot{q}''_{ext} + \dot{q}''_f - \sigma T_{ig}^4 \text{ for } t > t_{ig}. \quad (8)$$

The remaining symbols are identified below:

$\alpha$  thermal diffusivity

$k$  thermal conductivity

$c$  specific heat

$\rho$  density

$\Delta H_v$  heat of vaporization

$L$  heat of gasification,  $\Delta H_v + c(T_{ig} - T_i)$

$T_i$  initial and ambient temperature

$T_{ig}$  ignition temperature, and assumed equal to a constant vaporization temperature

$T_s$  surface temperature

$\sigma$  Stefan-Boltzmann constant

$h_c$  convective heat transfer coefficient

$\dot{q}''_{ext}$  incident external radiant heat flux

$\dot{q}''_f$  incident total flame heat flux.

Experiments have been conducted in a Cone heater assembly to measure the burning rates for polymethylmethacrylate, nylon 6/6, polyethylene, and polypropylene. Typical results are presented in Figures 1-4. The ignition temperatures and kpc were determined from the ignition data. Attempts were also made to measure the surface temperatures at ignition. The results follow:

	PMMA	Nylon 6/6	Polyethylene	Polypropylene
measured, C	250-360	≈ 500	320-390	315-330
inferred, C	180	380	300	

From the steady burning rate data as a function of irradiance, the flame heat flux and the heat of gasification was found. Based on the inferred ignition temperatures, the flame heat fluxes are given as follows:

	PMMA	Nylon 6/6	Polyethylene	Polypropylene
Flame flux kW/m <sup>2</sup>	30	30	25	14

The formulation appears to yield good results for the time to ignite and transient burning rate in term of effective properties determined from data. this provides a potential basis for using cone data in the prediction of the burning behavior in general provided the flame heat flux is known. The study is currently investigating a similar methodology for charring materials.

#### Reports and Papers

1. Quintiere, J. and Iqbal, N., "An Approximate Integral Model for the Burning Rate of a Thermoplastic-like Material", *Fire and Materials*, Vol. 18, 89-98 (1994).
2. Rhodes, B. T., "Burning Rate and Flame Heat Flux for PMMA in the Cone Calorimeter", M.S. Thesis, Dept. of fire Prot. Engrg., Univ. of Maryland, College Park, May 1994.
3. Hopkins, D. Rhodes, B. and Quintiere, J., "Predicting the Rate of Thermoplastic-like Materials in the Cone Calorimeter", submitted for the NIST 1994 Annual Fire Conference.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution                   The University of Texas

Grant No.                    60NANB3D1436

Grant Title                 Modeling of Combustion, Fluid Mechanics, and Radiation  
in Buoyant Turbulent Fires

Principal Investigator     Professor O.A. Ezekoye  
Department of Mechanical Engineering  
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Other Personnel            Z. Zhang, Doctoral Candidate

NIST Scientific Officer     Dr. Katherine Butler

Technical Abstract

Introduction Recent experimental results indicate that transient effects in the temperature and soot volume fraction distributions within a fire significantly contribute to the measured radiative heat transfer rates from the fire. For large pool fires, the radiative heat transfer rates control the burning rate. Thus, it is imperative that these transient couplings be properly specified in order to correctly model the burning process. The goal of this project is to develop a computational technique focused towards the simulation and modeling of large scale fire phenomena. The method being developed is transient in formulation and should properly characterize many experimentally noted features of fires.

It is presently computationally prohibitive to use a single global model to resolve all the necessary temporal and spatial scales present in a large geometric scale fire. Many methods have been developed to characterize the burning process of large nonpremixed flames. The laminar flamelet method has been used with varying degrees of success in specifying the burning phenomena in such flames. For typical large fires, significant amounts of soot will be produced within the fire. It does not appear that soot evolution can be nonarbitrarily included in the current (stationary) Laminar Flamelet formalism. In order to place soot evolution into turbulent flame computations, the soot evolution equations are often averaged and then computed on the relatively coarse convection grid. Averaging of the source and sink terms in the soot evolution equations may also produce some errors. An alternative to requiring an average of the governing combustion conservation equations may be found by pursuing a Lagrangian or Particle in Cell (PIC) formulation of the combustion processes.

The basis of such a formulation relies on the description of the evolution of a fuel element through a fire on the Lagrangian scale. It is assumed that the element and products formed from the element remain contiguous. It is clear that the environment of the fuel element will determine its burning history. At the same time, the rate of consumption of the fuel, the internal temperature distribution of the element, and the amounts of product species within the element will influence the large scale flow field and thus the trajectory of the element. The total flow field description is consistent with PIC computational methods in which there are generally considered to be three interactions: the particle properties are interpolated onto the grid, the particle trajectory is specified by the updated flow field, and the grid resolved properties are interpolated onto the particles.



The PIC formalism is being applied in this project to specify the burning properties of several fire flow fields. In terms of implementation a fuel particle burning history is computed in a separate fine scale mesh. An initial mass of fuel is surrounded by a much larger mass of air. The subsequent burning process of the fuel is computed. The effects of both finite rate kinetics and also of diffusion limited reactions have been examined. The results of these investigations are presented in (1). The feasibility of using the particle computation in a large scale flow field was demonstrated in reference (2). In (2), a three dimensional, reacting, flow field satisfying the Navier Stokes equations was computed by use of the Lagrangian formalism. The flow field was specified to be the sum of an analytical vortex solenoidal velocity field (Hill's vortex) and an irrotational velocity field computed on the large scale flow field using the heat release rate information (i.e., expansion rates) of the particles. The particles were coupled to the large scale flow field using the convective time scale of the flow field. In reference (2) the particle burning history was specified in the fast chemistry limit. All the particles were released at the same time into the flow, and their burning histories were identical.

Since that work, we have generalized the form of the solenoidal velocity field. We are presently investigating the Lagrangian description of a jet flame. For the jet flame, we initially formulated the particle introduction and indexing in a similar manner as was used within the Hill's vortex flow. The index for the burning process was the convective time variable. After a particle was released into the flow, its "clock" would start and it would evolve in the flow time. This indexing scheme resulted in the flame core temperatures being too large at relatively small axial distances away from the jet nozzle. Particles which should not have had enough air entrainment to react considerably were reacting. The solution to this problem lay in redefining the particle index. As with the conventional laminar flamelet methodology, the index was chosen to be the mixture fraction. The burning properties of the element had to be redefined in terms of the average mixture fraction of the element. In the element scale, time advance is associated with average mixture fraction retreat. As the mass of fuel decreases, the mass fraction of fuel, which is directly related to the average mixture fraction of the element, also decreases. All relevant quantities in the thermal element can therefore be indexed in terms of the average mixture fraction for the element. On the large scale grid, an average mixture fraction is ideally computed at every time step. For a steady flow, the average steady mixture fraction may be computed.

The element (flamelet) library is now constructed using a single step finite rate mechanism on the thermal element. A phenomenological soot evolution model is also specified within the element scale. Several quantities are placed into the library. The average particle temperature, fuel mass, soot mass, products mass, and combustion energy are written out at different mixture fraction values. The particle temperature is averaged over the mass of species corresponding to the average mixture fraction. The heat release rate is integrated with respect to time to yield the amount of converted energy at any small scale time step; recall that any element time corresponds to an average mixture fraction value. In the large scale flow, as a particle moves from one spatial location to another, the mean mixture fraction of the particles environment may change in the convective time of  $dt$ . The heat release rate for this particle is arrived at by dividing the change in its converted energy as specified by the library by the convective flow time,  $dt$ . Thus, a particle that quickly moves from a mixture fraction of unity to a mixture fraction corresponding to stoichiometry has a considerably higher heat release rate than one that sees a slower change in its environment.

Preliminary results for a jet diffusion flame have been computed. In particular, attention is focused on the jet entry region ( $x/D < 15$ .) in which we previously had difficulty modeling. In the accompanying figure are several realizations of temperature, mixture fraction, and soot volume fraction for a jet flow ( $Re=20,000$ ). The solenoidal component of the velocity was computed using a modified version of the GENMIX (Patankar, 1980) algorithm. A mean (steady) value of the mixture fraction was computed for the solenoidal field. A transient computation was then carried out in which particles were introduced at the inlet of the jet. As the particles were convected downstream, the environment changed and the particles took on the characteristics of their environments. In all the figures presented below, a center section is cut out of the actual three dimensional jet to get the two dimensional contours shown. In figure (a), the temperature profile is shown for a long time calculation in which the first particles introduced into the flow have been carried outside of the computational domain. It is important to note that there are two methods to compute the grid temperature profile. One method uses the mixture fraction averaged temperature of the elements and interpolates this value onto the grid using a triangulation technique. One might think of this method as a computation on an adaptive irregular grid. Any errors in the grid

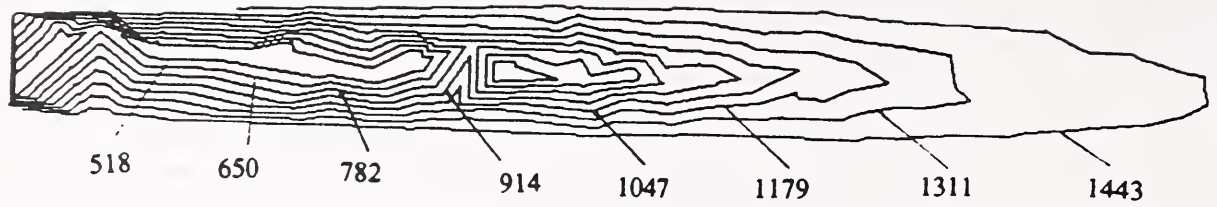


determined scalar values are a result of excessively large average particle separation distances (i.e., grid spacing). If the particular interpolation scheme is linear, then the grid errors at any location are also linear in the particle separation distance. A more conventional method to compute the temperature profile is to place the particle heat release on the regular mesh and to compute the energy equation on the mesh. In all the figures presented below, the former method was used. Estimates of the grid resolution error associated with the inter-particle spacing can be found by looking at figure (b) in which the particle based average mixture fraction is triangulated onto the grid. Compare figure (b) with the average mixture fraction profiles specified by the solenoidal flow in figure (c). With increasing particle numbers (decreasing inter-particle spacing) the two profiles are identical. For the case shown, errors appear at the jet inlet where there are not enough particles to accurately specify the temperature and the mixture fraction. Next, the soot volume fraction profile is examined in figure (d). Consistent with the chemistry prescribed on the small scale element, soot species begin to appear at relatively high values of the mixture fraction in the core of the jet. The phenomenological model specified for the soot evolution allows high temperature fuel species to pyrolyze and form soot.

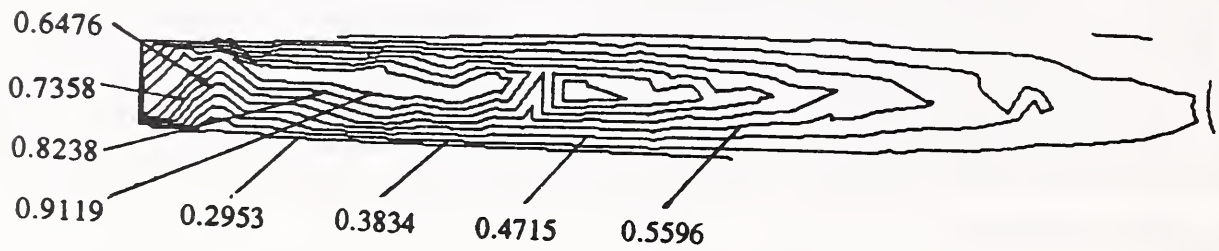
It is emphasized that the Lagrangian element's combustion model can incorporate varying degrees of complexity. The combustion and soot generation components of the model may be refined and corrected according to the most recent developments in these areas. The flow field specification for the model is also quite general. There has been continued collaboration and interaction with Kevin McGrattan and Howard Baum of BFRL with respect to the implementation of the latest developments in the Lagrangian model into the pool fire computations that they are presently carrying out. In the future we intend on making careful comparisons of this methodology with experimental data and also to investigate a series of canonical flow fields. We also intend to begin the large scale radiation component of this work.

#### **Publications and Reports**

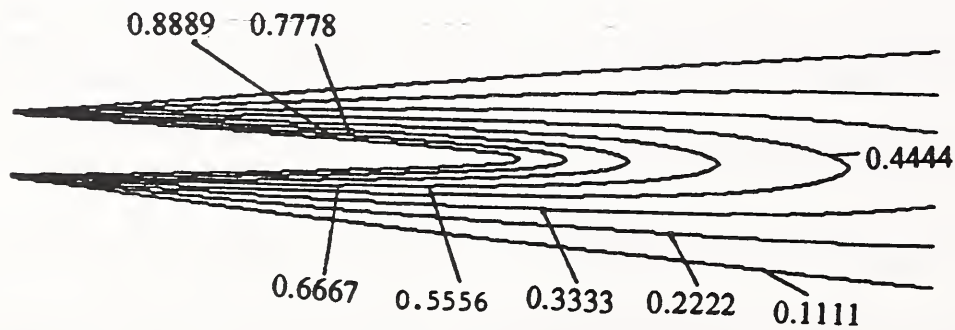
1. O.A. Ezekoye and Z. Zhang, "Modeling of a Lagrangian Flamelet with Radiation Interaction", *Combustion Science and Technology*, in review 1994.
2. O.A. Ezekoye, H.R. Baum and H.E. Rushmeier, "A Thermal Element Model of Fires", *Comb. and Flame*, in review 1994.
3. H.R. Baum, O.A. Ezekoye, K.B. McGrattan, and R.G. Rehm, "Mathematical Modeling and Computer Simulation of Fire Phenomena", *Theoretical and Computational Fluid Dynamics*, in press 1993.
4. Z. Zhang and O.A. Ezekoye, "Combustion of a Spherical Diffusion Flame in a Radiative Field", to appear in *HTD bound vol.* ASME WAM, Chicago, Ill December 1994.
5. H.R. Baum, O.A. Ezekoye, K.B. McGrattan, and R.G. Rehm, "Large Eddy Simulation of Fire Phenomena", Ninth Symposium on Turbulent Shear Flows Kyoto, Japan, August 1993
6. O.A. Ezekoye and H.R. Baum, "A Lagrangian Element Analysis of Combustion Processes in Fires", Central & Eastern States Sections of the Combustion Institute joint meeting, New Orleans, LA, 1993.



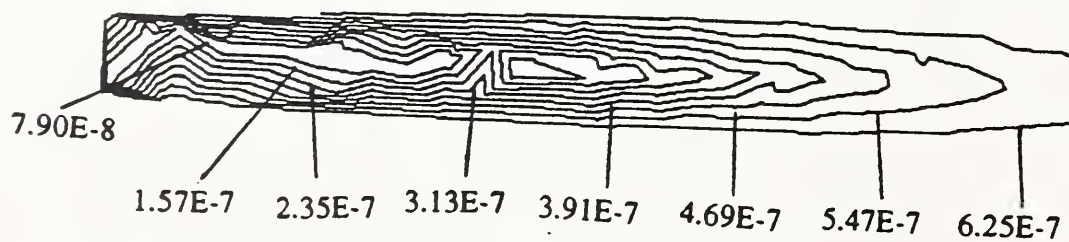
a) Temperature contour(K)



b) Mixture fraction (particle)



c) Mixture fraction (k-e)



d) Soot volume fraction



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT- FY94

Institution Purdue University

Grant No. 60NANB2D1291

Grant Title A Study of Entrainment and Flow Patterns in Pool Fires Using Particle Imaging Velocimetry (PIV)

Principal Investigator Professor J. P. Gore  
School of Mechanical Engineering  
Purdue University  
West Lafayette, IN 47907-1077

Other Personnel Y. R. Sivathanu, Research Professor  
X. C. Zhou, Doctoral Candidate

NIST Scientific Officers Dr. Anthony Hamins, Dr. Takashi Kashiwagi

Technical Abstract

Entrainment flows around pool fires and coupled radiation and soot kinetics properties are being studied.

Entrainment into Pool Fires

Introduction Entrainment rate of air into pool fires determines flame size and shape, degree of partial premixing, and consequently smoke production, radiant emission and fuel depletion. These parameters are important in models of hazard, egress time and suppression techniques for a variety of fires. Motivated by these applications, measurements of entrainment rates into pool fires have been made in the past by many investigators. However, the data show approximately a factor of two scatter depending upon the fire size, fuel type, ambient conditions, lip height (for liquid fueled pools), and measurement technique. During the present work, it has been determined that a part of the scatter in the data originates in the different definitions of entrainment rate. Considering the importance of entrainment rates in fire safety, the objectives of the research are: to improve current understanding of the process, to develop a non-intrusive technique for the measurement of entrainment defined in a unique manner, and to obtain a large enough data base for the construction of engineering correlations as well as for use in computational fluid dynamics (CFD) based fire models.

In the fluid mechanics literature, the entrainment rate is defined as the increase in the axial mass-flow rate of the gases with distance from the pool surface:

$$m_{ent} = 2\pi \frac{d}{dz} \int_0^R r \rho v dr \quad (1)$$

where  $z$  is the distance from the pool surface,  $v$  is the velocity in the axial direction,  $\rho$  is the density,  $r$  is the radial distance from the axis, and  $R$  is infinity. If a radial location at which the axial velocity is zero can be found at each  $z$ , then the integral in eq. (1) can be evaluated by

equating  $R$  to the radius of this location. Since the source flow is not a function of  $z$ , the entrainment rate is equal to the rate of change of mass flow of the surrounding fluid set in motion. Only a part of the mass of air set in motion by the fire enters the visible surface and even a smaller part actually takes part in the chemical reaction. The processes that lead to the determination of the above parts are coupled and can be completely described only in terms of an overall fire flow-field. However, for construction of engineering models, it is desirable to obtain separate estimates of the mass flow entrained by the fire. The total mass flow rate of room air set in motion is important in determining the composition and the temperature of the upper layer and the gases that flow into surrounding rooms and corridors. Thus, the significance of the total air flow increases in later stages of a fire when a sufficiently large mass of products is generated. However, fire detection, control, protection, and rescue methods can be most effective at a time prior to such fire growth. Hence, the mass flow entering the fire near the source, which is potentially available for combustion and determines the fire size and shape during the early period of fire growth, is of utmost significance.

Experimental Method PIV was used to measure mean and instantaneous air velocities in the vicinity of pool fires. The mass flow rate of air entering the fire was obtained by integrating the dot product of the local velocity vectors and local small area elements over the visible interface. The fires were enclosed in a 100 cm x 100 cm x 250 cm enclosure with air seeded with  $Al_2O_3$  particles entering at the symmetrically at the bottom through 25 cm screened opening as shown in Fig. 1. A stable interface of combustion products was formed at a height of 64 cm above the pool surface. A floor of 51 cm diameter was attached to the pool at the top surface. The cooling water flow rate was adjusted to maintain a constant burning rate of 83 mg/s and the exhaust fan speed was adjusted to maintain a constant interface height.

The PIV arrangement is shown schematically in Fig. 2. A 13 W CW  $Ar^+$  laser source pulsed by a mechanical chopper generated the illuminating light sheet. A galvanometer controlled oscillating mirror mounted in front of a 1.2 MB digital CCD camera provided an image shift between laser pulses to remove directional ambiguity in the measurements. A digital pulse delay generator, with input from the chopper controller was used to send synchronizing signals to the camera, the A/D board, and the mirror controller. The system was calibrated using a stationary object pin and a calibration jet flow. Approximately 100 images of the flow field were captured to obtain the mean and fluctuating components of the entrainment flow field.

Results and Discussion Figure 3 shows the mean entrainment flow around the 7.1 cm toluene fire. Very near the flame surface, data from images involving strong flame luminosity and high acceleration due to the density gradient are lost, introducing a downward bias in the mean velocity. The entrainment flow velocity is in the radial direction near the floor and at locations away from the flame surface. Near the flame surface and at farther positions from the pool surface, a significant axial velocity component is observed. Mean entrainment mass flow rate into a surface defined by the maximum visible flame position amongst the 100 images is calculated using the individual velocity vectors near this surface. The entrainment rate expressed in the coordinates of a recent correlation is plotted together with the data from the literature and LDV data for the present pool in Fig. 4. Reasonable agreement with the LDV data is observed. The present data are in agreement with some of the previous data but higher by as much as a factor of two compared to the correlation and the data on which it is based. The effect of pool diameter may be a factor but the limitation of the past measurement techniques in defining an exact value of  $R$  for entrainment flow calculation is a major contributor to the differences.

#### Radiation and Soot kinetics Interactions

Introduction Radiation heat transfer from flames depends on the instantaneous soot volume fractions and temperatures. In strongly radiating flames, it has been shown that radiation and soot



kinetics calculations need to be coupled to correctly predict observed soot volume fractions. Motivated by this observation, the present study seeks to investigate this coupling of radiation and soot kinetics in weakly radiating flames. A simplified soot kinetics model is used to determine the soot volume fractions present in a laminar methane/air diffusion flame while radiation is calculated using detailed narrow band calculations.

Numerical Methods The parabolic boundary layer equations for an axisymmetric laminar reacting flow are solved using a finite difference simulation. The dependent variables considered in the simulation are the velocity, mixture fraction, enthalpy, soot mass fraction and soot number density. The source terms for both the soot mass fraction and the soot number density are modeled using a kinetic mechanism that involves soot formation, growth and oxidation. Nucleation and growth are linked to a indicative species which is acetylene and oxidation by both  $O_2$  molecules and OH radicals is considered. The concentrations of OH radicals and all stable major gas species including  $C_2H_2$  are obtained from state relationships. The calculations of the source term for enthalpy which includes emission and absorption by the gas molecules are performed using the narrow band algorithm RADCAL in conjunction with a multiray computation.

Results and Discussion Figure 5 shows the predicted variation of peak soot volume fractions with axial distance in a laminar methane/air diffusion flame. There are four different curves shown in Fig. 5. The solid lines show results of the coupled soot kinetics and radiation calculations including the effects of oxidation due to both  $O_2$  molecules and OH radicals. The soot volume fraction reaches a peak of around 0.07 ppm and decreases rapidly when it passes through the flame zone. Eventually, all the soot produced by the flame is oxidized within it. The long-dashed line shows the results of a fully coupled calculation in which oxidation by OH radicals is neglected. The soot volume fraction reaches a peak of 0.11 ppm and then decreases slowly with soot being emitted from the tip of the flame, contrary to experimental observations, highlighting the importance of OH oxidation. The dotted-line and the short-dashed line represent soot kinetics calculations obtained using a fixed 20% or 5% radiative heat loss fraction respectively. If a fixed value of 20% radiation heat loss fraction (which has been experimentally measured) is used, the peak soot volume fractions reach only 0.03 ppm and oxidation is much slower. This is due to the lower temperatures restricting both soot growth and oxidation. To match the peak observed in fully coupled calculations, an unrealistically low value of 5% radiative heat loss fraction has to be used. The lack of coupling between radiation and soot kinetics causes soot growth to be delayed and soot oxidation to be more rapid as shown in Fig. 5.

Figure 6 shows the development of mixture fraction and peak local radiative fraction as a function of axial distance. Close to the burner, the radiative fraction is zero and increases to around 18% at the stoichiometric flame height. If oxidation of soot from OH radicals is neglected, there is very little change in the peak radiative fraction profile. This implies that radiation is primarily from gas molecules since the soot levels with and without OH oxidation are vastly different.

#### Reports and Papers

X. C. Zhou and J. P. Gore, 1994, "Air Entrainment Flow Field Induced by a Pool Fire," *Twenty Fifth Symposium (International) Combustion*, to be published in a special volume of *Combustion and Flame*, in press.

X. C. Zhou and J. P. Gore, 1994, "Particle Imaging Velocimetry of Flow Field Induced by a Small Toluene Pool Fire," Open Session on Fire and Combustion Systems, *ASME Winter Annual Meeting*, Chicago, IL., in press, also *Combustion and Flame*, submitted.

X. C. Zhou and J. P. Gore, 1993, "Laser Doppler Velocimetry and Particle Imaging Velocimetry Based Measurements of Air Entrainment into Pool Fires," *Proceedings of the Annual Conference on Fire Research, National Institute of Standards and Technology*, Gaithersburg, MD, pp. 63-64.



Y. R. Sivathanu and J. P. Gore, 1993, "Oxidation and Thermophoresis of Soot in Laminar Acetylene/Air Diffusion Flames," *Proceedings of the Fall Technical Meeting of the Eastern States Section of the Combustion Institute*, pp. 307-310, Princeton, New Jersey.

Y. R. Sivathanu and J. P. Gore, 1994, "Soot Kinetics/Radiation Interactions in Methane/Air Diffusion Flames, *Annual Conference on Fire Research*, also *Combustion and Flame*, to be submitted.

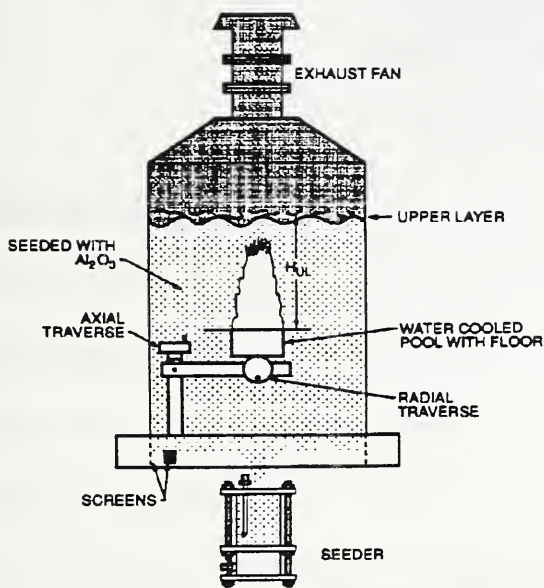


Figure 1. Schematic of an experimental arrangement for the measurement of fire induced flows.

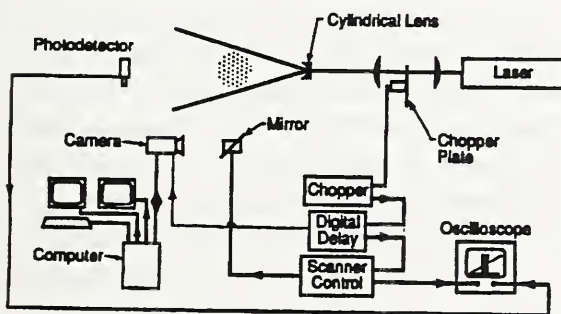


Figure 2. PIV instrument for the measurement of entrainment flows.

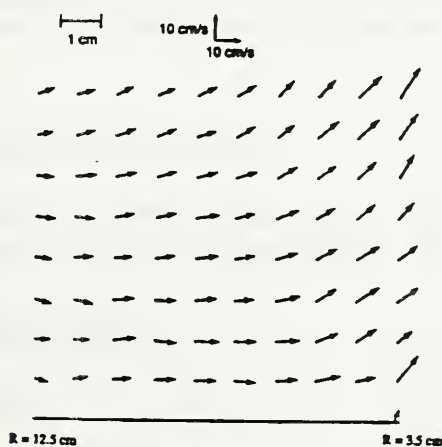


Figure 3. Mean velocity vectors around a 7.1 cm toluene fueled pool fire.

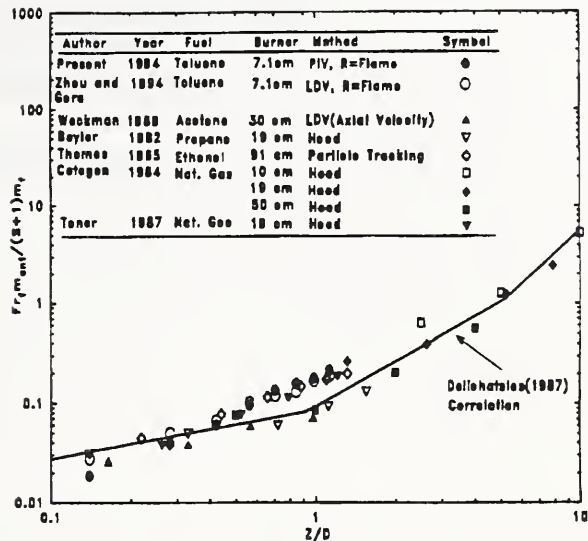


Figure 4. Measurements and correlation of entrainment rate into pool fires.

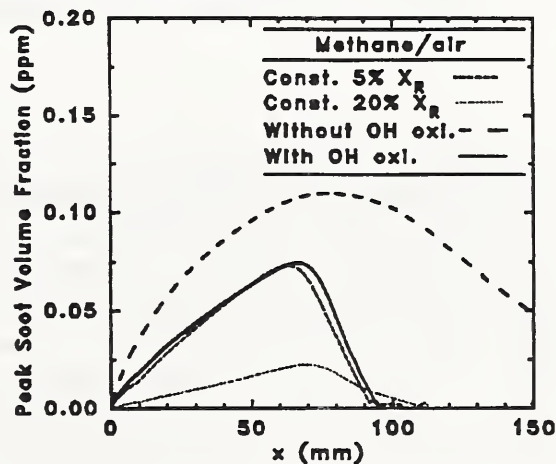


Figure 5. Axial variation of peak soot volume fractions in a laminar methane/air diffusion flame.

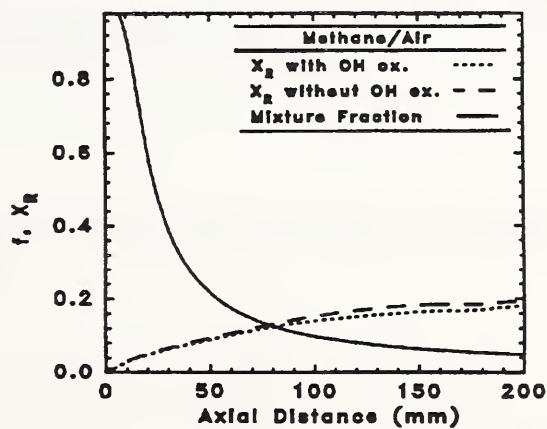


Figure 6. Axial variation of mixture fraction and radiative heat loss fraction in a laminar methane/air diffusion flame.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

FLAME RETARDANT STUDY

Funding Agency

General Electric Co.

Professional Staff

Takashi Kashiwagi, Project Leader

Project Objective

To understand the effects of polymer structure and certain flame retardant treatments on flammability properties of engineering thermoplastics and advanced structural composites.

Technical Accomplishments

Various flammability properties, (ignition, flame spread rate, heat release rate, CO, soot yields and smoke extinction), are measured for various GE's polycarbonates, polyimides and polyphenyleneoxides with and without flame retardant treatments. The flammability properties of polycarbonate/silicone copolymer samples were measured in a Cone Calorimeter. The effects of weight fraction of silicone in polycarbonate on flammability properties were determined. Furthermore, the effects of silicone chain length on flammability properties were also determined at the same weight fraction of silicone in polycarbonate. The silicone chain length effects on gasification rate were determined in a nitrogen atmosphere at the external radiant flux of 38 kW/m<sup>2</sup>. It was found that the amount of intumescent char is highly sensitive to the silicone chain length. All char samples were collected and analyzed by solid state NMR to determine their chemical structure.

The effects of the addition of glass fibers in polycarbonate and also in polyphenyleneoxides on flammability properties were determined. Furthermore, the effects of the amount of fibers, fiber diameter and length and its structure on flammability properties were also obtained.

Reports and Publications

"Effects of Sample Mounting on Flammability Properties of Intumescent Polymers", Kashiwagi, T and Cleary, T.G., Fire Safety J., 20, 203-225 (1993).

Related Grants

None



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT-FY1994

POLYMER FLAMMABILITY MODELING

Professional Personnel

Marc R. Nyden, Research Chemist  
James E. Brown, Research Chemist

Project Objective

To develop a technical basis for the design of a new generation of fire retardants and fire resistant materials.

Scope

The demand for better, cheaper and safer products has lead to a rapid proliferation of high performance and specialty polymers. This development has created a pressing need for new and more versatile approaches to increasing fire resistance. There is a strong correlation between char yield and fire resistance. This follows because char is always formed at the expense of combustible gases and because it protects the underlying polymer from the heat generated in combustion reactions. The presence of a surface char layer also acts as a physical barrier which obstructs the flow of gases produced in the degradation of the interior and thereby depresses the concentration of fuel in the gas phase. In principle, the tendency of a polymer to char can be increased by chemical additives and/or by altering its molecular structure. We have demonstrated that factors which promote char formation are revealed in molecular dynamic simulations of degrading polymers. In particular, we observed that cross-linked model polymers charred more readily than their linear counterparts. This prediction has been confirmed by Cone Calorimeter measurements made on  $\gamma$  and electron beam - irradiated polyethylene (PE), as well as, on chemically cross-linked poly(methyl methacrylate). We are now investigating the efficacy of chemical additives which, though inert at ambient temperatures, will promote cross-linking at the onset of the thermal degradation of the bulk polymer.

Technical Accomplishments

During FY94 our work has focused on augmenting the molecular dynamics model to facilitate investigation of the flammability properties of a wide range of vinyl polymers.



### Reports and Publications

"An Investigation of the Thermal Stability and Char Forming Tendency of Cross-linked Poly(methyl methacrylate)," S.M. Lomakin, James E. Brown, Robin S. Breese and Marc R. Nyden, *Polymer Degradation and Stability* **41**, 229 (1993).

"A New Generation of Fire Resistant Polymers: Part I Computer-Aided Molecular Design," Proceedings of the Joint Panel Meeting of the UJNR Panel on Fire Research and Safety, 257, 1992.

### Related Grants

None

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

COMBUSTION OF SILICONE

Funding Agency

Dow Corning Co.

Professional Staff

Takashi Kashiwagi, Project Leader  
Anthony Hamins  
Robert Buch, Dow Corning Co.

Project Objective

To understand the combustion mechanism of siloxane and specifically why the heat release rate, HRR, (as measured in the Cone Calorimeter) of burning siloxane is nearly independent of external thermal radiant flux.

Technical Accomplishments

Measurement of the steady burning rate and radiative heat loss fraction ( $\chi_R$ ) for siloxanes having different chain lengths was determined for pool flames with diameters of 10, 30, and 60 cm. Flame ignition for the longer chain length fluids could only be accomplished after heating to more than 100 °C. The measured burning rate was found to be a strong function of chain length. Ash was observed both in the gas phase and on the surface of the liquid pool, where it collected and with time submerged. The rate of ash deposition was largest for the slow burning long chain length fluids. The collected ash was analyzed for carbon, silicon, and hydrogen content and found to be predominantly silicon dioxide (silica). Silicon dioxide was apparent in the emission spectra of the siloxane flames as determined using an open-path FTIR spectrometer. Differences in the emission spectra between heptane and siloxane flames were related to broad band emission in the 8-10  $\mu\text{m}$  region of the siloxane which was attributed to silica. Radiative emission was measured at multiple locations on the surface of a cylindrical control surface surrounding the pool flame. Results showed that for the shorter chain length siloxane,  $\chi_R$  increased from  $\approx 0.3$  to 0.5 as the burner diameter increased from 10 to 60 cm. For the longer length siloxanes, however,  $\chi_R$  remained nearly constant or decreased with pool diameter.

Reports and Publications

None

Related Grants

None



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

MATERIAL FLAMMABILITY PREDICTIVE TECHNIQUES/METHODS

Funding Agency

U.S. Navy, David Taylor Research Center

Professional Personnel

James E. Brown, Research Chemist  
Thomas J. Ohlemiller, Chemical Engineer  
Thomas G. Cleary, Chemical Engineer  
John Shields, Physical Scientist

Project Objective

To assess for the U. S. Navy by September, 1994 the ability of existing models to predict the full-scale upward flamespread behavior of composite materials.

Technical Accomplishments

Most materials of interest to the Navy are sufficiently fire resistant as to require some external heat flux before they will yield upward flame spread in a flat wall configuration. For this reason, and to meet other program goals, we have built a medium-scale radiant panel facility which can be used under the hood of our furniture calorimeter. This facility allows uniform irradiation on samples 38 cm wide by 122 cm tall. The spread of flames and the resulting heat release process can be measured simultaneously. This facility was applied previously to a pair of non-flame retarded resin/woven glass composites and is now being applied to a heavily retarded version of one of these. Flame spread behavior is measured as a function of external flux and of igniter size. The heat flux into the surface is measured at several points during the flame spread process. The flux is also measured on these same materials in Cone Calorimeter scale experiments. One goal is to determine the appropriate external flux conditions for small-scale measurements intended to be input into flame spread models. A second goal is to test the ability of existing spread models to predict the observed full-scale behavior. Comparisons of model predictions with results on the unretarded composites shows reasonable, semi-quantitative agreement which implies that these models can help make useful decisions regarding composite usage. Assessment of the ability of the models to deal with the more difficult retarded material is still underway.

Reports and Publications

Ohlemiller, T., Cleary, T., Brown, J. and Shields, J., "Assessing the Flammability of Composite Materials", J. Fire Sciences, 4, July/August, 1993, p. 308

Related Grants

None

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

RADIATIVE IGNITION AND SUBSEQUENT FLAME SPREADING  
IN MICROGRAVITY ENVIRONMENT

Funding Agency

NASA Microgravity Science Program

Professional Personnel

Takashi Kashiwagi, Project Leader

Howard R. Baum

Kevin B. MacGrattan

Project Objective

Develop a theoretical model to be able to predict ignition and subsequent flame spreading over a thin cellulosic material in a microgravity environment using the material characteristics determined in normal gravity by September, 1994.

Technical Accomplishments

Two-dimensional, two-dimensional axisymmetric, and three-dimensional time-dependent ignition and subsequent flame spread with slow forced flows from 0 to 10 cm/s in microgravity has been developed. Its gas phase model is based on irrotational flow mainly controlled by the slow forced flow, gas expansion and mass addition from a degrading condensed fuel with one-step oxidative reaction with energy and chemical species equations. Its condensed phase model is based on the thermally thin cellulosic sheet with three global degradation reactions, pyrolysis reaction and oxidative degradation of the sheet to generate char and gaseous products, and oxidative char degradation. The results show that ignition parameters, the size of irradiated area, its duration and flux, have significant effects on transition to flame spread. The effects of flow velocity, oxygen concentration, the size and its duration of external radiant flux, with and without a pilot, and many other parameters (gas phase reaction kinetics,...) on transition from ignition and flame spread are being studied. Determination of kinetic constants of the three degradation reactions was completed using TGA analysis with multiple heating rates and oxygen concentrations and by continuous evolved gas analysis of CO, CO<sub>2</sub>, H<sub>2</sub>O and O<sub>2</sub>. A series of experiments corresponding to the above calculation are being conducted using the 2.2 and 5.5 seconds NASA's drop towers and a Lear jet and also will be planned in the glovebox of a shuttle mission which is scheduled to fly in February 1996. The effects of external wind velocity and the size of irradiated area on ignition, the transition to flame spread and flame spread process will be determined for comparison with the predicted results.

This project will be funded by NASA for additional three years starting October 1, 1994.



### Reports and Publications

1."Heat Transfer from Radiatively Heated Thick Material in a Low Reynolds Number Microgravity Environment", Yamashita, H., Baum, H.R., Kushida, G., Nakabe, K. and Kashiwagi, T., *J. Heat Transfer*, 115, 418-425 (1993).

2."Ignition and Transition to Flame Spread Over a Thermally Thin Cellulosic Sheet in a Microgravity Environment", Nakabe, K., McGrattan, K. B., Kashiwagi, T., Baum, H. R., Yamashita, H. and Kushida, G. to appear in *Combustion and Flame*.

### Related Grants

None

BUILDING AND FIRE LABORATORY  
FIRE SCIENCE DIVISION  
STRS PROJECT-FY94

CHAR STRUCTURE AND FLAMMABILITY

Professional Personnel

T. Kashiwagi, Group Leader  
Jeff Gilman, Polymer Chemist

Project Objective

To characterize the chemical structure of polymer residues which are generated at well-defined fire simulated conditions; the study in FY 94 is a seed project which hopefully will be extended to a more long range project for determining the links between original polymer structure, char characteristics and flammability properties for polymeric materials.

Scope

Currently, due to concerns over the environmental effects of halogenated compounds, there is an increasing international demand for the control of polymer flammability without the use of halogenated or metal based additives. One alternative flame retardant approach is to form char during polymer burning. This approach is ideal in that carbon retained in the condensed phase, as char, lessens the available fuel for combustion even as it helps insulate the polymer from the heat of the flame. However, at present, there is very little quantitative information about the relation between polymer structure, char properties and realistic flammability properties. Our approach to this issue is first to characterize the fundamental condensed phase processes and structures which lead to char formation during polymer combustion and then to use this information to design new strategies which increase char formation and, therefore, will reduce polymer flammability but without the use of halogenated or metal based additives.

Technical Accomplishments

The polymer we chose to investigate was poly(vinyl alcohol), PVA, because of its linear aliphatic structure, low char yield and commercial applications (paper, textile and adhesives).

We prepared PVA chars in a flow pyrolysis apparatus with an inert atmosphere ( $N_2$ ) at several temperatures. This experimental setup allows study of the condensed phase decomposition processes in the absence of gas phase oxidation. The physical appearance, hydrogen-to-carbon ratio and char yields are shown in Table 1.

Table 1. Material	Appearance	H/C Ratio	Char Yield (%)
PVA	white solid	2:1	NA
250 °C Char* (30 min)	yellow-orange foam	1.9:1	60
300 °C Char* (30 min)	tan rigid foam	1.4:1	47
350 °C Char* (30 min)	dark brown foam	1.2:1	17
400 °C Char (30 min)	black powder	1:1	5

\* We use the term "char" here to refer to the polymer residue after heating. This reference does not infer that the residues are necessarily graphitic or purely carbon.

The chars were characterized using CP/MAS <sup>13</sup>C NMR and elemental analysis. The results suggest that, in addition to the well known chain-stripping elimination reaction of H<sub>2</sub>O, a random chain scission reaction is also in progress. We also see evidence of formation of carbon-carbon bonds at all char temperatures and of conversion of the polyene products from the elimination reaction into aliphatic groups, possibly via Diels-Alder and/or radical reactions. This information was used to select a class of non-halogenated additives, i.e.. maleimides for study. Chars of PVA with three different maleimides were made at 300, 350, and 400C in the nitrogen flow pyrolysis tube. The chars were characterized using solid phase <sup>13</sup>C-NMR and C/H & N elemental analysis. These results show an increase of 50-100% in the char yields for one of the maleimide additives.

#### Reports and Publications

J.W.Gilman, T.Kashiwagi and D.L.Vander Hart, Thermal Decomposition Chemistry of Poly(vinyl-alcohol): Char Characterization, ACS-PMSE, Fire and Polymers Symposium, Preprint for ACS National Meeting, August 1994.

#### Related Grants

None at this time



Building and Fire Research Laboratory  
Fire Research Program  
National Institute of Standards and Technology  
Grantee Project - FY94

Institution Virginia Polytechnic Institute and State University

Grant No. 70NANB3H1434

Grant Title The Synthesis, Characterization, and Systematic Fire Safety Evaluation of High Volume and Specialty Hydrolytically Stable Phosphine Oxide Containing Polymeric Materials

Principal Investigator Professor James E. McGrath  
Department of Chemistry  
NSF Science and Technology Center:  
High Performance Polymeric Adhesives and Composites  
Blacksburg, Virginia 24061-0344

Other Personnel Dr. Tae Ho Yoon  
Mr. Daniel Knauss  
Mr. I-Wan Yuan

NIST Scientific Officer Dr. Takashi Kashiwagi

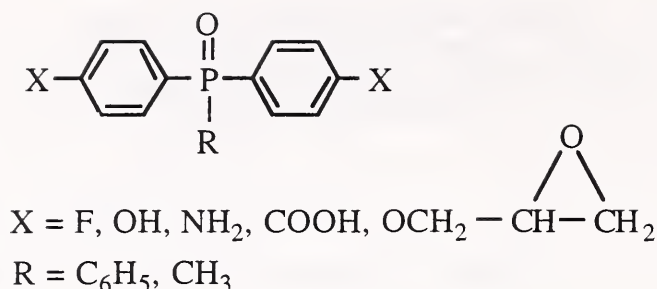
Technical Abstract

The objectives of this research project are to investigate hydrolytically stable phosphine oxide comonomers for both high volume thermoplastic materials, such as polyesters, polyamides, and polycarbonates, and important thermosetting systems, such as epoxy resin networks. In addition, the effort extends to high performance materials, such as polyimides and poly(arylene ether ketone)s. However, the latter effort is of secondary importance.

The research is attempting to determine whether or not chemically incorporated hydrolytically stable phosphorus systems can produce major improvements in fundamental fire resistant behavior. This chemically incorporated approach contrasts with the normal industrial method of physically adding fire retardants to the material systems. The disadvantage of the current approach includes the ideas that mechanical properties are impaired by the physical additives. Secondly, the additives may be extractable under conditions of use, possibly even producing unattractive, toxic byproducts. In contrast, the chemically incorporated systems will not be extracted by detergents or subjected to environmental degradation by normal humidity in the air. Preliminary small scale burning tests and dynamic thermogravimetric analysis methods have been very encouraging. The NIST project is the first effort achieving a more fundamental understanding through the use of cone calorimetry methodologies, which permit determination of heat release rate, heats of combustion, smoke generation, and carbon monoxide generation. The first year's achievements are promising and are documented below.

Introduction

During the past year it has been possible to synthesize a number of triphenyl phosphine oxide containing monomers, including the diamine, the dicarboxylic acid, the bisphenol, the diglycidyl ether, and to use these monomers to prepare polyesters, polyamides, polycarbonates and to generate epoxide networks. The structures of the most utilized monomers are provided below.



The emphasis thus far has included generating a series of polyamides which contained 10, 20 and 30 weight percent of the corresponding triphenyl phosphine oxide dicarboxylic acid. **The interest here was the possibility of making a semicrystalline high volume fiber forming material which would show inherent flame resistance.** The 10 and 20 mol percent samples were observed to be semicrystalline, although with a reduced melting point, as one would expect from a random copolymer. The 30 mol percent sample did not crystallize under compression molding conditions. We have not examined fiber drawing at this point, and it is possible that orienting the chains might induce some level of morphological order. The materials have been compression molded and initially evaluated at the NIST Fire Center via cone calorimetry. Briefly, the heat release rate and heat of combustion were definitely decreased by the introduction of the phosphine oxide comonomer (Figure 1). However, on the negative side, additional soot and carbon monoxide concentrations were observed under the conditions evaluated. The efforts in this area are more thoroughly summarized in a paper which has been prepared for presentation at the American Chemical Society meeting on fire resistant materials in August of this year.

Polycarbonates are also high volume engineering thermoplastics and it was of great interest to investigate whether the phosphine oxide bisphenol could be synthesized and copolymerized with the high volume bisphenol-A component. This, in fact, was achieved by both academic routes and possibly a more pragmatic scalable route involving first the synthesis of the bisaryldichloride followed by hydrolysis to the desired starting bisphenol material. The initial results on copolymerization of the phosphine oxide bisphenol with bisphenol-A under commercial polycarbonate synthesis conditions have been quite promising. It has been possible to prepare a range of copolymers, thus far up to 50 weight percent phosphine oxide bisphenol, and tough ductile transparent materials have been obtained which are compression moldable. Secondly, the observed increase in char yield as a function of phosphine oxide bisphenol has been realized. These samples are currently being prepared for evaluation by cone calorimetry.

The third polymer system investigated during the reporting period has been the epoxy diamine cured networks (Figure 2, Figure 3, and Table 1). These systems are more or less the backbone of aerospace matrix resin materials and fire resistance improvement is of great interest, for example, for aircraft interiors and also for marine applications, including ships, submarines, commercial vessels, composite oil drilling rigs, etc.. Our first approach was to utilize our diamine hardener. Initial experiments were conducted wherein 30 mol percent of the conventional diamino diphenyl sulfone (DDS) curing agent was substituted with BAPPO. The reason for limiting the concentration to 30 percent was the question of availability of the BAPPO. We have since produced a larger quantity. Nevertheless, the characteristics of the 30 mol percent BAPPO cured Epon resins were evaluated by an initial study by cone calorimetry. The resulting networks, even with only 30 percent of the curing agent containing phosphorous, were moderately encouraging and heat and combustion reduction for this system was demonstrated.

This effort is continuing and additional progress has been made on the synthesis of wholly phosphorus containing monomers. At this point it has been demonstrated that the phosphorus containing materials show a significantly higher char yield than their nonphosphorous conventional counterparts, as shown in Figure 3 below. **The logic for investigating this series of materials has been that firstly, it increases the percent phosphorus in the compound, and secondly, it does reduce the aromatic content of the structure which may enhance the reduction of soot and/or carbon monoxide.** Recall that the earlier experiments described above with copolyamides showed attractive reduction in heat release rate but did demonstrate significant soot yields. The synthesis of the first



materials have been generated by utilizing the reaction of trimethoxy phosphine with methyl halides, which produces a carbon phosphorous bond and two residual phosphorous methoxy units. The resulting methoxy compound has been converted to the chloride with thionyl chloride and then reacted with alkyl aromatics via electrophilic aromatic substitution chemistry. The resulting route is then a precursor to the analogous diamine, dicarboxylic acid or bisphenol structures that have already been demonstrated with the triaryl systems.

Future research plans will include first an evaluation of the copolycarbonates by cone calorimetry. The char yield improvement demonstrated is very encouraging and we are optimistic that it may be possible to prepare transparent tough ductile polycarbonate engineering copolymers that will have inherently increased flame resistance. That will be our first priority in the near future.

We intend to scale up the methyl diphenyl phosphine oxide copolymers and related monomers to include polyesters, polyamides, polycarbonates, and poly(arylene ether)s. Our goal will be to learn whether the increased phosphorus content and decreased aromatic structure will improve both heat release rate and at the same time retard or even diminish carbon monoxide generation. Thirdly, we intend to investigate the epoxy networks more thoroughly than has been conducted during the first nine months. This will particularly utilize the newly synthesized diamine structure 4, which can be prepared from commercially available triphenyl phosphine. There is already a high volume of this material produced, and it has applications in several areas including antioxidants for polyolefins. In the past year we have developed ways for selective di-nitration which produces the resulting phosphine oxide diamine after suitable reduction.

#### Acknowledgements

The principal investigator acknowledges the many discussions with Dr. Takashi Kashiwagi, as well as the cone calorimetry measurements that he provided for this research.

#### Reports and Papers

Wan, I-Yuan, Kashiwagi, T., and McGrath, J. "Synthesis, Characterization and Flame Retardancy Behavior of Triaryl Phosphine Oxide Containing Nylon 6,6 Copolymers," *Polymeric Materials: Science and Engineering*, 71, 233, 1994.

Knauss, D., Kashiwagi, T. and McGrath J. "Copolycarbonates Containing Hydrolytically Stable Phosphine Oxide Comonomers," *Polymeric Materials: Science and Engineering*, 71, 229 1994.

#### Figures and Tables

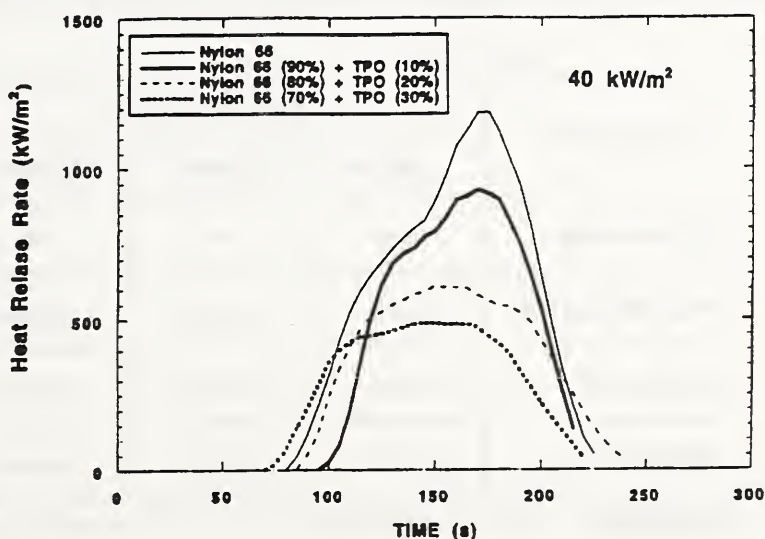


Figure 1  
Heat Release Rate of Triaryl Phosphine Oxide Containing Nylon 6,6, Copolymers



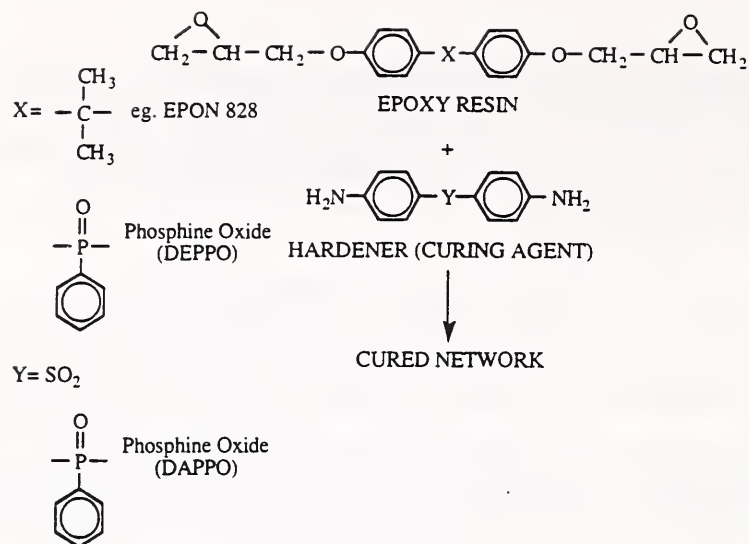


Figure 2  
Development of Fire Resistant Cured Epoxy Network Matrix and Adhesive Materials

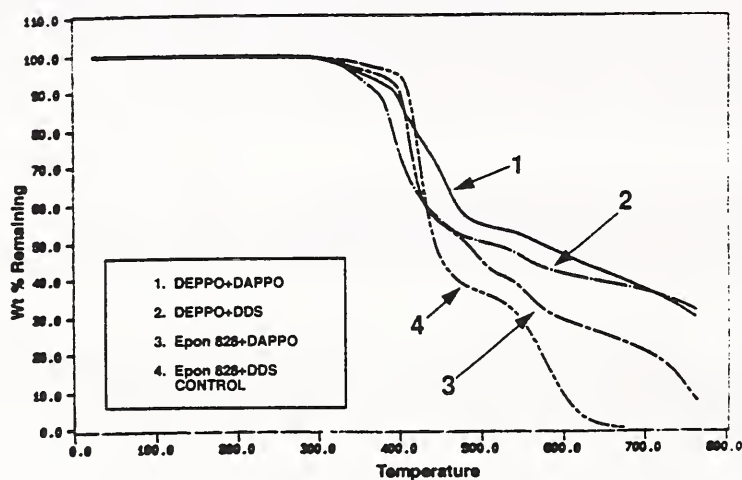
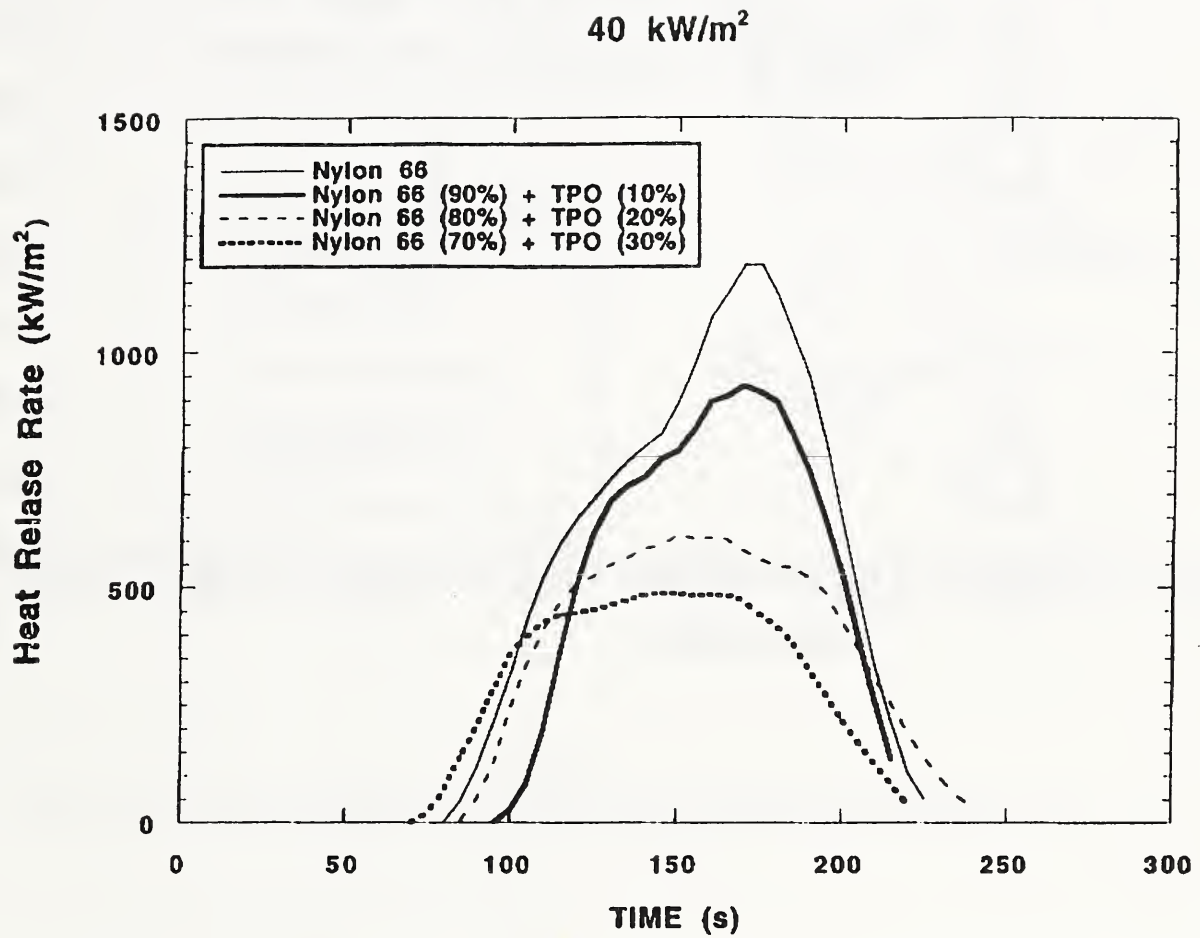


Figure 3  
High Char Yields are Generated When New Epoxy Polymers are Degraded in Air

Epoxy Sample	Weight Remained		
	at 600 °C	at 700 °C	at 760 °C
EPON 828+DDS	8.4%	0%	0%
EPON 828+DAPPO	29.0%	20.6%	8.25%
DEPPO+DDS	41.5%	36.8%	32.2%
DEPPO+DAPPO	46.3%	37.0%	29.6%

Measured in Air

Table 1  
Thermal Stability of Epoxy Polymers 1



**Figure 4.38** Heat release rate of triarylphosphine oxide containing nylon 6,6 copolymers [156]

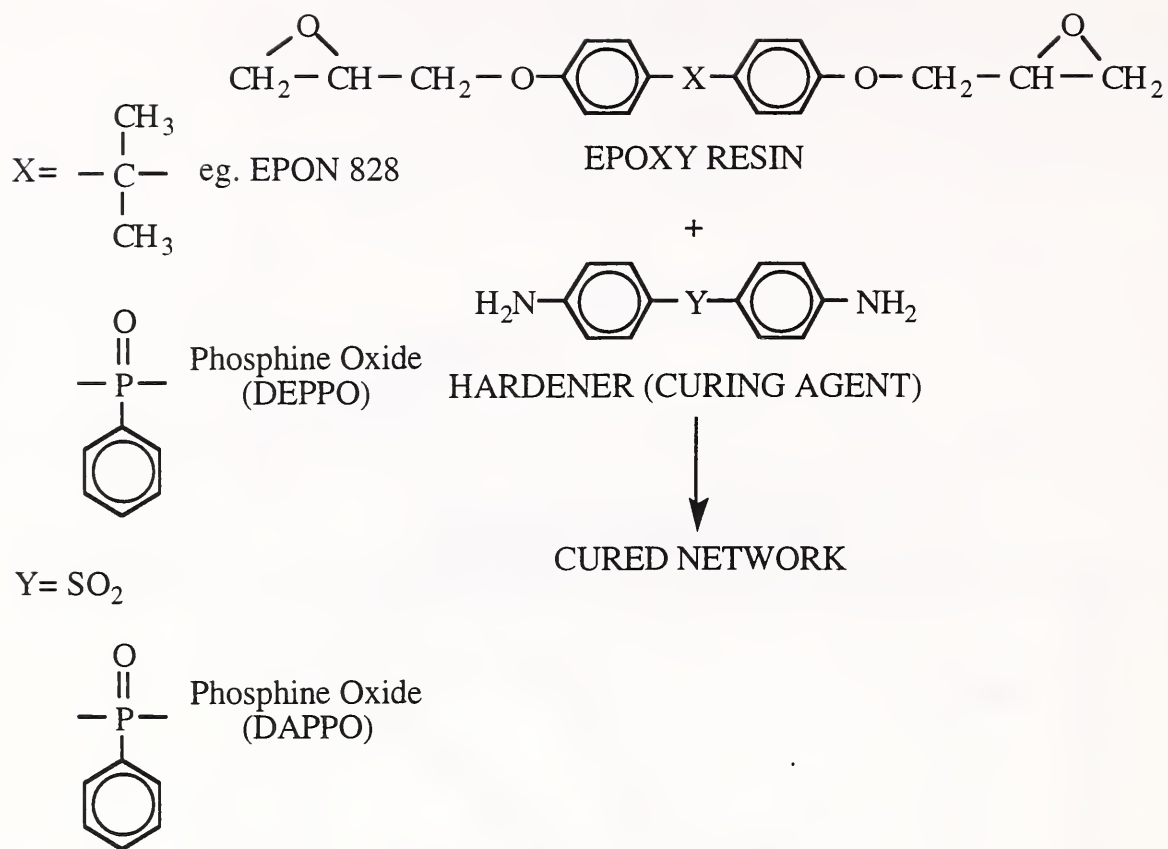


Figure 2  
Development of Fire Resistant Cured Epoxy Network Matrix and Adhesive Materials



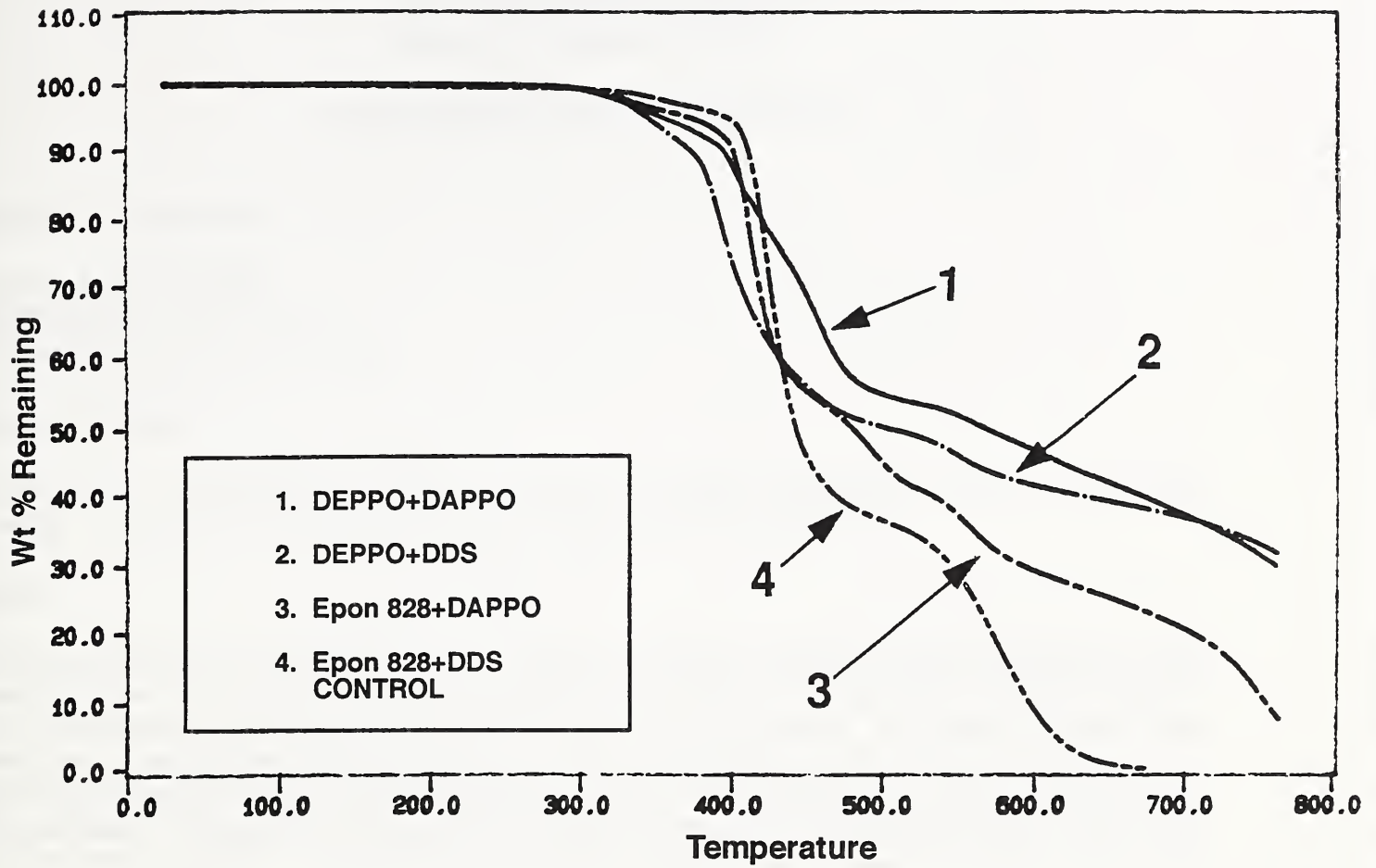


Figure 3  
High Char Yields are Generated When New Epoxy Polymers are Degraded in Air

Table 1  
Thermal Stability of Epoxy Polymers 1



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY 94

INTUMESCENT CHAR MODELLING

Professional Personnel

Kathryn Butler, Physicist  
Howard Baum, NIST Fellow  
Takashi Kashiwagi, Group Leader

Project Objective

To develop an understanding of the mechanisms of thermal protection provided by intumescent coatings through the numerical modelling of underlying physical principles.

Scope

Design of intumescent coatings, which protect the underlying surface from fire by swelling into a thick insulating char, has proceeded largely by systematic testing of a variety of formulations, since the physical mechanisms governing behavior are not as yet well understood. The numerical model being developed to understand this phenomenon is fully three-dimensional and time-dependent, and includes the dynamics of the swelling phenomenon, heat transfer through the coating, and chemistry of gasification. Simplified assumptions for these processes are eventually replaced with more sophisticated submodels. Qualitative and quantitative comparisons are made with laboratory results.

Technical Accomplishments

In this new project, the swelling phenomenon is modelled numerically by considering the collective behavior of a large number of bubbles expanding within a fluid volume of variable viscosity. This provides a physical representation of the chemical reactions that cause the intumescent material to successively melt, generate a large volume of gas in a multitude of small bubbles, and eventually solidify as a multicellular insulating foam.

Model development begins with the dynamics of a single bubble as it expands and travels through the surrounding fluidized material. The viscosity of intumescent material is known to be a strong function of temperature, which varies considerably through the coating during exposure to fire. Under the influence of a viscosity gradient, an expanding bubble in a fluid of infinite extent feels a force in the direction of decreasing viscosity. Because the Reynolds number for the small bubbles of interest is small, the induced velocity field can be obtained analytically as a perturbation solution to the Stokes equation driven by the viscosity gradient force term. The bubble also feels a buoyancy force and pressure drag; the sum of all forces determines the net velocity of the bubble through the fluid.

The velocity fields generated by individual bubbles are summed to describe the swelling of the intumescent coating. Initially, the coating is represented by a rectangular volume of fluid with bubble nucleation sites randomly distributed throughout. The upper surface of the coating is exposed to a constant heat flux representing the fire source, and the temperature within the coating begins to rise. When the local temperature at a given bubble site exceeds a specified value, the bubble begins to



expand. Its path through the fluid is determined by its own expansion rate, the local viscosity gradient, and the sum of the fields from all of the other bubbles, including a mirror image beneath the bottom surface to maintain the boundary condition of zero normal velocity at the rigid substrate. Bubble location and size are incremented in time according to a Runge-Kutta scheme. Merging of two overlapping bubbles is handled by replacing them with a single bubble of the combined volume located at the center of mass. The flexible upper surface of the intumescent material also feels the forces from all bubbles within the volume, and the locations of points on the surface are incremented accordingly.

Currently, the heat transfer model assumes simple conduction, with uniform conductivity through the coating thickness. In the near future, the detailed temperature field in the intumescent melt will be solved, using Lagrangian coordinates to take advantage of the simple initial geometry. Improvements are also planned for calculating the growth rate of each bubble, which is determined by the chemistry of gasification. An approximate expression for growth by diffusion in an oversaturated liquid-gas solution will be replaced by calculations that include the concentration of the blowing agent and locate temperature and viscosity.

An example of the results from this three-dimensional model is shown below. Figure 1 shows the grid describing the locating of the upper surface after integration of each node location over several time steps. The side view in Figure 2 shows that the bubbles near the bottom surface are much smaller than those near the top, since they have not had as much time to grow. At the time shown here, the temperature near the bottom surface is not yet hot enough to cause nucleation of the bubbles in this region.

This approach to the modelling of the dynamics and thermodynamics of an intumescent system provides a physical picture of its behavior. Calculations for up to 10000 bubbles have been run on a workstation.

#### Reports and Publications

Butler, K.M., Baum, H.R., and Kashiwagi, T., "A Kinetic Model of an Intumescent Material," in preparation.

#### Related Grants

None

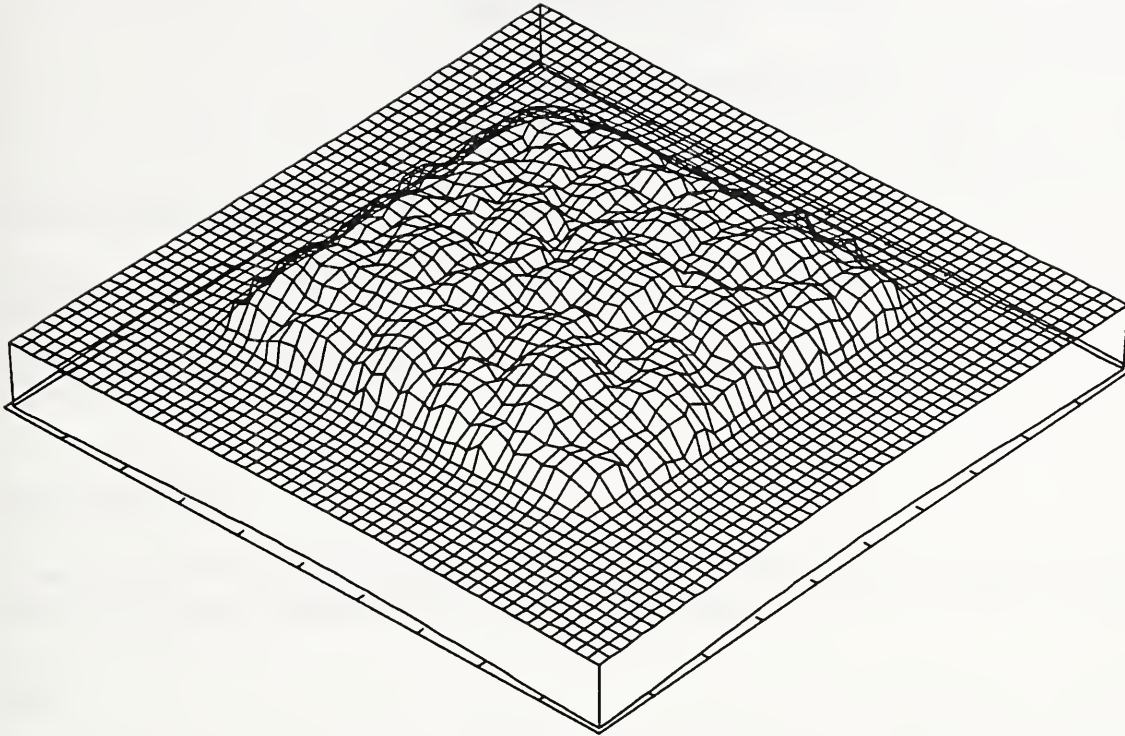


Figure 1: The intumescent surface grid after development in time of 10000 bubble sites randomly distributed between  $(-3,3)$  in  $x$  and  $y$  directions in a  $10 \times 10 \times 1$  rectangular slab.

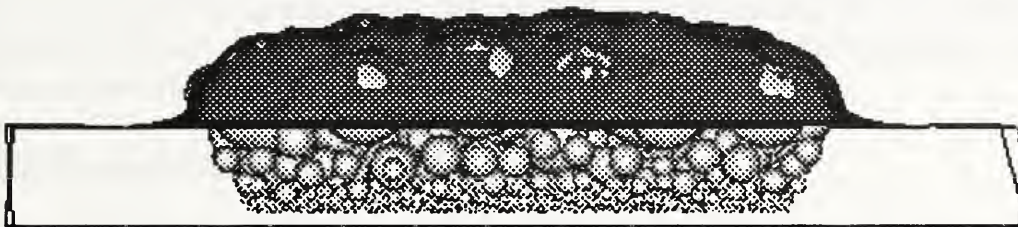


Figure 2: Same as Figure 1 showing a side view of bubbles and the intumescent surface.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY 94

FURNITURE FLAMMABILITY

Professional Personnel

Thomas J. Ohlemiller, Chemical Engineer  
Walter Jones, Physicist  
Rebecca Portier, Mathematician  
John Shields, Physical Scientist

Project Objective

Develop by 1997 an initial set of guidelines by which manufacturers can predict the peak rate of heat release of furniture designed for low rate of heat release.

Scope

Initially the work on interliners (protective fabrics placed between the decorative fabric and the polyurethane foam) is being completed because this technically has great promise for reducing the heat release of all types of upholstered furniture. Then, using mockups, we will systematically examine the effect on heat release rate of design factors such as heat release and flame spread rate of the fabric, seat width, seat back height and angle, and arm height. Based on information from these mockup burns and from the videotapes of full-scale tests, a predictive model of the burn process will be developed. The model will address the initial ignition pattern of various heat sources including the California TB133 gas burner, flame spread across the surfaces, burning rate of the furniture, and, finally, the possible ignition of other items. The predictive model, combined with a room fire model, will be used to calculate the impact of various sized ignition sources and various levels of flammability on residential furniture fires. Rules for designing low heat release furniture and calculation procedures for predicting mockup and full size item performance from Cone calorimeter and LIFT data will be developed. These rules and calculation procedures will finally be tested against commercially available furniture items.

Technical Accomplishments

A series of full-scale mock-up tests on twenty seven material combinations (seven fabrics, four interliners and two polyurethane foams) has been completed in our furniture calorimeter facility. In addition to heat release rate, data were taken on physical behavior and, to a limited extent, heat fluxes to the burning surfaces. The typical mock-up yielded two peaks of heat release, the first near the end of the gas burner exposure and the second usually much later, though frequently more intense. During the first peak, the geometry of the mock-up is largely preserved (except for macroscopic movements of the fabric) thus making it possible to consider whether this peak correlates in a simple manner with the behavior seen in the Cone Calorimeter. To assess this, all of the material combinations were tested in the Cone at 35 kW/m<sup>2</sup> incident flux. There is a tendency for

the two types of results to show a similar trend but the scatter in the relationship makes it of dubious practical value. Further analysis of the processes which lead to the peaks of heat release is underway.

#### Reports and Publications

"The Influence of Ignition Source on the Flaming Fire Hazard of Upholstered Furniture", Cleary, T., Ohlemiller, T. and Villa, K., to be published in Fire Safety Journal

#### Related Grants

None

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT-FY1994

FIRE RESISTANT AIRCRAFT MATERIALS

Funding Agency

Federal Aviation Administration

Professional Personnel

Marc R. Nyden, Research Chemist  
James E. Brown, Research Chemist

Project Objective

To formulate treatments for increasing the fire resistance of existing aircraft materials and to develop the technical basis for the design of a new generation of fire resistant polymer grafts and composites for use in the interiors of commercial aircraft.

Technical Accomplishments

The flammability properties of honeycomb composite materials, which are currently used in the interior cabin compartments of commercial aircraft, were examined. Analyses of the gases evolved during the thermal degradation of the components indicated that the phenol-formaldehyde resin makes a significant contribution to the flammabilities of these composites. The possibility that a more fire resistant formulation could be synthesized was examined by testing a series of resins which differed in the relative amounts of phenol and formaldehyde used in the reaction mixtures. The flammabilities of resins synthesized in excess phenol were measurably less than those synthesized in excess formaldehyde.

Publications

"Computer-Aided Molecular Design of Fire Resistant Aircraft Materials," Proceedings of the International Conference for the Promotion of Advanced Fire Resistant Aircraft Interior Materials, 147 1993.

"Flammability Properties of Honeycomb Composites and Phenol-Formaldehyde Resins," Proceedings of the Fire and Polymers International Symposium, 1994.



Related Grants

None

## **C. ADVANCED FIRE SENSING AND SUPPRESSION**





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

ADVANCED FIRE DETECTION SYSTEMS

Professional Personnel

William Grosshandler, Project Leader  
Richard Smith, Physical Scientist  
Margaret Jackson, Co-op Student

Project Objectives

To demonstrate to U.S. industry novel techniques for sensing products of and precursors to a fire, to suggest standard fires for evaluating the performance of detectors for various applications, and to investigate the chemical and physical products formed very early in fires which will allow one to discriminate between a fire and non-fire interfering signal.

Technical Approach

A properly designed detection system must be able to identify in a matter of seconds a fire event which may occur only once in one hundred years, and the identification must lead to an action which is appropriate to the space being protected. This disparity in time scale and the variability in geometry, content and occupancy of the space impose great demands on the system. False alarms, maintenance problems, incomplete or inaccurate information, and inappropriate suppression responses are problems which can plague current fire detection systems, especially when cost is an overriding constraint. The phase out of halons and the increased capital investment in modern industrial processes make early sensing and suppression even more imperative.

Interaction with representatives from the fire detector systems industry is required to more adequately understand their needs and to transfer our results directly to those who can use them. The current test procedures will be reviewed and a methodology will be developed for characterizing fires that will be useful for the evaluation of detectors. Various mechanisms for handling information provided by conventional detectors, from the description of the space being protected and from knowledge of different likely ignition events will be investigated to assess the impact of different approaches to fire protection and aid in the decision-making process.

Technical Accomplishments

A summary of the results of a workshop held in 1993 was distributed to members of the fire detection industry for their comments. A research plan which was to have come out of that workshop is still evolving. An evaluation of the impact of further research into improved fire detection was made, and the following issues will be kept in mind to ensure the research plan is cost effective: approximately 80% of residential fires occur in the 20% of residences that do not have working fire (smoke) detectors; fire detection is just one of a number of tactics for reducing fire losses; detection is not a cure-all; some technologies already exist which may provide for an adequate level of fire detection (including holding the false alarm rate to a reasonable level); and there are already large research efforts aimed at improving commercial detectors (e.g., one large international company has over 100 persons doing research relating to improving fire detection).

Research facilities at the University of Duisburg, Germany, and at Cerberus in Switzerland were visited as further background for the research plan. Residential applications do not have a high priority in the European research programs. Adapting the methodology used for European commercial/industrial applications to U.S. residential applications is thought to be fruitful. The challenge is to design a gas/particle/temperature sensing package and data processing unit which can be produced by the hundreds, and to devise ways to install them in and retrieve them from the field. In-situ environmental learning algorithms are not being developed in Europe, nor is the use of deterministic in conjunction with stochastic models being exploited.

The concept of a universal fire simulator/detection system evaluator is being developed in this project to supplement existing UL and EN standards involving prescribed full-scale room fires or smoke-flow boxes and to develop an environmental chamber in which velocity, individual gas species, particulate matter and temperature could be controlled as a function of time. A detector would be placed inside the chamber and the desired environmental program would be selected to emulate either a fire or interfering signal. The objective would be to have a facility in which alternative systems could be compared and new concepts evaluated on a level playing field. It would eliminate the run-to-run variation which is unavoidable in full-scale tests and allow more well controlled environments with realistic multiple stimuli. Support for such a facility needs to be obtained from the fire protection industry, UL, FM and NFPA.

An internal report was written entitled *Performance Parameters of Fire Detection Systems*. This report is a formal, functional analysis of fire detection systems' requirements. The performance parameters of fire detection systems are given as conditional probabilities, which are identified by the objective analysis of the functions of a fire detection system. It was demonstrated that using the false alarm rate to specify the malfunctioning of a threshold detection system is inadequate. The principal function of fire detection systems is the notification of anti-fire agents of the probability of an unwanted fire. The evaluation of the information provided by a detector system is central to its worth.

A summary of novel sensor developments was presented in a paper to the SFPE and NFPA.



The work done last year on detecting fires in a full-scale room using acoustic emission was reported to the International Association of Fire Safety Science. The AE research continues to attract the interest of different industries, although further work is not currently planned.

The literature has been reviewed to determine the extent to which fires have been characterized in their early phase (smaller than 100 kW). In particular, measurements of CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, O<sub>2</sub>, smoke and temperature have been collected from tests performed by other laboratories simulating the UL and EN test protocols. Figure 1 is a plot of CO concentration measured in the six standard European fires (TF1 through TF6), a UL test, and a test performed with a transformer fire (CERB) [Jackson, M.A., and Robins, I., "Gas Sensing for Fire Detection: Measurements of CO, CO<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>, and Smoke Density in European Standard Fire Tests," *Fire Safety Journal* 22, 181-205 (1994); Pfister, G., "Detection of Smoke Gases by Solid State Sensors - A Focus on Research Activities," *Fire Safety Journal* 6, 265-174 (1983)]. Not surprisingly, the variation in magnitude and rate of growth vary dramatically with fuel type and geometry. The variation is also large between repeat runs of the same tests (TF1, TF2 and TF3). When scaled by estimated mass consumed of fuel (Figure 2), the different standard fires can be seen to group a bit more systematically. The measuring location for one series of TF1, TF2 and TF3 fires was three meters off the centerline, while the others were made directly above the center of the fuel.

Additional measurements of species, temperature and velocity just above the flame are planned for next year to get a more complete footprint of each fire type. Similar measurements of non-fire nuisance sources are likely to be required in order to discriminate between a fire and non-threatening situation with a high degree of certainty.

Organization of a follow-on detector workshop to be held early in FY 1995 has begun. Development of an environmental chamber with a programmable temperature, velocity, composition, and radiation field designed to emulate a fire and interfering signals will be proposed to the industry group.

### Reports and Publications

Grosshandler, W., and Jackson, M., "Acoustic Emission of Structural Materials Exposed to an Open Flame," *Fire Safety Journal* 22, 209-228 (1994).

Grosshandler, W., and Braun, E., "Early Detection of Room Fires Through Acoustic Emission," Fourth International Symposium on Fire Safety Science, Ottawa, June 13-17, 1994

Smith, R.L., "Performance Parameters of Fire Detection Systems," NISTIR 5439, June 1994.

### Related Grants

Plumb, O.A. and Richards, R.F., "Development of an Economical Video-based Fire Detection and Location System," Washington State University.



Milke, J.A. and McAvoy, T.J., "Smart Fire Detection Using Neural Networks," University of Maryland.

Serio, M.A., "Advanced Infrared Systems for Detection of Building Fires," Advanced Fuel Research, East Hartford, CT, Phase I SBIR.

Shwe, M., "Decision-theoretic Control of Centralized Fire-alarm Systems," Knowledge Industries, Palo Alto, CA, SBIR Phase I.

Roby, R., "Advanced Fire Detection Based on Combined Smoke and CO Sensors," Hughes Associates, Inc., Columbia, MD, SBIR Phase II.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution Washington State University

Grant No. 60NANB2D1290

Grant Title Development of an Economical Video Based Fire Detection and Location System

Principal Investigators O.A. Plumb and R.F. Richards  
Department of Mechanical and Materials Engineering  
Washington State University  
Pullman, WA 99164-2920

Other Personnel K. Padakannaya, Doctoral Candidate  
B. Munk, Master's Student

NIST Scientific Officer W.L. Grosshandler

Technical Abstract

A video based system to detect, locate, and size accidental fires is being developed and its effectiveness investigated. The system involves a video camera which monitors color-changing, temperature-sensitive sensors to gather transient temperature information around a fire, and an inverse problem solution algorithm which uses the transient temperature data to predict the fire's location and heat release rate. Software implementing the inverse problem solution algorithm has been written. An evaluation of the accuracy of the inversion algorithm is described. The effects of errors in the fire model used by the inversion algorithm and measurement errors from the video system on system accuracy are quantified. In addition, a working prototype of the proposed fire detection system has been built.

Introduction

The video based fire detection system consists of color-changing, temperature-sensitive sensors, a video camera, a frame-grabber and a PC based inversion algorithm. Temperature-sensitive labels are arranged in a grid on the ceiling of a room. A video camera is placed in the room at a vantage point such that the temperature-sensitive sensors are within its field of view. If a fire is accidentally ignited, a buoyant plume of hot combustion gases will be generated. The buoyant plume rises to the ceiling of the compartment and upon reaching the ceiling will turn and then flow radially outward as a ceiling jet. As the ceiling jet flows across the ceiling, temperature sensitive labels are heated to their detection temperature and one by one will display a visible color change. Transient temperature information about the expanding ceiling jet is passed on to the PC by the frame grabber in the form of a time-series of digitized video images. The series of digitized images is then analyzed in the PC to provide the data needed by the inversion algorithm to predict the fire's location and size.

Inversion Algorithm

The problem of locating a fire and determining its growth rate can be formally posed as an inverse problem. In the present study the problem is taken to be one of parameter estimation, in which only three

unknown parameters are sought:  $x$ ,  $y$ , and  $\alpha$ . The location of the fire is assumed to be completely described by the Cartesian coordinates,  $(x,y)$ , defined to lie in the plane of the compartment floor. The functional form of the fire heat release rate is assumed to be quadratic in time:

$$Q = \alpha t^2 \quad (1)$$

where the parameter  $\alpha$  controls the fire growth rate. Here  $Q$  is the fire's convective heat release rate in kW and  $t$  is the elapsed time starting from the ignition of the fire.

The solution of the inverse problem involves two steps. First the forward problem is solved for a set of fire scenarios. For each scenario (each value of the ordered triple  $(x,y,\alpha)$ ) the time-to-activation for each of the sensors in the ceiling mounted grid is predicted. In the present study the solution of the forward problem is found using the compartment fire model LAVENT. LAVENT, developed at NIST, is a two-zone fire model employing semi-empirical models of the buoyant plume and ceiling jet to compute convective heat fluxes. Second, the predicted times-to-activation are compared to the actual sensor times-to-detection acquired by the video system. More specifically, the inversion algorithm proceeds by subtracting measured times-to-activation from predicted times-to-activation for the  $n$  sensors which change color in a given fire scenario and then summing the squares of the differences:

$$\sum_{i=1}^n (t_{a,i} - \hat{t}_{a,i})^2 \quad (2)$$

The solution to the inverse problem is taken to be the particular scenario  $(x,y,\alpha)$  which minimizes the sum of squares over the complete set of fire scenarios. In the present work, the number of sensors used by the inversion algorithm is taken to be  $n=5$ .

### Evaluation

The performance of the inversion algorithm was evaluated by simulating fires in a compartment and then using the algorithm to predict  $(x,y,\alpha)$  values for the simulated fire. To provide a statistical basis for the evaluation, each test consisted of 1000 simulated fires, each with a randomly chosen location  $(x,y)$ . The location and size determined by the inversion algorithm were then compared with the "actual" location and size of each simulated fire. Statistics concerning location and sizing errors were recorded and probability density functions (pdf's) determined.

In the present study, fires to be detected by the inversion algorithm were simulated using LAVENT. To include the effect of uncertainty that would inevitably arise in a real system, both random and systematic errors were introduced into the simulations. To account for uncertainty inherent in the fire model used to produce the forward solution, a systematic error was added to the LAVENT simulated sensor times-to-activation. The systematic error was assumed to be linear. To account for the measurement error inescapable in a fire environment, random values were also added to the simulated sensor times-to-activation. In this case, the error added was randomly chosen from a Gaussian distribution with a mean value of zero. Simulated times-to-activation,  $t_{sim,i}$  are then:

$$\hat{t}_{sim,i} = \hat{t}_{LAV,i} + (a + b\hat{t}_{LAV,i}) + G(\sigma) \quad (3)$$

where  $t_{LAV,i}$  is the time-to-activation of the  $i$ th sensor as calculated by LAVENT,  $a$  and  $b$  are constants, and  $G(\sigma)$  is a random number chosen from a normal distribution with standard deviation  $\sigma$ .

To validate the use of LAVENT simulated fire data (with added error), in evaluating the inversion algorithm, the results of the evaluation using simulated data were compared to an evaluation using experimental fire data. Transient temperature measurements from full scale experimental burns reported by Heskestad and Delichatsios were used to predict sensor times-to-activation. The experimentally derived times-to-activation were then used as data for the inversion algorithm



## Results

The results of the evaluation of the inversion algorithm can be seen in Figs 1 through 4. Figure 1 shows pdf's times-to-activation for the first and fifth sensors for a slow-growing fire ( $\alpha=2.98 \text{ W/s}^2$ ) and a fast-growing fire ( $\alpha=42.6 \text{ W/s}^2$ ). Upon activation of the fifth sensor the inversion algorithm has sufficient information to locate the fire. The slow-growing fire is seen to be located in three minutes and the fast-growing fire within one minute.

Figure 2 shows pdf's for location and heat release rate errors associated with the inversion algorithm's predictions for the slow-growing and fast-growing fires respectively. In order to show the effect of random error, fires were simulated with no random error ( $\sigma=0 \text{ sec}$ ) and moderate random error ( $\sigma=5 \text{ sec}$ ) and no systematic error (i.e. assuming LAVENT is a "perfect" model). Location error (Fig. 2a) is reported as the distance between predicted and actual fire locations, given in centimeters. Heat release rate error (Fig. 2b) is reported as the ratio of heat release rate predicted by the inversion algorithm at the time of the fifth sensor activation, divided by the actual fire's heat release rate (See equation 1). Random error is seen to broaden all of the error pdf's, although the effect is significantly greater in the fast-growing fire.

Figure 3 shows the effect of systematic or model error on the accuracy of the inversion algorithm to predict the fire location and fire size. Pdf's are shown for both the slow-growing and fast growing fires. The curves shown are for cases with random error  $\sigma=5\text{s}$  and systematic error corresponding to  $a=0\text{s}$  and  $a=40\text{s}$  for the slow-growing fire and  $b=0.0$  and  $b=0.6$  for the fast-growing fire. Figure 3a shows the surprisingly small effect of systematic error on error in location predictions by the inversion algorithm. On the other hand Fig. 3b shows the large errors in fire size predictions that systematic errors in the fire model used in the inversion algorithm can lead to.

Figure 4 shows the comparison between location and heat release rate error pdf's as determined using LAVENT simulated fire data and as determined using the experimental bum transient temperature measurements. The LAVENT simulated data has an added random error with  $\sigma=5\text{s}$ , and systematic error corresponding to  $a=20\text{s}$  and  $b=0.20$ . Both the location (Fig. 4a) and heat release rate error (Fig. 4b) pdf's are seen to be nearly identical for the evaluations using the LAVENT simulated data and the experimental data.

## Summary

An evaluation of a algorithm to be used in a video based fire detection system has shown the potential of the system to locate and size accidental fires. The algorithm has been shown, under simulated circumstances, to reliably locate fires within two meters, even when the algorithm is assumed to be based on a relatively inaccurate fire model. In contrast, the ability of the algorithm to size accidental fires is more limited, and more dependent on the accuracy of the fire model it incorporates. Finally, the use of LAVENT simulated fire data, with appropriate random and systematic errors added in, has been shown to give results essentially indistinguishable from those found using experimental data.

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Munk, B.N., Evaluation of an Intelligent System to Detect and Locate Fires, M.S. Report, Washington State University, Dept. of Mechanical and Materials Engineering, April, 1994

Richards, R.F., Munk, B.N., and Plumb O.A., Fire Detection and Location through Inverse Problem Solution, submitted to Fire Safety Journal.

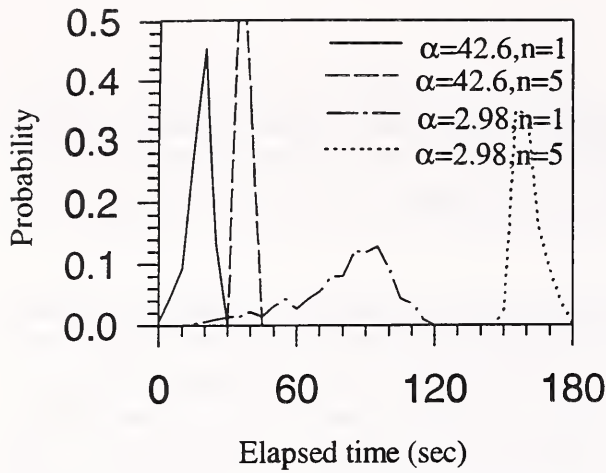


Fig. 1 Time to activation of sensors

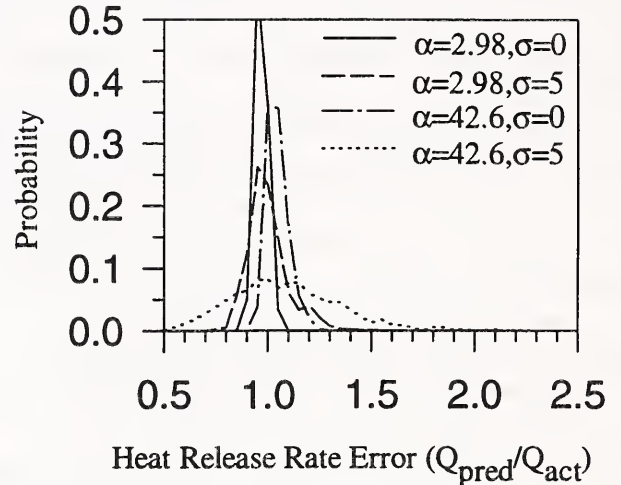
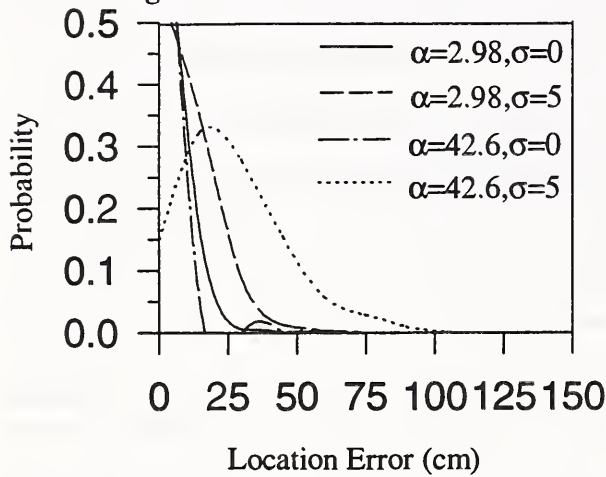


Fig. 2a,b Effect of random error on location and heat release rate predictions

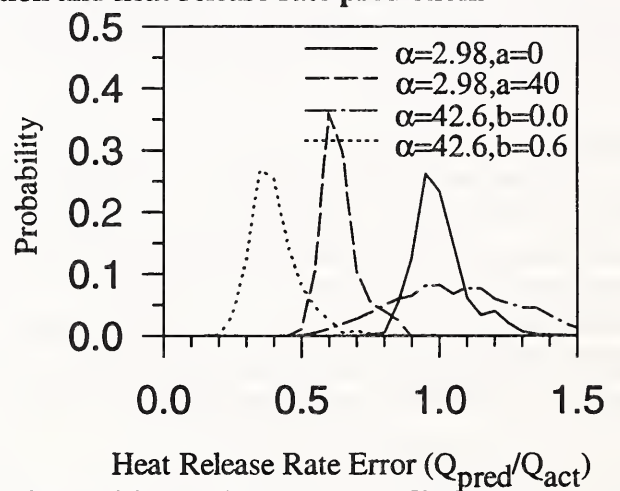
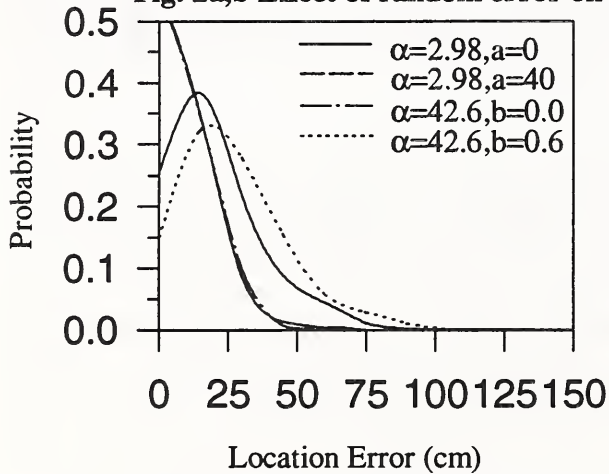


Fig. 3a,b Effect of systematic bias on location and heat release rate predictions

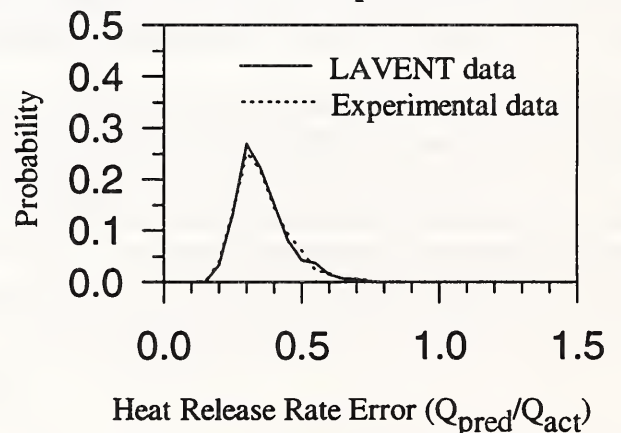
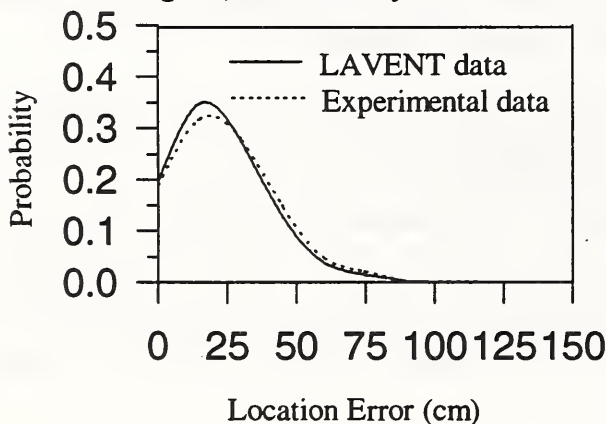


Fig. 4a,b Comparison of evaluations using LAVENT data and experimental data

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution University of Maryland at College Park

Grant No. 60NANB2D1300

Grant Title Large-Scale Experiments of Fire Signatures to Develop a Discriminating Fire Detector

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Technical Abstract

Incorporating intelligence into a fire detector can provide the capability to promptly react to smoke while discriminating between smoke from fire and non-fire sources. The primary purpose of this study was to investigate the patterns of signatures associated with fire and environmental signatures via experiments. During the most recent phase of research, work is being conducted to supplement the small-scale experimental effort reported previously [1]. The research is being conducted at the University of Maryland by teams in the Departments of Fire Protection Engineering and Chemical Engineering. The fire protection engineering team is concentrating on identifying signatures from fire and non-fire sources. The chemical engineering team is investigating the applicability of neural networks to discriminate between fire signatures.

In the initial phase of effort, small-scale tests were conducted to characterize the signatures from fire and non-fire sources. The experiments were designed to be conceptually similar to those by Okayama [2]. Modifications in the experimental program by Okayama



were incorporated to provide a greater range of measurements for describing the signature.

The small-scale experimental apparatus was a simplified tunnel which included a means for generating odors, measurement equipment and sensors. Measurements of light obscuration, temperature, and gas species concentrations (CO, CO<sub>2</sub> and O<sub>2</sub>) and presence of any oxidizable gas are provided. The presence of oxidizable gases was measured by a Taguchi metal oxide sensor. Sources of the smoke or odor were placed under a hood at the inlet end of the apparatus. Smoke and odors were produced from a wide range of conditions: samples with flaming and pyrolyzing combustion, heated samples and samples maintained at ambient conditions where the odor was introduced into the box via an atomizer. The specific fuels and environmental sources were intended to be representative of a residential environment.

The following patterns in the small-scale experimental data were evident: the maximum CO<sub>2</sub> concentrations for flaming fires were at least 1500 ppm, while the maximum CO<sub>2</sub> concentration for the non-flaming fires (pyrolyzing fires, heated liquids and environmental odors) were all less than 1500 ppm. The non-flaming sources can be distinguished based on the CO and metal oxide sensor peak measurements. All but three of the pyrolyzing solids had peak CO concentrations of at least 28 ppm and a signal of less than 6 V from the Taguchi detector. Based on these observations, an elementary expert system appears to be capable of identifying the source of the odor.

The level of success attained from the small-scale experimental program indicated the feasibility of the concept presented by Okayama. However, the success of the expert system only relates to the limited range of fuel sources investigated and the small-scale test apparatus. A large-scale experimental program is being conducted to determine whether the trends identified in the small-scale experimental effort also can be observed in large-scale environments. The large-scale experiments being conducted at the University of Maryland are conceptually similar to the small-scale experiments. Signatures from fires and environmental sources involving a wide variety of fuel sources are monitored. As in the small-scale study, patterns are being sought, with the applicability of an expert system or neural network investigated.

The large-scale experiments are being conducted in a 12 x 12 ft room with a height of 8 ft. Measurements include temperature, mass loss of the fire sources, CO, CO<sub>2</sub> and O<sub>2</sub> concentrations and the voltage output from three different metal oxide sensors. The three metal oxide sensors respond to the presence of CO, oxidizable gas and environmental odors respectively.

In addition to the large-scale experiments being conducted, results from a wide variety of large-scale experiments conducted at international research institutions including NIST, VTT, SP, SINTEF and DIFT are being analyzed to describe early fire signatures. This data

is useful to describe signatures only from flaming and non-flaming fuel sources, excluding signatures from environmental sources.

This work is ongoing. Analysis of experimental data and application of neural network will be reported.

### Acknowledgements

The guidance of Dr. William Grosshandler, NIST, is greatly appreciated on technical issues related to the project. In addition, the assistance of Mr. Randy Edwards, Fire Control Instruments, and Mr. Seth Cowles, Notifier Division of Pittway, is recognized in lending assistance with commercial smoke detection systems used in the study.

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BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

SPECIES PRODUCTION FOR TURBULENT FLAME MODELLING

Professional Personnel

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Project Objectives

Develop an accurate data base and phenomenological descriptions to establish models for in-flame species concentrations and post-flame species yields as a function of residence time, equivalence ratio, temperature, and strain and scalar dissipation rates by the year 2000. Customers include the CFAST Team, Mass Burning Rate Project, Smart Sensor Project, and the Large Fire Project.

Technical Accomplishments

Combustion involves complex interactions between high-temperature chemical reactions, fluid mixing processes, and the production of gaseous fuel components via both thermal and chemical degradation. Although our knowledge of fuel production pathways and rates is in its infancy for the general case of condensed-phase fuel decomposition, significant progress has been achieved in identifying the key gas-phase chemical reactions and the associated fluid mechanical mixing phenomena which occur under high-temperature combustion conditions. As a consequence, increasing attention is now focussed on elucidating the strong coupling which occurs between chemical heat release and turbulent mixing, i.e., chemistry-turbulence interactions.

Soot formation is an example of a process which is especially sensitive to the local combustion conditions, since the pre-particle soot inception chemistry is relatively slow. In recent years several new attempts have been made to utilize the extensive experimental data currently available from steady flames to develop integrated models of soot formation and evolution. Although the various modelling approaches differ a good deal, there are several common threads. The local temperature, mixture fraction, and residence time have been

identified as important variables in soot production, in addition to the chemical structure of the fuel. In complex flowfields many possible combinations of residence times, temperature histories, and local stoichiometries exist for soot production and destruction, as well as a wide variation of strain and scalar dissipation rates. One might anticipate that chemistry-flowfield interactions will have a dramatic impact upon soot formation, and indeed we have found this to be the case.

While the chemical growth reactions play a key role in regard to the total amount of smoke produced, the actual structure of the smoke leaving the flame region is determined by a physical agglomeration process of particles sticking and forming a cluster. The agglomerate structure consists of a number of primary particles with diameters of about 30 nm connected in a rather open structure. The light extinction coefficient and light scattering coefficient, both of which affect the visibility through smoke, are not well characterized for agglomerate structures. The aerodynamic properties, which control smoke deposition in the respiratory tract, are also poorly specified. Understanding the relationship between the geometric structure of an agglomerate and its properties is a key research topic in both aerosol research and condensed matter physics.

#### 1. Soot Production in Flickering Hydrocarbon Diffusion Flames

As our understanding of gas-phase chemistry in steady diffusion flames has matured, increased focus has been directed toward more practical, turbulent diffusion flames. A critical assumption in applying chemical models developed in laminar flames to turbulent combustion is that the limited combinations of residence times, temperature histories, local stoichiometries (mixture fraction), and strain rates (scalar dissipation) sampled in laboratory-scale steady laminar flames are sufficient to quantitatively describe chemical processes in turbulent environments. In order to critically evaluate the validity of this assumption, an experimental facility for performing optical measurements in time-varying, laminar diffusion flames has been developed at NIST. This apparatus provides an environment for in-situ investigation of flame chemistry which allows the systematic examination of the time-dependent interaction of variable-strength external vortex rings with the flame structure.

Quantitative measurements of the local soot volume fraction have been made in a co-flowing, flickering  $\text{CH}_4$ /air diffusion flame burning at atmospheric pressure. Acoustic forcing of the fuel flow rate is used to phase lock the periodic flame flicker close to the natural flicker frequency. Our results show that soot production is four times greater for a forcing condition in which flame tip clipping occurs, compared to a steady flame burning with the same mean fuel flow velocity. The soot field in the flickering flame has been characterized using tomographic reconstruction of extinction data obtained at 632.8 nm, laser-induced incandescence (LII) images calibrated against steady  $\text{CH}_4$ /air extinction results, and vertically polarized scattering data. The LII method is found to track the soot volume fraction closely and to give better signal-to-noise than the extinction measurements in both the steady and time-varying flowfields. A Mie analysis of these results suggests that the flickering flame



exhibits similar number densities but larger particle sizes than the corresponding steady flame.

## 2. Smoke Agglomerates

This portion of the project focusses on the properties of the smoke agglomerates above the flame zone. During the past year we began a program to assess the accuracy of optically measuring soot volume fraction in the post-flame environment. While soot volume fraction measurements using optical techniques have become common over the past decade, there has been no critical assessment of the accuracy of the measurements.

The key element in this study was the development of an accurate method for measuring soot volume fraction. The method consists of iso-kinetically sampling the soot at a known flow rate, measuring the mass of soot collected, and determining the density of soot by helium pycnometry. The uncertainty in the measurement ( $2\sigma$ ) is found to be about 12% of the measured value.

The experiment consisted of producing a well mixed flow of smoke and then simultaneously measuring the light extinction and sampling the smoke. A 6 cm diameter water-cooled flat-flame McKenna burner was positioned inside a 65 cm long cylindrical quartz chimney. To cool the soot/gas mixture, nitrogen was injected into two ports on the side of the quartz tube. A 2.1 cm diameter tripper plate was positioned 18 cm above the burner and the sampling location was six tube diameters downstream of a tripper plate. A wire mesh was placed 2 cm upstream of the laser beam/soot collection point to enhance the uniformity of the smoke concentration. The radial variation in the soot concentration was characterized.

The optical measurements were performed using a 15 mW 632.8 nm He-Ne laser and a silicon photodiode. To prevent air entrainment into the chamber, light tubes were used at the entrance and exit of the glass cylinder. Nominally 60% of the incident light was transmitted through the smoke produced by the acetylene flame. Measurements were performed at equivalence ratios of 2.3, 2.5, and 2.7.

The key result of this study is the determination of a dimensionless extinction coefficient of  $8.6 \pm 1.5$  for  $\lambda = 632.8$  nm. The mass specific light extinction coefficient is found to be  $8.0 \text{ m}^2/\text{g}$ . This quantity can be used for inferring mass concentration from light extinction measurements.

### Publications

K.C. Smyth, J.E. Harrington, E.L. Johnsson, and W.M. Pitts, *Combustion and Flame* 95, 229 (1993). Greatly Enhanced Soot Scattering in Flickering  $\text{CH}_4$ /Air Diffusion Flames.



R. Puri, R.J. Santoro, and K.C. Smyth, *Combustion and Flame* 97, 125 (1994). The Oxidation of Soot and Carbon Monoxide in Hydrocarbon Diffusion Flames.

C.R. Shaddix, J.E. Harrington, and K.C. Smyth, *Twenty-Fifth Symposium (International) on Combustion*, in press. Quantitative Measurements of Enhanced Soot Production in Flickering Methane/Air Diffusion Flame.

J.E. Harrington, C.R. Shaddix, and K.C. Smyth, *SPIE International Symposium on Laser Diagnostics in Combustion*, Vol. 2124, Paper 20 (1994). Laser Imaging of Chemistry-Flowfield Interactions: Enhanced Soot Formation in Time-Varying Diffusion Flames.

G.W. Mulholland and N.P. Bryner, *Atmospheric Environment* 28, 873 (1994). Radiometric Model of the Transmission Cell-Reciprocal Nephelometer.

R.A. Dobbins, G.W. Mulholland, and N.P. Bryner, *Atmospheric Environment*, 28, 889 (1994). Comparison of a Fractal Optics Model with Light Extinction Measurements.

#### Related Grants

1. Fundamental Studies of Diffusion Flame Chemistry  
J. Houston Miller, George Washington University.
2. Aerosol Fractal Aggregates: Light Scattering, Diffusion and Aggregation  
Christopher M. Sorensen, Kansas State University
3. Experimental Study of the Optical Properties of Soot & Smoke  
Mun Young Choi, University of Illinois
4. Mixing and Radiation Properties of Buoyant Luminous Flame Environments  
Gerald M. Faeth, University of Michigan

**BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94**

Institution: The Pennsylvania State University

Grant No.: 60NANBOD1035

Grant Title: Fundamental Mechanisms of CO and Soot Formation in Diffusion Flames

Principal Investigator: Professor Robert J. Santoro  
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240 Research Building East  
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Other Professional Personnel: R. Puri, Doctoral Student  
S. Léonard, Graduate Student

NIST Scientific Officer: Dr. Kermit C. Smyth

Technical Abstract:

Introduction: Since CO inhalation is one of the major causes of fire fatalities, significant effort has been directed towards obtaining an understanding of CO production in fires. Numerous workers have observed a correlation between the amounts of CO and soot produced in diffusion flames [1] as well as compartment fires [2]. There have also been several studies of the species produced by underventilated turbulent flames [3,4]. In these studies, there is an abrupt increase in the CO concentration at a global equivalence ratio of 1.0. This large increase in CO is of concern in regards to safety implications for fires in structures and is a motivation for the present study of simpler underventilated laminar diffusion flames.

The focus of the present study is to provide a quantitative data base on the production of CO and smoke particulates from laminar underventilated diffusion flames à la Burke and Schumann [5]. Advantages of the underventilated laminar diffusion flame system include a wide range of  $\Phi$  up to at least 4, the ease in measuring  $\Phi$  and the yields of CO and smoke, and the potential for theoretical analysis of the generation rates of the combustion products. In the present study, emphasis is given to the general trends observed for both CO and soot production in terms of the global equivalence ratio. The trends in the CO and soot yields in these underventilated laminar flame studies differ distinctively from results observed in overventilated diffusion flames. Additionally, the very nature of the soot formed in these flames is different from that observed in the more widely studied overventilated conditions.

Experimental Approach: Underventilated diffusion flames refer to conditions where the amount of oxidizer flow is insufficient to result in the oxidation of all of the fuel to carbon dioxide and water. In the present study, the fuel-to-oxidizer ratio is characterized by the overall equivalence ratio,  $\Phi$ , based on the ratio of the inlet fuel and air flow rates, where  $\Phi$  greater than one correspond to fuel-rich conditions.



The burner consists of two concentric tubes which could be varied in size to investigate the sensitivity of the results to burner geometry effects. Results for a single burner will be presented which are representative of the general behavior observed for the CO and soot yields. This burner had a fuel tube of 0.73 cm i.d. and outer air annulus with a 2.9 cm i.d. Both methane ( $\text{CH}_4$ ) and ethene ( $\text{C}_2\text{H}_4$ ) fuels were studied. For the methane flames, fuel flow rates of 10  $\text{cm}^3/\text{s}$  and 20  $\text{cm}^3/\text{s}$  were examined, while for ethene, flow rates of 3.2 and 6.4  $\text{cm}^3/\text{s}$  were considered. The air flow rates were selected in each case to allow the overall equivalence ratio  $\Phi$ , to be varied between 0.5 and 4.0. Measurements of CO and  $\text{CO}_2$  concentrations were obtained using individual NDIR instruments, while soot particles were collected separately using filters and analyzed for mass deposited by a weighing procedure. Yields for CO and soot on a mass basis were determined from the measured concentrations and known flow rates of the gases supplied to the burner. Detailed species concentration profiles were obtained using intrusive probe techniques followed by gas chromatographic analysis. Complementary temperature measurements were made using thermocouples. These measurements were used to investigate the evolution of flame structure of these underventilated laminar diffusion flames as a function of radial and axial position.

**Results and Analysis:** It is convenient to express the results in terms of a yield based on the mass of CO or soot produced per mass of fuel entering the burner. The CO yield increases abruptly with  $\Phi$  to a peak value of 0.37 for methane and 0.47 for ethene. As shown in Fig. 1, the peak in the methane curve occurs at a slightly smaller  $\Phi$  than for ethene, 1.3 relative to 1.7. Additional measurements were performed at other fuel flow rates and with a second burner configuration to determine the generality of this shift, and the results were inconclusive in regard to the difference being attributed to fuel chemistry. Decreasing the fuel flow rate for ethene by a factor of two to 3.2  $\text{cm}^3/\text{s}$  was observed to shift the peak to the left by an amount similar to the difference between ethene at 6.4  $\text{cm}^3/\text{s}$  and methane at 10  $\text{cm}^3/\text{s}$ .

The smoke yield curve peaks at smaller  $\Phi$ , near 1.0, compared to the result for CO yield. Also for large  $\Phi$ , the percentage decrease for smoke is much greater than for CO, and the smoke yield decreases sharply for  $\Phi > 1.5$ . This is the same trend as for the CO yield. The large reduction in the smoke yield at  $\Phi = 0.5$  for the 3.2  $\text{cm}^3/\text{s}$  fuel flow rate case is expected since the fuel flow rate is then below the smoke point for the overventilated flame.

The filter samples for smoke generated at large  $\Phi$  appeared lighter in color and the deposit on the combustion burner tube had a liquid character. In fact, for methane at  $\Phi = 4$ , the filter had a yellowish appearance. Thermo-optical analysis of the smoke collected on the quartz filters indicated that as  $\Phi$  increased, the organic fraction of the smoke increased relative to the elemental carbon fraction (see Table 1). For  $\Phi \geq 2$ , the organic-to-elemental carbon ratio exceeded 0.5 for both the methane and ethene flames. Such large amounts of organic carbon in the soot particles is viewed to be quite interesting and differs from observations in overventilated flames where a ratio closer to 0.1 is usually observed. Additional evidence of the difference in character of the high  $\Phi$  smoke compared to the low  $\Phi$  smoke was obtained from electron micrographs of the ethene smoke collected at  $\Phi = 4$  and  $\Phi = 1$ . In both cases the smoke was observed to have an agglomerated structure, however, at  $\Phi = 4$  the agglomerate appeared to be agglutinated, indicating the presence of a liquid-like component.

The peak CO yields for methane and ethene differ only by 20%, while the peak smoke yields differ by about a factor of five. This result that the CO and smoke yields seem uncorrelated for underventilated burning differs markedly from the strong correlation between CO and smoke yields for overventilated burning observed for gaseous hydrocarbons [1] and for plastics and lumber [6].

**Summary:** An investigation of the generation of CO and smoke for underventilated laminar diffusion flames has revealed both strong similarities and differences with studies considering overventilated conditions. In particular, the proportionality between smoke yield and CO yield observed for the post-



flame (overfire) region of overventilated flames for a wide range of fuels is not found to be valid for the underventilated case. In fact, the soot observed in the underventilated flames is observed to vary considerably in terms of the chemical structure from that typically observed in overventilated flames. The highly organic nature of the soot implies that the structure of the soot may be more similar to early agglutinated soot particles recently observed in diffusion flames than to the more aged aggregates typical of the post-flame region for overventilated flames. Based on additional results, comparisons in terms of the ratio of CO and CO<sub>2</sub> as a function of global equivalence ratio in the post-flame region of the underventilated flames show a similar behavior to that previously observed for in-flame measurements for both overventilated and underventilated diffusion flames which examined the dependence of this ratio on local equivalence ratio conditions. This suggests that for the in-flame fuel-rich region, the chemical environment excluding soot is correlated with equivalence ratio in a similar way for both an overventilated flame and an underventilated flame. The low production of CO in the post-flame region of overventilated flames is simply a result of the oxidation of CO to CO<sub>2</sub> in the upper region of these flames. Finally, the present studies illustrate the utility of the study of underventilated flame environments where product yields and trends can be quite different from overventilated conditions. These studies should have significance for combustion phenomena in which underventilated conditions are typical, such as in fires.

Acknowledgement: The work done at The Pennsylvania State University was supported under grant 60NANB0D1035 from the National Institute of Standards and Technology.

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TABLE 1

Organic and Elemental Carbon Analysis

Methane 10 cm <sup>3</sup> /s					
$\Phi$	Organic Carbon $\mu\text{g}/\text{cm}^2$	Organic Carbon Error	Elemental Carbon $\mu\text{g}/\text{cm}^2$	Elemental Carbon Error	Organic/Elemental
1	1.0	0.2	21	1	0.05
2	8.4	0.5	4.9	0.3	1.7
4	3.4	0.3	0.4	0.1	8.5
4	5.2	0.4	1.0	0.2	5.2

Ethene 6.4 cm <sup>3</sup> /s					
$\Phi$	Organic Carbon $\mu\text{g}/\text{cm}^2$	Organic Carbon Error	Elemental Carbon $\mu\text{g}/\text{cm}^2$	Elemental Carbon Error	Organic/Elemental
0.50	0.7	0.1	19	1	0.04
1	1.3	0.2	27	1	0.05
2	7.2	0.5	15	0.9	0.48
4	7.0	0.5	6.2	0.4	1.13

BUILDING AND FIRE RESEARCH LABORATORY  
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FY 94

**Institution:** The George Washington University

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**Grant Title:** Fundamental Studies of Diffusion Flame Chemistry

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**Technical Abstract:**

This year our work was divided into three projects, two of which were continuations of work begun in prior funding years and the third marking a new experimental program. Given the space limitations of the current document, only a briefly summary of progress made in each of these projects will be presented here.

*Validation of the Conserved Scalar Relationship in Laminar CH<sub>4</sub>/Air Diffusion Flames*

State relationships for temperature and species concentrations as functions of one (mixture fraction,  $\xi$ )<sup>1,2</sup> or two (mixture fraction and scalar dissipation,  $\chi$ )<sup>3</sup> scalar variables have been extensively investigated for laminar and turbulent flames in order to create libraries for these correlations. These efforts resulted in the establishment of the laminar flamelet concept<sup>3</sup> which allows the decoupling of chemistry and fluid mechanics during non-premixed combustion. This concept is based upon the hypothesis that the chemical production rates for each species and thermal energy are locally balanced by the diffusive transport rate in the direction which is orthogonal to the mixture fraction isopleths. Bilger proposed that individual species conservation equations could be written as

$$w_i = -\frac{1}{2} \rho \chi \left( \frac{\partial Y_i}{\partial \xi} \right)$$

Equation 1

<sup>1</sup> R.W. Bilger, *Combust. Flame* 30, 277-284 (1977).

<sup>2</sup> Y.R. Sivathanu and G.M. Faeth, *Combust. Flame* 82, 211-229 (1990).

<sup>3</sup> N. Peters, *Twenty-First Symposium (International) on Combustion.*, p. 1231 (1988).



where is the scalar dissipation rate, and  $Y_i$  is a species' concentration expressed as mass fraction.

Utilizing this hypothesis, species mass and energy conservation equations can be reduced to a spatially-invariant form where the mixture fraction is an independent scalar variable and the scalar dissipation is a parameter which, in general, may vary across the reaction zone. Despite some recognized limitations, the flamelet approach is widely utilized for turbulent flames modeling. However, several important questions have not been fully addressed:

- What role does the differential diffusion of different flame species have in the applicability of Eq. 1?
- Does the data collected in (or calculated for) laminar flames sample enough of  $(\chi, \xi)$  space to be useful for turbulent combustion models?

In this past year the results of direct numerical calculations for laminar axisymmetric methane/air diffusion flame were used to test Eq. 1. The original calculations were done for an unbounded coflowing flame where fuel was introduced into the flame through an inner tube of radius 0.2 cm with the inlet velocity 35 cm/s and the coflow air through a concentric tube of radius 2.5 cm with the same inlet velocity. The reaction mechanism included 83 reversible reactions and 26 species including  $C_1$  and  $C_2$  chemistry. Different diffusivities were utilized in this calculation for the temperature and each species. We showed that Eq. 1 worked well for major species whose diffusivities were close to that of the mass-averaged mixture, but less well for minor species such as hydrogen atom which diffuse significantly faster than the mixture. Recently, we have further quantified this effect and explored the relative importance of the inclusion of differential diffusion into Eq.1 and transport along mixture fraction isopleths.

To illustrate the importance of differential diffusion the magnitude of  $w_i$  calculated from transport rate (Eq. 1) has been compared with the chemical production rate calculated from chemical kinetics for various flame species. For major species such as methane little improvement in the correlation between these two quantities is apparent when using the specific diffusivity for methane as opposed to that for the mixture as a whole. However, for hydrogen atom, which diffuses much faster than the average flame mixture component, a considerably more accurate approximation to net chemical production rate results from the use of the species-specific diffusion coefficient in the conserved scalar species conservation equation (Eq. 1).

The strong correlations between chemical production and transport terms which are found for both methane and H atom suggests the validity of the flamelets hypothesis for these coflowing laminar diffusion flame. Our conclusion may also explain the excellent agreement found between the results of calculations for axisymmetric flames and measurements in a two-dimensional flame supported on a Wolfhard-Parker burner. These experimental and calculated profiles were matched for heights in the flame where  $\chi(\xi)$  profiles were similar and differential diffusion effects as well as the effects of transport along mixture fraction isopleths would also be approximately the same in magnitude.

#### *Tunable diode laser absorption spectroscopy measurements of Carbon Monoxide Concentrations in Ethylene/Air Diffusion Flames*

Tunable diode laser absorption spectroscopy has been used to map carbon monoxide concentrations and temperature in a series of laminar ethylene/air, axisymmetric diffusion flames. Early studies in these flames by Santoro and coworkers have provided quantitative information on the formation, growth, and burnout of soot particles<sup>4</sup> and was later extended to include measurements of temperature and velocity<sup>5,6</sup>. In a later study,

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4. R.J. Santoro, H.G. Semerjian, and R.A. Dobbins, *Combust. and Flame*, 51, 203-218 (1983).

5. R. J. Santoro, T.T. Yeh, J.J. Horvath, and H.G. Semerjian, *Combust. and Sci. and Tech.*, 53, 89-115(1987).

6. P.R. Soloman, P.E. Best, R.M. Carangelo, J.R. Markham, and PO-Liang Chien, and R.J. Santoro and H.G. Semerjian, *Twenty-First Symposium (International) on Combustion*, The Combustion Institute, Pittsburg, 1986, p1763-1771.

temperatures were measured in the ethylene flames using Coherent Anti-Stokes Raman Spectroscopy (CARS)<sup>7</sup>. Both of these studies observed a decline in flame temperatures near the tip as soot loading increased. More recently, measurements of hydroxyl radical concentrations were made which allowed for the quantitative assessment of soot oxidation processes<sup>8</sup>.

In our work temperatures at the tip of the flames were found to decrease as the quantity of soot increased. Carbon monoxide concentration profiles were also found to depend on soot levels in the flames, with the most dramatic differences apparent along the centerline above the stoichiometric surface. These measurements were combined with literature data to calculate oxidation rates for both particles and carbon monoxide. It was found that the oxidation rate for CO low in the flames was faster than that at the tip, attributable to both lower temperature and hydroxyl radical concentrations. Further, soot particle oxidation, which is believed to form CO, is slightly faster in non-smoking and incipient smoking flames; in the smoking flame the soot oxidation rate becomes almost twice that of CO's, thus leading to carbon monoxide emission.

### *The Oxidation of Smoke above Flames*

In fires, the concentrations of soot and carbon monoxide are found to be strongly correlated<sup>9</sup> and a significant fraction of the CO emitted from fires is believed to originate from soot particle oxidation. There have been a number of studies of particle oxidation within flames<sup>10, 11, 12</sup> and in shock tubes<sup>13, 14</sup>, but little research on post-flame oxidation<sup>15, 16</sup>. We have recently initiated a study of the transformation of post-flame smoke with an emphasis on the chemical transformation of surface-adsorbed polynuclear aromatic hydrocarbons and the subsequent formation of gas phase molecular oxidation products.

In our studies we use a burner which consists of a central fuel tube that is 1/4 inch diameter surrounded by a ~3/4 inch diameter air co-flow tube to stabilize the flame. This burner is fitted into a 1 inch diameter sleeve which allows for vertical movement of up to 3.5 inches. There is a six way cross above the burner region which allows for optical and/or probe sampling of either the flame or immediate post-flame gases. A 1 inch diameter, 25 inch long quartz tube is enclosed by a tube furnace which operates at 400 - 1500 degrees Celsius. Above this is another six way diagnostics cross. The test sections are equipped to perform a variety of optical and/or extractive sampling diagnostics.

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<sup>7</sup> L.R. Boedeker, G.M. Dobbs, *Combust. and Sci. and Tech.*, **46**, 301-323 (1986).

<sup>8</sup> R. Puri, M. Moser, R.J. Santoro, and K.C. Smyth, *Twenty-Fourth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, 1992, 1015-1022.

<sup>9</sup> Köylü, U., and Faeth, G.M., "Soot Emission from Liquid Fueled Buoyant Turbulent Diffusion Flames," *Combustion and Flame*, **87**, 61-76 (1991).

<sup>10</sup> Puri, R., Santoro, R.J. and Smyth, K.C., "The Oxidation of Soot and Carbon Monoxide in Hydrocarbon Diffusion Flames," *Combustion and Flame*, **97**, 125-144 (1994).

<sup>11</sup> Santoro, R.J., Yeh, T.T., Horvath, J.J. and Semerjian, H.G., "The Transport and Growth of Soot Particles in Laminar Diffusion Flames," *Combustion Science and Technology*, **53**, 89-115 (1987).

<sup>12</sup> Megardis, C.M. and Dobbins, R.A., "Comparison of Soot Growth and Oxidation in Smoking and Non-Smoking Ethylene Diffusion Flames," *Combustion Science and Technology*, **66**, 1-16 (1989).

<sup>13</sup> Park, C. and Appleton, J.P., "Shock-Tube Measurements of Soot Oxidation Rates," *Combustion and Flame*, **20**, 369-79 (1973).

<sup>14</sup> Roth, P., Brandt, O. and Von Gersum, S., "High Temperature Oxidation of Suspended Soot Particles Verified by CO and CO<sub>2</sub> Measurements," *Twenty Third Symposium (International) on Combustion*, The Combustion Institute, 1485-1491 (1990).

<sup>15</sup> Noirot, R., Gilot, P., Gadiou, R., and Prado, G., "Control of Soot Emission by Filtration and Post-Combustion. A Laboratory Study of the Regeneration of an Organic Particulate Trap Assisted by Hydrocarbon Injection," *Combustion Science and Technology*, **95**, 139-160 (1994).

<sup>16</sup> Schug, K.P., Manheimer-Timnat, Yaccarino, P. and Glassman, I., "Sooting Behavior of Gaseous Hydrocarbon Diffusion Flames and the Influence of Additives," *Combustion Science and Technology*, **22**, 235-50 (1980).



Because the system is fully enclosed, it is possible to vary the global equivalence ratio,  $\phi_{\text{GLOBAL}}$ , within the furnace. In our preliminary work, we have been able to vary  $\phi_{\text{GLOBAL}}$  from overventilated to slightly underventilated. With ethylene as a fuel we have observed soot volume fractions above the flame in the range of 1-10 ppm, with the highest values observed for  $\phi_{\text{GLOBAL}} = 1$ . For all stoichiometries, the soot volume fraction measured above the tube furnace was found to decrease with furnace temperature. The soot volume fraction is shown on the figure below. We are currently analyzing this data to extract kinetic information for soot oxidation.

**Publications during this reporting Period:**

"The Structure of axially-symmetric diffusion flames: computations and optical diagnostics"

R. Reed Skaggs, Khanh N Le, J. H. Miller, D R. Honnery, and J.H. Kent  
 Combustion Fundamentals and Applications (1993) pp167-170.

"Tunable Diode Laser Diagnostics in Ethylene/Air Axially-symmetric Diffusion Flames"

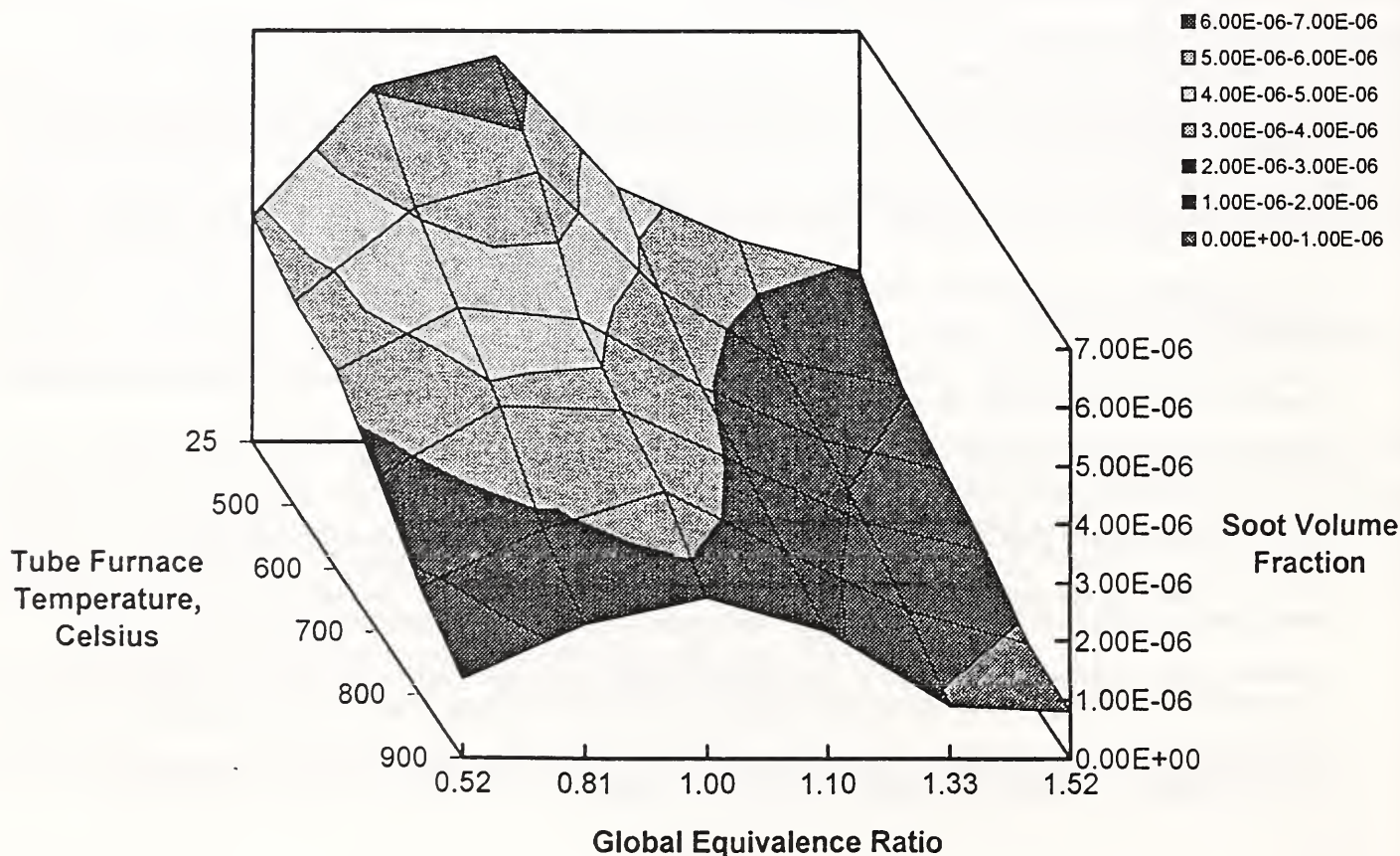
R. Reed Skaggs and J.H. Miller, Combust. Flame, in press.

"The Validation of the Conserved Scalar Relationship in Laminar CH<sub>4</sub>/Air Diffusion Flames."

M.A.T. Marro and J.H. Miller, Chemical and Physical Processes in Combustion (1993), p. 279

"Tunable Diode Laser Absorption Detection of Polyatomic Species in Hydrocarbon Diffusion Flames: Some Cautions and Measurement Strategies."

M. Tolocka and J.H. Miller, Microchemical Journal, in press.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

STUDY OF SMOKE AGGLOMERATES

Funding Agency

National Aeronautics and Space Administration, NASA Headquarters, Solar System Exploration Division

Professional Personnel

George W. Mulholland, Principal Investigator  
Raymond D. Mountain, Co-Principle Investigator  
Nelson Bryner, Chemical Engineer

Objective

To test the validity and utility of fractal concepts in describing the growth and properties of large smoke agglomerates.

Technical Accomplishments

The differential scattering component of the Large Agglomerate Optics Facility has been fabricated. The facility consists of a 10 cm diameter by 100 cm long optical cell for studying the properties of smoke agglomerates as they grow. The acceptance angle of the detector is limited to  $\pm 0.3^\circ$  allowing accurate small angle scattering measurements. In a series of preliminary measurements with a co-annular acetylene burner, the fractal dimension was obtained from light scattering measurements at large angles and the radius of gyration was obtained from the small angle scattering measurements. Substantial design development was required to overcome reflections from the cell, three orders of magnitude variation in scattering signal, and angle dependent scattering volume. From a theoretical analysis of light scattering by agglomerates, estimates were obtained for the validity of the Rayleigh-Debye method for computing the fractal dimension and the radius of gyration of the agglomerate. The computational method also suggests a direct optical measurement of the primary sphere size.

## Reports and Publications

G.W. Mulholland and N.P. Bryner, *Atmospheric Environment* 28, 873 (1994). Radiometric Model of the Transmission Cell-Reciprocal Nephelometer.

G.W. Mulholland, C.F. Bohren, and K.A. Fuller, accepted by *Langmuir*. Light Scattering by Agglomerates: Coupled Electric and Magnetic Dipole Method.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

STUDY OF HEAT AND SMOKE MOVEMENT  
AND THEIR INFLUENCE ON DETECTOR AND SPRINKLER RESPONSE  
IN ENCLOSED SPACES WITH COMPLEX CEILING GEOMETRIES

Funding Agency

National Fire Protection Research Foundation

Professional Staff

Richard W. Bukowski, Project Leader  
Glen Forney  
William Davis

Project Objective

To examine the effect of complex ceiling geometry and obstructions on the distribution of heat and smoke in order to optimize requirements for automatic fire detector location found in NFPA 72E and for automatic sprinklers as covered by NFPA 13, 13D, and 13R.

Technical Accomplishments

At present, recommendations for the placement of automatic fire detectors found in the NFPA Standard on Detection Devices (72E) are based either on engineering judgement or on experiments done by Heskestad and Delichatsios on flat, unobstructed ceilings. In the implementation of these data, tables and curves were developed from calculations with a zone model which are also only applicable for flat, unobstructed ceilings. Since 72E includes recommendations for placement of fire detectors in spaces with sloping or peaked ceilings, or with open beams and joists, some validation of these recommendations is necessary. Further, detector siting problems associated with stratification and high air movement from HVAC systems are mentioned in the standards, but only limited installation guidance is provided which are based only on judgement.

In the first year of this planned four year effort, the use of CFD models was validated by reproducing the results of full-scale experiments conducted a decade ago by Heskestad and Delicatsios. Parametric studies were then conducted on a set of independent variables including fire size, ceiling height, beam depth and spacing, and room volume, and constant response surfaces were plotted for the principal types of fire sensors. FY94 represented the second year of the project in which ceiling slope (up to a pitch of 15/12) was added as another independent variable.

In a "special case" study the question of the size of the gap between a single obstruction and the ceiling such that the obstruction need not be considered in the sensor placement was addressed. As was done for the first year, the technical report will go beyond reporting



research results by including suggested wording for changes to the standards based on the results.

Reports and Publications

Forney, Glenn P., Bukowski, Richard W., and Davis, William D., Field Modeling: Effects of Flat Beamed Ceilings on Detector and Sprinkler Response, International Fire Detection Research Project Technical Report (year 1), Nat. Fire Prot. Research Foundation, Quincy, MA 02269 (1993).

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

REAL-TIME SUPPRESSANT CONCENTRATION MEASUREMENT

Funding Agency: Departments of Air Force, Navy, and Army and FAA

Professional Personnel: William M. Pitts, Project Leader  
Brett D. Breuel, Mechanical Engineer  
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Michael P. Glover, Technician  
David Hess, Research Engineer  
Richard H. Harris, Jr., Chemist  
Erik L. Johnsson, Mechanical Engineer  
George W. Mulholland, Research Chemist  
Michael R. Smith, Technician

Project Objective

To evaluate possible methods for real-time measurement of concentrations of alternative fire fighting agents for dry bay and nacelle applications. If one or more feasible approaches are identified early in the investigation, a demonstration system will be developed for characterization under actual test conditions.

Scope

The U. S. Air Force is coordinating the search for alternative fire fighting agents for dry bay and nacelle fires on aircraft. They have narrowed their search to four candidates--HFC-227, HFC-125, FC-218, and CF<sub>3</sub>I. A method is required for measuring real-time concentrations of these agents during full-scale nacelle and dry bay tests. Existing measurement techniques do not have the required temporal resolution.

The effort is broken down into two major parts. The first is a search of the measurement literature to identify possible methods for concentration measurement, in addition to those to be tested under the current plan, which might meet the needs of the Air Force. The second is the testing and characterization of two instruments--a differential infrared broad-band absorption device developed under an Air Force SBIR and supplied to NIST by the Air Force and an aspirated hot-film concentration probe used for qualitative flow characterization during last year's effort on agent screening. Provision is included for testing one of the instruments in Wright Patterson's full-scale test facilities if one of the techniques appears to be viable.

Technical Accomplishments

The original project plan only provided for NIST to perform an assessment of two existing instruments--a commercial aspirating hot-film concentration probe and a prototype instrument developed by John Brown Associates, Inc. based on infrared absorption which was supplied by the sponsor. However, it was quickly determined that both instruments, as delivered, could not provide

the required measurement capability. The decision was made to make modifications to both instruments and to try to improve their capabilities.

The following sections describe progress thus far.

## 1. Aspirated Hot-Film

A hot-film anemometer is a device designed to measure the heat loss from a small heated cylinder when placed in a fluid flow. The heat loss depends on a number of parameters including flow velocity, temperature difference between the sensor surface and the surroundings, fluid pressure, thermal conductivity of the fluid passing over the sensor, and the geometry of the sensor.

Hot-films are normally used to measure velocity in uniform gases by calibrating in a known flow field and characterizing the response of the hot-film to the unknown flow field. However, if the velocity of the flow over the sensor is held constant, the sensor is sensitive to flow composition due to variations in the thermal conductivity of the fluid with composition. In an aspirated hot-film the gas is drawn through a small tube into a narrow orifice. When the downstream pressure is sufficiently low, the orifice becomes sonically choked and the flow through the orifice is independent of upstream velocity at the sampling port. The choked mass flow rate still depends on upstream temperature and pressure. A hot-film placed in such a flow is expected to be subjected to a constant velocity and thus should only be sensitive to composition changes assuming the ambient pressure and temperature are unchanged. It had been previously demonstrated that these probes are capable of accurate concentration measurements with excellent temporal and spatial resolution in a number of binary gas flows .

In considering the application of these probes for agent concentration measurements a problem immediately became apparent. The agents, which are gases at room temperature, are normally released as high-pressure liquids which undergo rapid vaporization and cooling. As a result, temperature variations are to be expected when measuring concentration. As noted above, the sensor responds to temperature variations and this sensitivity interferes with the concentration measurement.

In order to overcome the sensitivity of the probe to temperature, a modified probe was developed which incorporated a cold wire to directly record the temperature. A cold wire is essentially a resistance thermometer. The temperature is determined by passing a small constant current through the device which gives a voltage proportional to temperature.

It is necessary to calibrate the cold wire as a function of temperature and the aspirated hot-film as a function of both temperature and concentration of a gas in a mixture of two gases. Once these calibrations are available it is possible to make measurements in unknown mixtures of the two gases where the temperature is varying.

A special system was designed and constructed which is capable of delivering specified agent/air mixtures at variable temperatures. Figure 1 shows calibrations for the aspirated hot-film as functions of concentration and temperature for mixtures of FC-218 and air. Figure 2 shows the response of the cold wire to temperature variations. Using these two sets of calibrations the concentration for unknown air/FC-218 mixtures can be determined over a wide temperature range.

Testing revealed an unexpected problem with the application of these probes for concentration measurement. The probe incorporates a choked sonic orifice which is designed to control the mass flow rate and hence provide a constant velocity over the hot-film sensor for a given concentration. Excellent velocity control is required since the hot-film sensor not only responds to temperature and composition changes, but is also sensitive to velocity changes. It was found that the probe was sensing turbulent velocity fluctuations. This result was a complete surprise since there are a number of papers in the literature which have used identical probes for concentration measure-



ments and have not reported a velocity sensitivity. A full understanding of the cause of the velocity sensitivity is still not available.

The response to velocity is a problem because it results in a fluctuating voltage output which is interpreted as concentration changes in the analysis procedure and ultimately degrades the signal-to-noise ratio for the measurement. Such fluctuations significantly increase the uncertainty in a measurement of agent concentration.

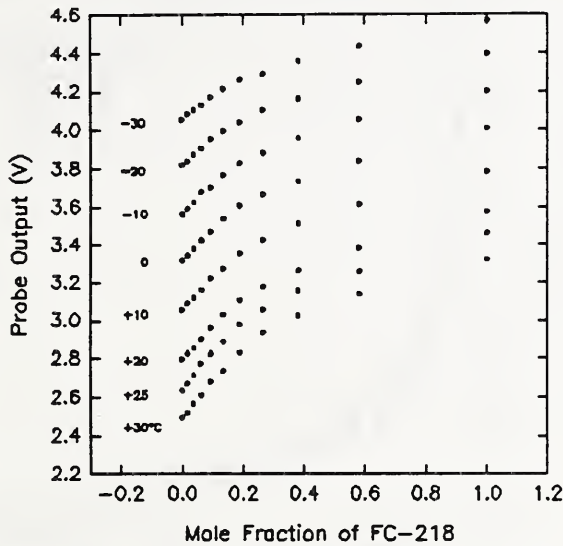


Figure 1 Calibration results for the aspirated hot-film are shown as a function of temperature and FC-218 mole fraction.

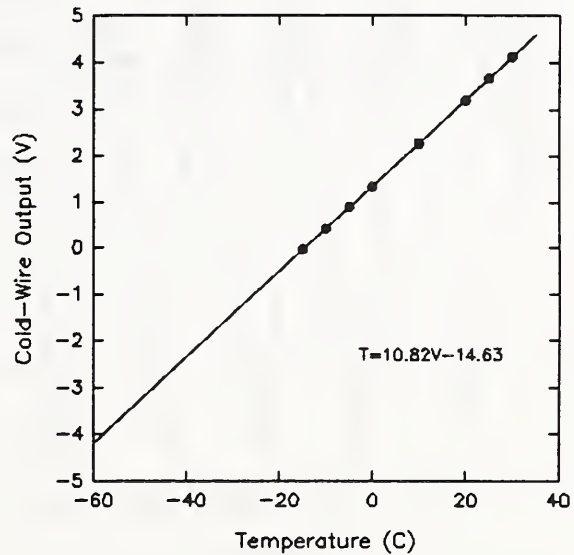


Figure 2 Calibration of the cold-wire for variations in temperature.

Work is underway to characterize the effects of the velocity sensitivity on the accuracy of the concentration measurements and to see if the probe can be redesigned to mitigate its effects.

## 2. Infrared Sensor

The performance of the Fire Extinguishment Agent Sensor (FEAS) developed by John Brown Associates, Inc. was evaluated in regard to its suitability for monitoring the concentration of candidate halon replacement agents during large-scale tests. Two major issues were its response time and the concentration sensitivity of the sensor.

The instrument operated much like a single-pass infrared absorption spectrometer. Thermal radiation from a heat source (filament with a current passing through it) was allowed to pass through an open volume. The light was then filtered by a narrow band-pass filter centered at  $8.654 \mu\text{m}$  (corresponding to the strong C-F stretch absorption band for the agents) and detected by a pyroelectric detector. Subsequent amplification yielded a voltage signal proportional to the infrared intensity reaching the detector. The absorption of infrared radiation by agent in the observation volume leads to a reduction in the intensity detected by the pyroelectric.

In order to evaluate the instrument supplied by the Air Force, a chopper was placed in the observation volume and the response of the device was recorded as a function of the chopper frequency using a storage oscilloscope. The sensor was found to respond to changes over a narrow frequency range of about 2 - 100 Hz. The maximum frequency response was roughly a factor of ten less than the desired value of 1 kHz. The observed voltage outputs as a function of frequency had

a maximum around 10 Hz and fell off sharply on either side of this frequency, instead of having the flat response required for absorption measurements.

The basis of operation of a pyroelectric detector is that it possesses a spontaneous polarization in the absence of an applied field. This polarization is a function of temperature. Thus a temperature change due to infrared energy radiation striking the surface produces a change in the polarization, which in turn produces a current flow. One difficulty in calibrating the sensor is that it is only sensitive to a change in temperature; that is, for a constant illumination the sensor

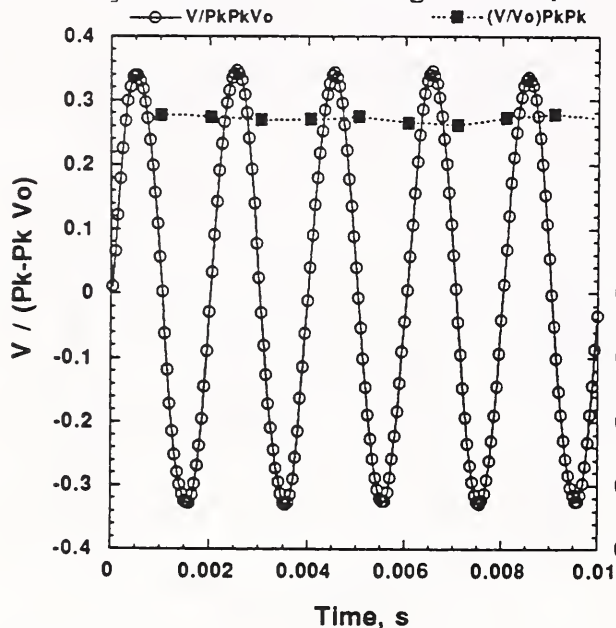


Figure 3 Real time voltage and peak-to-peak voltage versus time for a 10% HFC-125/air mixture.

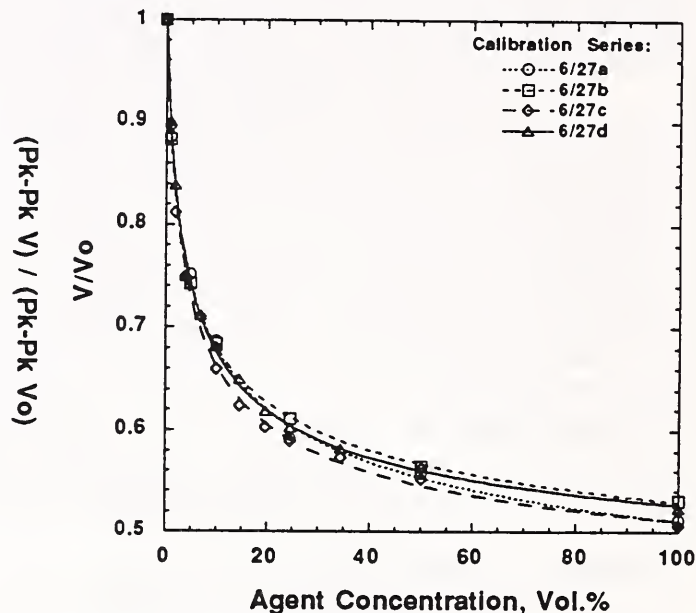


Figure 4 Calibration curves (four repeats) for voltage ratio versus HFC-125 concentration.

temperature is constant so there is no current flow and no signal. This is the reason for the observed behavior of the Air Force-supplied instrument.

Analysis indicated that it would be possible to substantially modify the instrument and create a system which would meet the design goals. To overcome the limitations in the FEAS design, the following changes were made: replacing the 1 mm detector with a 5 mm detector, use of an improved amplifier, focusing the IR source on the detector to improve sensitivity, and using a broader bandpass filter. The most important modification was to incorporate a chopper in the light path operating at 500 Hz. This chopper provided differential detection where the output signal became time varying and the signal amplitude was proportional to the infrared intensity reaching the detector. Measurements could be recorded every half cycle or at a rate of 1000 Hz.

Figure 3 illustrates the amplified voltage output from the pyroelectric sensor recorded by the computer with the chopper operating at 500 Hz and the computer acquiring data at 20,000 Hz. The agent concentration is 10% by volume and the signal is normalized by the signal in air. The peak-to-peak signal is derived from the periodic signal and is also plotted.

The voltages are normalized by the peak-to-peak values for air. The IR device was calibrated using 12 different air-agent concentrations over the range 0 to 100% HFC-125. The calibration curve has a hyperbolic shape with approximately 50% attenuation of the IR beam at 100% concentration of agent (see Figure 2).

The variation in successive peak-to-peak values determines the uncertainty in the concentration measurement. The  $\sigma$  for the ratio of the peak-to-peak value of the 10% mixture to the value

for air,  $V/V_0$ , for the data shown in Fig. 1 is 0.0041. This value of  $\sigma$  is typical of values measured for other concentrations.

The modified instrument appears very promising for measuring agent concentrations. Efforts to characterize its operation and evaluate its accuracy and precision are continuing.

Reports and Publications: Series of monthly reports to the sponsor.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

DYNAMICS OF FIRE SUPPRESSION

Professional Personnel

Gregory T. Linteris, Project Leader  
Grzegorz Gmurczyk  
Arnold Liu  
Michelle King

Project Objective

To provide a fundamental understanding of the action of inert and chemical flame inhibitors to the fire protection community to enable the development of the next generation of suppression agents and technologies.

Scope

Halogenated hydrocarbons are effective and widely used as fire suppressants. However, because of their suspected destruction of stratospheric ozone, the production of these agents, the most popular being Halon 1301 ( $\text{CF}_3\text{Br}$ ), will be discontinued in 1994. There exists a need to develop alternatives to the Halons, to establish the relative effectiveness of alternative inhibitors, and to understand the mechanism of inhibition of existing agents as well as agents which show extraordinary inhibitory effects.

Technical Approach

Despite their widespread use, and notwithstanding the abundant experimental information on the quantities of inhibitors necessary to inhibit and extinguish flames, surprisingly little is known about the fundamental mechanisms by which some widely used suppressants work. Consequently, efforts to optimize the delivery and effectiveness of existing suppressants are limited. It is believed that improving the fundamental understanding of extinction and suppression will facilitate the development of more effective delivery systems and agents and provide a basis for comparison of alternative suppressants. The approach in this project is to study the chemical and physical mechanisms of existing suppressants through detailed flame structure measurements in a laboratory scale burners to establish the relationship between the characteristic times of the chemistry and fluid dynamics. In order to understand the simultaneous thermodynamic, fluid mechanic and chemical kinetic effects of the inhibitors, the experimental results will be interpreted through numerical calculations of the flame structure using existing well developed codes. These experimental and modelling results should lead to a unified method of describing, and an improved fundamental understanding of the mechanisms of flame inhibition, extinction, and stabilization relevant to the advanced suppression of fires. This combined numerical and experimental examination of the action of flame inhibitors is being performed for the widely used inhibitor  $\text{CF}_3\text{Br}$  to serve as a baseline, as

well as for chemicals such as  $\text{CF}_3\text{H}$  which are representative of those likely to be used in the near future as  $\text{CF}_3\text{Br}$  replacements. In addition, the mechanism of several highly effective chemicals, such as  $\text{TiCl}_4$  and  $\text{Fe}(\text{CO})_5$  will be studied to provide information on their mode of action. This information may provide insights into approaches for developing new agents or techniques with vastly improved flame inhibition properties.

### Technical Accomplishments

Halogenated agents have been and will remain for some time the most commonly used chemical flame inhibitors. Consequently, one of the goals of the early stages of this project is to understand the mechanisms of halogen (principally Br, I, and F) inhibition of hydrocarbon flames. The research in the past year has started with measurements and modeling of premixed flames. These experiments are being conducted in concert with continued development of a chemical kinetic model of halogen inhibition. The fluorinated mechanism is being examined first since fluorine inhibition is a sub-mechanism of  $\text{CF}_3\text{Br}$  inhibition (the  $\text{CF}_3$  radical contributes to the inhibition by Br atoms for agents such as  $\text{CF}_3\text{Br}$ ). It is best to first gain confidence in the fluorine sub-mechanism before proceeding to a larger mechanism containing Br or I; likewise, premixed flames are studied first since their structure is simpler and more easily calculated and interpreted than those of inhibited diffusion flames. It should be noted that there is great synergism between this project and the other-agency project on HF formation in flames inhibited by halogenated hydrocarbons. Tests have also been initiated to study the mechanism of inhibition of  $\text{Fe}(\text{CO})_5$ . Although iron pentacarbonyl has been found to be among the best flame inhibitors ever discovered, its mode of inhibition has never been clearly delineated.

#### 1. Burning Rate Measurements

The premixed laminar burning velocity is a fundamental parameter describing the overall reaction rate, heat release, and heat and mass transport in a flame. In addition, the reduction in the premixed flame burning rate is useful for understanding the mechanism of chemical suppression of fires since diffusion flames often have a stabilization region which is premixed, and good correlation has been found between the reduction in burning rate and the concentration of inhibitors found to extinguish diffusion flames. Premixed flame burners have flow fields which are relatively easily characterized, making interpretation of the inhibitor's effect on the overall reaction rate straightforward. For these reasons, the laminar burning velocity has traditionally been one of the first parameters to measure in assessing the effectiveness and the chemical mechanism of flame inhibitors. The reduction in the laminar burning velocity is not as burner and flow-field dependent as the extinction concentration (for diffusion flames) and does not simultaneously include the effects of agent transport. Consequently, from a fundamental perspective, it is a more useful parameter for comparing the chemical effectiveness of agents. In addition, the burning velocity is the first parameter to compare when testing a chemical kinetic mechanism. Matching the burning rate, although not a sufficiently stringent test of a mechanism, can be considered an essential requirement of a mechanism. If the burning rate is wrong, it is unlikely that any other calculated parameter will be correct.

A Mach-Hebra converging nozzle burner amenable to flame speed measurements has been constructed and integrated with a computer controlled flow control system. The burner produces bunsen-type premixed flames with a co-flowing shroud gases whose velocity and composition can be



controlled. The nozzle shape provides straight-sided bunsen cones which have a well characterized flow field, making flame speed determination either by the total area method, cone angle method or by LDV measurements straightforward. A schlieren system was designed and built and integrated with a video-based digital image processing system so that both visible and schlieren images could be captured in real time.

Data have been obtained for methane-air flames for values of the fuel-air equivalence ratio  $\phi$  from 0.9 to 1.1. Burning rate data have been obtained for  $N_2$ , for the single carbon agents  $CF_4$ ,  $CF_3H$ ,  $CH_2F_2$ ,  $CF_3I$ ; for the two carbon agents  $C_2HF_5$ ,  $C_2H_2F_4$ ; and for  $C_3HF_7$  and  $C_3F_8$ . The gas velocities above the Mache-Hebra nozzle burner were measured with the PDPA used as a LDV. Data were obtained for cold flow and for a methane-air flame with and without inhibitor as a function of height above the burner. Temperature measurements were performed with coated fine-wire thermocouples of two diameters to obtain estimates of the gas temperature corrected for radiation losses, and calculations were performed of the adiabatic flame temperatures of these inhibited flames. In addition, numerical calculations of the structure of the premixed flames have been performed using a hydrocarbon mechanism with fluorine inhibition obtained from Chemical Science and Technology and Chemical Kinetics divisions at NIST. The measured burning rates for the inhibited flames were found to be in good agreement with the predictions of the numerical calculations, providing added confidence in the mechanism. These data represent the first burning rate values ever measured for these agents. The details of the inhibition mechanism are being studied; however, it is now clear that the inhibitors are not inert, and that the amount of reduction in the burning rate is greater than if they were. It will be possible in the near future to obtain valuable insights into the precise chemical mechanisms of inhibition of these agents.

## 2. Extraordinary Inhibitors

There exist some categories of inhibitors (for example organometallics and metal halides) that reduce the burning rate of premixed flames up to two orders of magnitude better than  $CF_3Br$ . While the effectiveness of these inhibitors has been known for decades, there is no conclusive explanation of their mechanism of inhibition. Experiments have been initiated to understand their behavior. An enclosed counterflow diffusion flame has been constructed suitable for measurements of the extinction strain rate of methane-air flames seeded with these compounds. Results will be available soon.

### Publications

Linteris, G.T., and Truett, L.F., "Burning rates of premixed methane-air flames inhibited by fluorinated hydrocarbons," Halon Options Technical Working Conference, Albuquerque, NM, May 3-5, 1994.

Linteris, G.T., King, M.D., Liu, A., Womeldorf, C., and Hsin, Y.E., "Acid gas production in inhibited diffusion flames," Halon Options Technical Working Conference, Albuquerque, NM, May 3-5, 1994.

Seshadri, K., and Ilincic, N, "The asymptotic structure of nonpremixed methane-air flames with oxidizer leakage of order unity," submitted for publication in *Combustion and Flame*, Feb., 1994.

Seshadri, K., and Ilincic, N, "The asymptotic structure of inhibited nonpremixed methane-air flames," submitted for publication in *Combustion and Flame*, April, 1994.

### Related Grants

"Chemical Inhibition of Methane-Air Diffusion Flames," K. Seshadri, University of California, San Diego.

"Basic Research on Fire Suppression," A. Atreya, University of Michigan.

**BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY 94**

Institution: The University of Michigan

Grant Number: 60NANB2D1293

Title: BASIC RESEARCH ON FIRE SUPPRESSION

Principal Investigators: Dr. Arvind Atreya  
Department of Mechanical Engineering and Applied Mechanics  
The University of Michigan; Ann Arbor, MI 48109-2125

Other Professional Personnel: Todd Crompton (M. S. candidate) & Jaeil Suh (Ph.D candidate)

NIST Scientific Officer: Dr. William Grosshandler

**TECHNICAL ABSTRACT:**

INTRODUCTION:

Fire suppression severely lacks quantitative results on the amount of agent required and the application rate needed to suppress fires and prevent their re-ignition. As a result, little comparison between various agents is possible. Also, qualitatively the suppression actions of various agents are known (such as cooling of the condensed-phase, isolation of fuel and oxidizer, etc.) but the quantitative details of the mechanisms responsible for the agent's action are not well known. Even for water, there is little quantitative understanding regarding the extinguishment mechanisms. Thus, it has not been possible to determine how much water is actually required and what should be the application strategy. The amount of water used is often about two orders of magnitude larger than that needed in controlled laboratory experiments. Most importantly, there does not exist a scientific basis for comparing the suppression effectiveness of various suppression agents. This prevents development of new, perhaps more efficient, suppression agents and application strategies. Thus, as a first step, this work attempts to provide a quantitative understanding of the chemical and physical mechanisms of fire suppression by water through an integrated approach of small-scale experiments and theoretical models.

Water is known to have two physical effects: (i) cooling of the burning solid by water evaporation, and (ii) smothering caused by dilution of the oxidizer and/or the fuel by water vapor. In addition to these two well known effects, there are three more effects, namely: (iii) enhanced radiative heat loss due to increased water concentration, (iv) enhanced mixing as a result of volumetric expansion caused by water evaporation, and (v) a little known but significant chemical enhancement effect which reduces the soot concentration and decreases the luminous flame radiation. Our experiments show that the last two effects considerably increase the combustion efficiency and reduce the suppression effectiveness of water (defined as: decrease in the heat release rate per unit mass application rate of the suppression agent). Since, the physical cooling effect of water [i.e. (i)] has been extensively studied earlier [1,2], the objective of this work is to quantify the gas-phase effects [i.e. (ii) through (v)] and model them. Understanding of these



gas-phase effects is very important for fire suppression by water mist.

#### SUPPRESSION EXPERIMENTS:

Experiments were conducted for different  $O_2$  concentrations (to change the soot volume fraction) and for different constant water application rates (applied both as liquid water and as water vapor). Methane and ethylene were used as fuels, and fuel and oxidizer flow rates were held constant to maintain constant strain rates. The overall transient species composition measurements in the exhaust of the stagnation-point flow apparatus were used to calculate the effect of water on the overall heat release rate. An increase in the  $CO_2$  production rate and the  $O_2$  depletion rate corresponds to an increase in the burning rate and vice versa. Also, detailed flame structure measurements in the presence of water vapor were made in the steady counterflow diffusion flame and numerical calculations were performed to help interpret the data and understand the suppression mechanisms. The dilution effect of  $H_2O$  is compared with the dilution by  $N_2$  &  $CO_2$ , enhanced radiative heat loss is calculated via a model and mixing and chemical enhancement effects are investigated experimentally and theoretically. A brief summary of the experimental results is presented below.

SUPPRESSION EXPERIMENTS WITH LIQUID WATER: These experiments began with liquid water applied to the surface of a burning PMMA sample. However, to eliminate the physical cooling effect of the solid, an uncooled porous ceramic methane burner was used and liquid water was gently applied to the surface of this burner while maintaining a constant methane flow rate. It was found that: (i) For a blue methane flame, fuel dilution due to water evaporation decreased the  $CO_2$  & CO production rates and the  $O_2$  depletion rate. Less hydrocarbons were burned and the hydrocarbon percentage increased until extinguishment was obtained. Thus, chemical enhancement was not observed. (ii) However, for a sooty methane flame, the  $O_2$  depletion rate and the  $CO_2$  production rate was observed to increase as the water application rate was increased. This implies an increase in the heat release rate (i.e. more efficient combustion). With further increase in the water application rate, dilution effects become dominant and the flame is extinguished.

The above results seem to contradict some previous work which claims that water simply acts as a diluent. Thus, to further eliminate the *possibility* of enhanced mixing due to flow disruptions that *may* be caused by volumetric expansion of liquid water (although not observed visibly in the experiments), these experiments were repeated with water vapor. Both stagnation-point flow and the steady counterflow diffusion flame apparatuses were used. The flame structure was measured and calculated with the help of a theoretical model which incorporates the SANDIA CHEMKIN code.

SUPPRESSION EXPERIMENTS WITH WATER VAPOR: In the experimental results presented below, different amounts of water vapor was added to the air side. The experiments were conducted both in the stagnation-point flow apparatus (to measure the cumulative transient effects and compare them with the previous results) and in the steady counterflow diffusion flame (to measure the flame structure and compare them with theoretical calculations).

*Transient Experiments:* Table 1 summarizes the measured mass flow rates in the exhaust both with and without water vapor application. In all these experiments the  $O_2$  concentration was held constant at 15% and different amounts of water was added to the air stream as replacement of  $N_2$  on a volumetric basis (cold air stream flow rate: 12 lpm). The fuel stream was pure  $CH_4$  (cold fuel flow rate: 1.5 lpm). Thus, the oxidizer flow with 30% water vapor contained 15%  $O_2$ , 30%  $H_2O$  and rest  $N_2$ . Normalized measured mass flow rates of  $CO_2$ , CO,  $O_2$  consumption & unburned hydrocarbons (THC) in the exhaust are plotted in figures 1 through 4. In these figures, values >1 represent production and values <1 represent consumption, except for  $O_2$  where consumption is plotted. The measured boundary and peak temperatures

are listed in Table I. There is a slight reduction in the peak flame temperature as water replaces  $N_2$  ( $\sim 20^\circ C$ ; Table I) but an increase in temperature elsewhere. Measured temperature profiles show that the reaction zone becomes wider upon water vapor addition. The temperatures at the fuel and oxidizer inlet also increase upon water vapor addition (see Table I). Visually, the flame becomes less bright and less sooty as  $N_2$  is replaced by water vapor.

The experiments in figures 1 through 4 were conducted by the following procedure: First, a steady diffusion flame was established with  $N_2$  in the air stream and then a predetermined amount of  $N_2$  flow rate was substituted with an equal molar flow rate of water vapor. Water vapor was turned off after about 900 seconds and an equal molar flow rate of  $N_2$  was re-substituted. While this procedure ensures that the initial and final flame conditions remain the same, it causes large fluctuations during changes. Thus, the useful data is at the two steady state conditions: i.e one without water and one with prescribed amount of water. This comparison is also shown in Table I. Note that for each experiment the initial steady state condition with  $N_2$  is nearly the same, indicating excellent repeatability.

The above results clearly show that more  $CO_2$  was produced as the concentration of water vapor was increased. This  $CO_2$  came from oxidation of  $CO$ , additional consumption of unburned hydrocarbons, and some additional consumption of  $O_2$ . Thus, the combustion efficiency was increased upon addition of water vapor. A corresponding increase in the flame temperature (except at the peak) was also observed despite a 25% larger  $\rho C_p$  for water vapor. These results are qualitatively consistent with previous experiments where liquid water was applied. Quantitative comparisons show that the effect is somewhat smaller - indicating additional enhancement due to mixing during application of liquid water.

These results are also consistent with the experiments conducted in sooty (fuel-rich) methane counterflow diffusion flames[3]. Here detailed flame structure measurements were made. It was found that by reducing the  $O_2$  concentration while maintaining the flame temperature by preheating the reactants (thus reducing the  $H_2O$  concentration in the reaction zone) led to an early soot inception and increased soot volume fraction. However, direct addition of only 3.6%  $H_2O$  (while holding all other conditions constant) resulted in delayed soot nucleation and a significant reduction in the soot volume fraction. These observations can be consistently explained by the mechanism of  $OH$  interference with soot inception. An increase in the  $H_2O$  concentration (brought about either by an increase in the  $O_2$  concentration or by direct addition) results in an increase in the  $OH$  concentration provided the flame temperature is high enough. This reduces the  $PAH$  and  $C_2H_2$  concentrations (the corresponding reduction in total hydrocarbons and  $CO$  was observed in the stagnation-point flow diffusion flame) and delays soot inception. This substantially decreases the ultimate soot loading and increases the combustion efficiency and hence the burning rate.

Acknowledgements: The many discussions with Dr. William Grosshandler regarding the direction of this work are gratefully acknowledged.

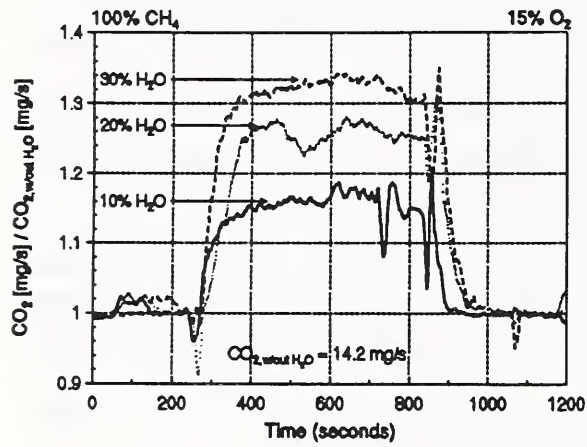
#### Reports, Papers & References

- [1] Abu-Zaid, M., and Atreya, A., "Transient Cooling of Hot Porous and Non-Porous Ceramic Solids by Droplet Evaporation," Presented in the Poster Session of the 22nd. Symposium (International) on Combustion and accepted for publication in the ASME J. Heat Transfer, being revised, 1992.
- [2] diMarzo, M.; Liao, Y.; Tartarini, P.; Evans, D. D.; Baum, H. R.; "Dropwise Evaporative Cooling of a Low Thermal Conductivity Solid," *IAFSS, 3rd International Symposium*, 1991.
- [3] Zhang, C., Atreya, A. and Lee, K., "Sooting Structure of Methane Counterflow Diffusion Flames with Preheated Reactants and Dilution by Products of Combustion," *Twenty-Fourth Symposium (International) on Combustion*, The Combustion Institute, 1992.

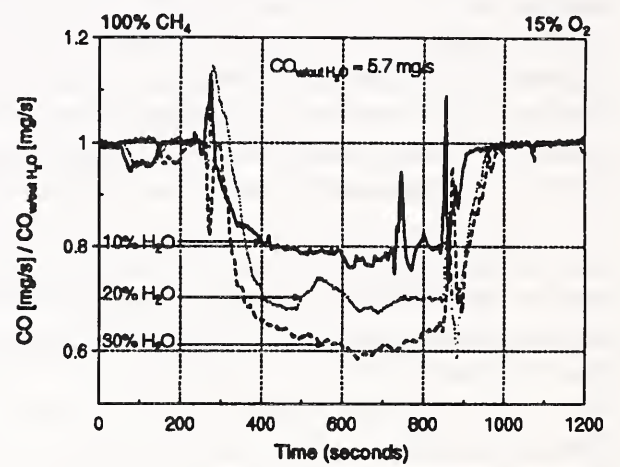


**Table I - Measured Exhaust Mass Flow Rates for experiments where Water Vapor Replaces Nitrogen in the Air Stream.**

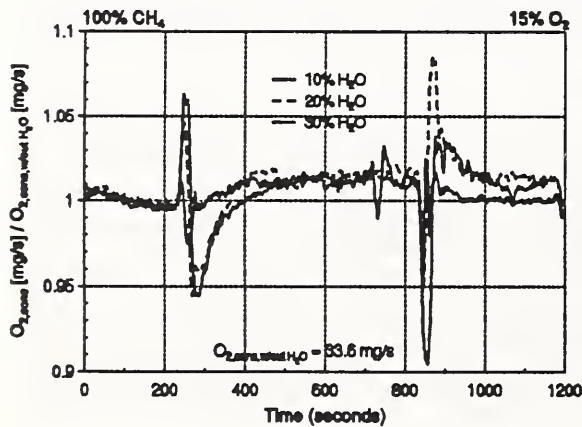
%H <sub>2</sub> O → Species↓	0% ----10%	0% ----20%	0%----30%
THC	8.4 ----- 8.1	8.4 ----- 7.9	8.4 ----- 8.0
CO (mg/sec)	5.7 ----- 4.4	5.7 ----- 4.0	5.7 ----- 3.5
CO <sub>2</sub> (mg/sec)	14.3 ----- 16.8	14.2 ----- 17.9	14.2----- 19.0
O <sub>2</sub> (mg/sec)	33.6 --- 34.1	33.6 -- 34.2	34.2 -- 34.6
O <sub>2</sub> Temp. (K)	751 ----- 754	751 ----- 760	750 --- 764
FuelTemp(K)	684 ---- 688	690 ---- 700	690 -- 707
MaxTemp(K)	1622 -- 1607	1623 -- 1605	1625 -- 1596



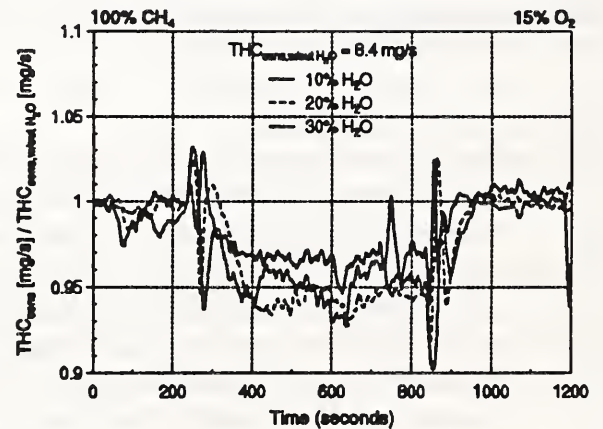
**Figure. 1:**  
Normalized CO<sub>2</sub> Production Rate Showing Excess CO<sub>2</sub>.



**Figure: 2**  
Normalized CO production rate showing reduction in CO



**Figure. 3:**  
Normalized O<sub>2</sub> Consumption Rate Showing Depleted O<sub>2</sub>.



**Figure. 4:**  
Normalized THC Consumption rate showing Unburned THC



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT-FY94

Institution The University of California at San Diego

Grant No. 60NANB3D1435

Grant Title Chemical Inhibition of Methane-Air Diffusion Flames

Principal Investigator Professor K. Seshadri  
Department of AMES  
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## Technical Abstract

### 1 Introduction

The principal objective of this study is to provide a clear understanding of the roles of fluid flow, transport processes and chemical-kinetics in the chemical inhibition of counterflow, methane-air diffusion flames by bromotrifluoromethane ( $\text{CF}_3\text{Br}$ ). An experimental, numerical and analytical study is in progress. This research was started in September 1993 and it is being performed in collaboration with Professor Norbert Peters at the Institut für Technische Mechanik, RWTH Aachen, Federal Republic of Germany and with Professor M. Smooke at Yale University. In this study efforts are being made to clarify the influence of the addition of the inhibitor on the basic flame structure and on the critical conditions of flame extinction. Considerable progress has been made in the asymptotic description of the structure of counterflow, inhibited methane-air flames. Two manuscripts describing the results of this research have been submitted for publication in Combustion and Flame [1,2]. In one of these manuscripts [2] the mechanisms of chemical inhibition by  $\text{CF}_3\text{Br}$  were addressed. Results of the asymptotic analyses were used to determine the critical conditions of flame extinction and the results were compared with previous measurements. Progress has also been made in the numerical description of the flame structure.

### 2 Numerical Calculations

Numerical calculations were performed, using a computer program developed by Professor Smooke to determine the structure of the two-dimensional, laminar, diffusion flames stabilized in the forward stagnation region of a porous cylinder. The flame structure is influenced by the value of the strain rate  $a$  which is defined as the normal gradient of the normal component of the flow velocity. The chemical-kinetic mechanism employed in the calculations contained 52 elementary reactions involving 29 chemical species excluding nitrogen. The flame structure was calculated for various values of  $a$  with different amounts of  $\text{CF}_3\text{Br}$  added to air. The results of the numerical calculations showed  $\text{CH}_4$  and  $\text{CF}_3\text{Br}$  to be consumed at different regions in the flow-field. For convenience, these regions were referred to as the "fuel-consumption zone," and the " $\text{CF}_3\text{Br}$ -consumption zone" respectively. The region between these zones was referred to as the "product-formation zone." The results of the numerical calculations also showed the peak values of the mole fractions of  $\text{H}_2$  and  $\text{CO}$  to be attained in the fuel-consumption zone and the peak value of the mole fraction of the radical  $\text{H}$  to be attained in the product-formation zone. The fuel-consumption zone and the  $\text{CF}_3\text{Br}$ -consumption zone were found to be sinks for radicals. Significant amounts of  $\text{O}_2$  was observed to leak through the fuel-consumption zone into the fuel-stream. These qualitative observations were used as a guide for the asymptotic analyses.

### 3 Asymptotic Analyses

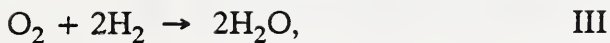
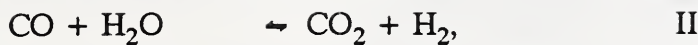
#### 3.1 The asymptotic structure of nonpremixed methane-air flames with oxidizer leakage of order unity

In previous rate-ratio asymptotic analyses it was assumed that fuel is completely consumed in the reaction zone and oxygen does not leak through the reaction zone to the leading order [3]. However measurements show that at conditions close to extinction, a significant amount of oxygen leaks through the flame. In view of these observations an alternative and simpler analysis of the flame structure was performed using a reduced three-step chemical-kinetic mechanism [1,3]. In this analysis fuel was presumed to be completely consumed in the reaction zone and oxygen was presumed to leak through the flame to the leading order. The results of this analysis are particularly useful for analyzing the structure of inhibited flames because the addition of the inhibitor enhances the leakage of oxygen through the reaction zone. *In fact the previous asymptotic models of uninhibited methane-air flames [3] failed to predict the inhibiting effects of halons on these flames because of insufficient leakage of oxygen through the reaction zone.* The values of the scalar dissipation rate at extinction calculated using the new asymptotic model [1] were found to agree well with the results of detailed numerical calculations. The techniques developed for analyzing the structure of the uninhibited flames were extended to inhibited methane-air flames.

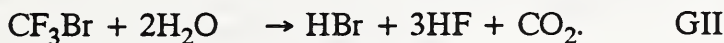
#### 3.2 The asymptotic structure of inhibited nonpremixed methane-air flames

An asymptotic analysis was performed to determine the influence of  $\text{CF}_3\text{Br}$  on the structure and extinction of nonpremixed methane-air flames [2]. The inhibitor  $\text{CF}_3\text{Br}$  was added to the air-stream of the diffusion flame. A reduced four-step mechanism was used to describe the chemistry taking place in the reaction zone. This four-step mechanism can be written as





The reaction rates of the overall reactions in the reduced mechanism can be related to the reaction rates of an appropriate elementary chemical-kinetic mechanism. The overall reaction I is effectively a chain-breaking step and represents the reaction between the fuel and the radicals to form the intermediate products CO and H<sub>2</sub>. The overall reaction II represents the oxidation of CO to form the final product CO<sub>2</sub>. The overall reaction III represents the three-body recombination steps and is also responsible for a major fraction of the heat released in the flame. The overall reaction IV is also a net chain-breaking step and represents the reaction between the inhibitor CF<sub>3</sub>Br and the radicals. In fact it was found that the chain-breaking effect of CF<sub>3</sub>Br is greater than that of CH<sub>4</sub> [2]. In the outer structure of the flame in the Burke-Schumann limit CH<sub>4</sub> and CF<sub>3</sub>Br were presumed to be completely consumed in two different infinitely thin zones. The chemistry in these infinitely thin zones was represented by the global steps



It is noteworthy that the global step GII does not involve O<sub>2</sub>. In the inner structure of the flame chemical reactions were presumed to take place in three distinct layers which were identified as the "fuel-consumption layer," the "oxidation layer" and the "CF<sub>3</sub>Br-consumption layer" [2]. Figure 1 shows comparison between the measured [4] and calculated values of the critical conditions of flame extinction for various amounts of CF<sub>3</sub>Br added to the air stream. The dotted line in Fig. 1 represents the measurements and the solid line represents the results of the asymptotic analysis. The measured results shown in Fig. 1 roughly represent the ratio of the strain rate at extinction for the inhibited flame  $a_q$  to that of the uninhibited flame  $(a_q)_u$ , where the subscript  $u$  refers to the uninhibited flame. The asymptotic results shown in Fig. 1 represent the ratio of the value of the scalar dissipation rate,  $\chi_q$  for the inhibited flame to that for the uninhibited flame  $(\chi_q)_u$ . The measurements and the calculations show the value of the strain rate at extinction to decrease with increasing amounts of CF<sub>3</sub>Br in the air stream. In comparison to the measurements, the asymptotic results show a weaker inhibiting effect and the differences are probably due to the approximations introduced in the asymptotic analysis. Research is in progress to improve the accuracy of the predictions of the asymptotic analysis.

## 4 References

1. Seshadri, K., and Ilincic, N., "The asymptotic structure of nonpremixed methane-air flames with oxidizer leakage of order unity," to appear in *Combustion and Flame*, 1994.
2. Seshadri, K., and Ilincic, N., "The asymptotic structure of inhibited nonpremixed methane-air flames," submitted for publication in *Combustion and flame*, 1994.



3. Seshadri, K., and Williams, F. A., in *Turbulent Reacting Flows* (Eds. P. A. Libby and F. A. Williams), Academic Press, pp 153--210, (1994).

4. Milne, T.A., Green, C.L., and Benson, D.K., *Combustion and Flame* 50: 89-97, 1983.

## 5 Acknowledgements

We wish to thank Professors N. Peters, F. A. Williams and A. S. Gordon for many helpful discussions.

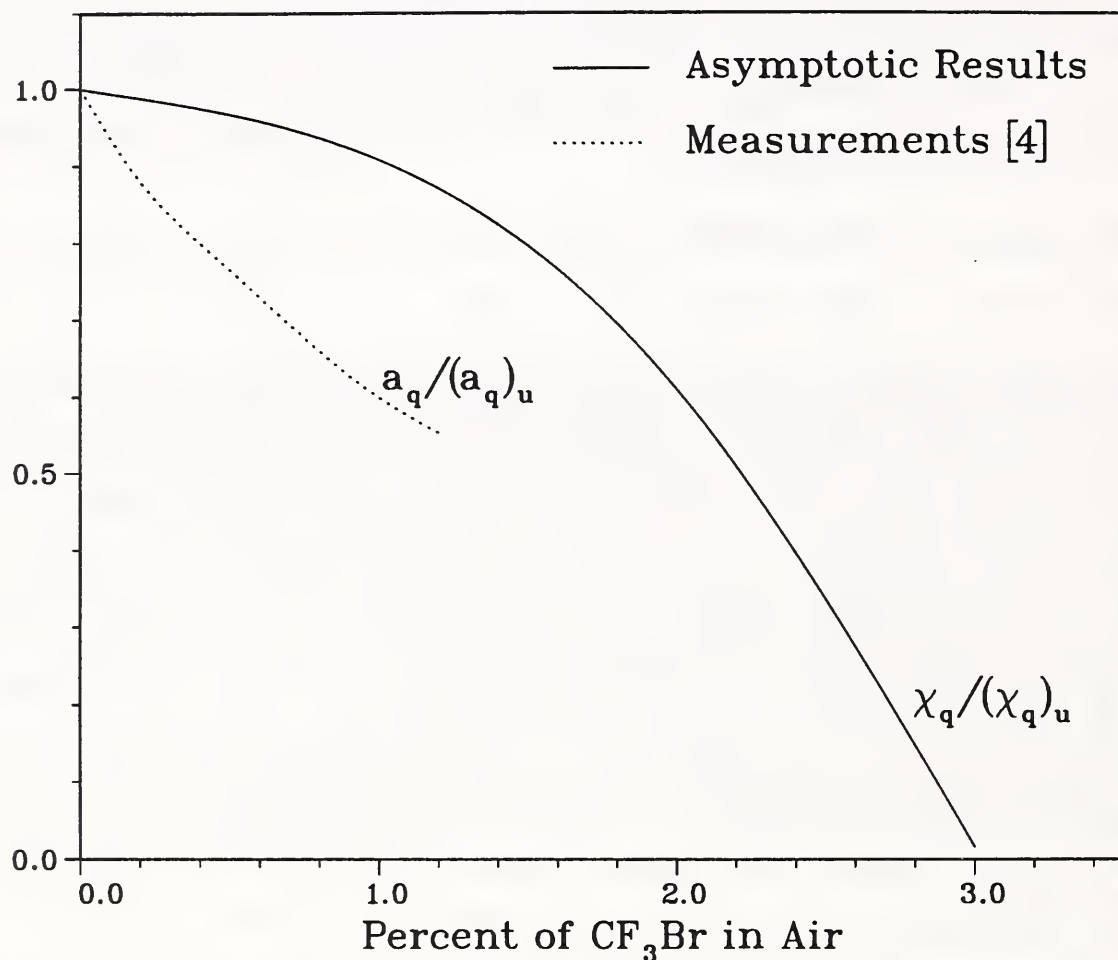


Figure 1: Comparison between measured [4] and calculated values of the critical conditions of flame extinction for various amounts (volume percent in air) of CF<sub>3</sub>Br added to the air-stream. The dotted line represents the measurements and the solid line represents the asymptotic results.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

OPTIMIZATION OF AIRCRAFT FIRE SUPPRESSION SYSTEM DISCHARGE

Funding Agencies

U.S. Air Force, U.S. Navy, U.S. Army and Federal Aviation Administration

Professional Personnel

Jiann C. Yang, Project Leader  
William L. Grosshandler, Group Leader, Fire Sensing and Extinguishment  
Thomas G. Cleary, Chemical Engineer  
Isa Vazquez, Chemical Engineer  
Carole Womeldorf, Civil Engineer  
Brett Breuel, Mechanical Engineer  
Grzegorz Gmurczyk, Visiting Scientist  
Lloyd Weber, Physical Chemist (Thermophysics Division)  
Marcia Huber, Chemical Engineer (NIST, Boulder Laboratory)  
Roy McLane, Engineering Technician  
Charles Boyer, Undergraduate Student  
Michelle King, Undergraduate Student

Project Objective

To ensure that the four recommended agents (HFC-227ea,  $CF_3I$ , HFC-125, and FC-218) for full-scale testing by the Air Force are delivered to the fire in an efficient manner so that an unbiased evaluation of system effectiveness can be made by the end of FY 94, and to provide generic scientific data to fire suppression system suppliers and airframe manufacturers in support of their efforts to design protective systems for existing and future aircraft.

Technical Accomplishments

A high pressure facility has been constructed to measure pressure-temperature relationship for agent/nitrogen mixtures at various fill densities and nitrogen charged pressures. Measurements obtained from our facility will provide safety guidelines for the structural integrity of fire suppression bottles when exposed to hostile environment. An apparatus has also been built to measure the amount of nitrogen dissolved in the agent. A computer code (named PROFISSY) for calculating the pressure-temperature characteristics of a fire suppression vessel has been developed. The code currently supports the four selected agents and halon 1301 although other agents can be easily incorporated into the code.

A facility which allows an agent to be discharged into the atmosphere in order to simulate dry bay discharge has been built. Various discharge mechanisms (valves and squibs), bottle geometries, and discharge orientation can be easily accommodated in this facility. The facility is also equipped with

a high-speed movie camera to record the discharge dynamics external to the vessel, laser attenuation for measuring the average speed of the dispersion front, and a vessel with sight glasses for observing the internal behavior of an agent during discharge.

A facility for studying two-phase pipe flow during the discharge of an agent from a vessel into a piping system has been constructed. The facility enables the experiments to be performed either quasi-steadily or transiently. A transparent section made of acrylic plastic can be installed in the piping system so that observation of the two-phase behavior of an agent flowing through the pipe can be made by using a high-speed movie camera.

#### Reports and Publications

Cleary, T.G., Grosshandler, W.L., and Yang, J.C., "Flow of Alternative Agents in Piping," paper presented at the Halon Options Technical Working Conference, May 3-5, 1994, Albuquerque, New Mexico.

Yang, J.C., Cleary, T.G., and Grosshandler, W.L., "Simulation of Dry Bay Discharge of Alternative Agents," poster presented at the Halon Options Technical Working Conference, May 3-5, 1994, Albuquerque, New Mexico.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

EFFECTS OF FIRE SUPPRESSANTS ON METAL FIRES

Funding Agency

U. S. Navy, Naval Air Warfare Center, Lakehurst, N. J.

Professional Personnel

Thomas J. Ohlemiller, Project Leader  
John Shields, Physical Scientist

Project Objective

To obtain a quantitative measure of the interaction between magnesium and titanium alloy fires and candidate substitutes for halon 1301. We wish to learn if these potential substitutes interact with (enhance) these fires more strongly than does halon 1301.

Technical Accomplishments

The project has been underway about three months. A test apparatus has been designed and is being assembled. This apparatus will permit controlled burning of thin rods of either magnesium or titanium 6-2-4-2 in an airflow at pressures up to 1380 kPa (200 psig). This airflow will carry controlled concentrations of the vapors of either halon 1301 or four candidate replacement agents past the burning metal. The halogens in these agents are expected to enhance, not suppress, the oxidation of the metal. The extent of the enhancement will be assessed by measurements of burning rate, radiative emissions and plume temperature.

Reports and Publications

None

Related Grants

None



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

AGENT SCREENING FOR HALON 1301 AVIATION REPLACEMENT

Funding Agency

U.S. Air Force, U.S. Navy, U.S. Army and Federal Aviation Administration

Professional Staff

William Grosshandler, Project Leader  
Richard Gann, Chief, Fire Science Division  
Anthony Hamins, Mechanical Engineer  
Marc Nyden, Research Chemist  
William Pitts, Research Chemist  
John Yang, Research Mechanical Engineer  
Michael Zachariah, Group Leader, High Temperature Reacting Flows

Project Objective

To produce a report on the comprehensive experimental program developed in FY 1992 and 1993 for screening eleven gaseous agents, sodium bicarbonate powder, and other promising chemicals as a means to identify (by 9/30/93) the best candidates for a subsequent full-scale aircraft fire extinguishment evaluation program.

Technical Approach

The major task leaders provided documentation on their particular aspect of the program. This was assembled into a single report, issued, upon sponsor approval, as a NIST Special Publication.

Technical Accomplishments

An increased understanding of the key issues which control extinguishment in aircraft engine nacelle and dry bay fires has been gained through a multi-year experimental program. A letter was delivered to the Air Force on September 28, 1993, which included a brief summary of the project, a list of agents recommended for full-scale testing in the Air Force facility in FY 1994, and a description of the rationale used to arrive at the recommendation. The specific agents recommended for large-scale testing in the simulated engine nacelle were HCFC-124 and HFC-125. Further testing of  $CF_3I$  was also thought to be warranted, and FC-218 was suggested for a back-up. FC-218 and HFC-125 were the top choices for the dry bay application, with HFC-227ea and  $CF_3I$  also possibilities. Sodium bicarbonate powder was found to be the most efficient flame extinguishing compound of all (even better than  $CF_3Br$  on a mass basis), but was recommended for testing only in the engine nacelle because the dry bay application places a premium on dispersion throughout the volume, greatly handicapping a condensed agent.



The task remaining for FY 1994 was to document the results and present them to the sponsors. The final report is a 900 page document which was completed with substantial contributions from 28 co-authors in addition to the primary staff listed above. Specific authorship is indicated at the beginning of each of the ten discrete sections. Copies of the document listed below are available from NIST, or from the Superintendent of Documents, U.S. Government Printing Office, Washington DC, 20402.

#### Reports and Publications

Grosshandler, William L., Gann, Richard G., Pitts, William M. (editors), *Evaluation of Alternative In-flight Fire Suppressants for Full-scale Testing on Simulated Aircraft Engine Nacelles and Dry Bays*, National Institute of Standards and Technology, NIST SP 861, April 1994.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

HALON 1301 SURROGATES FOR ENGINE NACELLE  
FIRE SUPPRESSION SYSTEM CERTIFICATION

Funding Agency

U.S. Naval Engineering Center, Lakehurst, NJ

Professional Staff

William Grosshandler, Project Leader  
Carole Womeldorf, Mechanical Engineer  
Jiann Yang, Mechanical Engineer

Project Objective

To determine the physical properties which dominate the dispersion process and recommend environmentally acceptable candidates for use in simulating the dispersion of ambient temperature halon 1301 in an aircraft engine nacelle.

Technical Approach

Existing Navy aircraft fire suppression systems require certification to ensure that the fire-fighting agent is present in sufficient quantity and for a long enough period of time to extinguish a possible fire. In the past, certification was accomplished by discharging halon 1301 and measuring its concentration over time at various locations in the nacelle. This procedure is no longer acceptable because (a) the reserves of halon 1301 are limited since it is no longer in production, and (b) halon 1301 released to the atmosphere contributes to the unwanted depletion of stratospheric ozone. An alternative chemical is thus needed to fill the certification role formerly played by halon 1301.

The properties of a wide range of chemicals are being reviewed for their physical similarity to halon 1301 (without regard to flame inhibition effectiveness) to identify prospective candidates for discharge certification. These include HFC-227 (FM 200), HFC-32/HFC-125 (AZ20) and SF<sub>6</sub>. Two chemicals (in addition to SF<sub>6</sub>) will be recommended for testing in light of limitations due to toxicity, flammability, current availability, and possible environmental impact. Tests with the recommended chemicals will be performed by Walter Kidde Aerospace in their full-scale fire bottle discharge facility and in their small-scale aircraft engine simulator, and discussions will be held on the results with NIST personnel. To give a broader understanding of the two-phase flow dynamics in the piping and the flashing discharge characteristics, additional experiments will be performed in NIST facilities. High speed photography will be used to reveal the physical behavior of the chemicals in both flow situations and permit a comparison between the surrogate candidates and halon 1301.

### Technical Accomplishments

The properties of a wide range of chemicals were assembled and reviewed. Two tiers of chemicals were identified as candidate surrogates: tier 1 contained SF<sub>6</sub> and HFC-125; and tier 2 contained HCFC-22, FC-218 and FC-216. The first tier candidates are much superior and are likely to have few problems when used to simulate halon 1301 discharges. Both of these have been recommended to the Navy for further testing by Walter Kidde Aerospace and NIST. The second tier chemicals are reasonably similar to halon 1301, but each suffers from either a non-zero ODP or excessive atmospheric lifetime. From the second tier, HCFC-22 was recommended as the third chemical for testing.

The second phase of this project is the laboratory-scale testing of the three candidates: SF<sub>6</sub>, HFC-125, and HCFC-22. Walter Kidde Aerospace will test the candidates in their full-scale fire bottle discharge facility and in their small-scale aircraft engine simulator. Two-phase flow dynamics in the piping and the flashing discharge characteristics of will be compared in the NIST facilities.

### Reports and Publications

Progress to date has been reported in meetings, presentations, and a letter report to the sponsors. In June, goals and preliminary results were discussed in a meeting at the Halon Options Technical Working Conference. Representatives from the Navy, WKA, Boeing, and the FAA attended. In July, NIST presented their recommendations and a letter report describing the selection process and the three candidates. In August a presentation was given by the Navy detailing these recommendations at the International Halon Working Group Meeting. A final report is expected at the end of 1994.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

PROTECTION OF DATA PROCESSING EQUIPMENT WITH WATER SPRAYS

Funding Agency

U.S. Fire Administration, Federal Emergency Management Administration

Professional Staff

William Grosshandler, Project Leader  
Kathy Notarianni, Fire Protection Engineer  
Darren Lowe, Computer Specialist

Project Objective

To determine, by 9/94, the ability of a water spray to protect data processing equipment from the threat of a fire.

Technical Approach

A water spray system is an attractive candidate for replacing halon 1301 in the protection of data processing equipment because water is an effective fire suppressant and is non-toxic, environmentally friendly and competitively priced. The dynamics controlling the transport of the liquid water droplets are different from the dynamics of prevaporized halon 1301; hence, the problem is to determine the applicability of a liquid spray system in an environment currently protected with a gaseous agent. The data processing industry and spray systems manufacturers were contacted to determine the where mist systems are most likely to be considered. A representative data processing cabinet and room geometry was defined and a likely ignition source and fuel load was identified. A test facility was built to emulate the physical parameters thought to control the actual fire suppression process and baseline studies will be performed to determine the amount of gaseous  $CF_3H$  required to extinguish the test fire. The influence on extinguishing efficiency of the nozzle geometry, location relative to the fire, water application rate, and the depth to which the fire is buried within the simulated cabinet are all parameters which are being examined. The experimental facility allows the droplet size distribution, velocity and obstructions to the flow to be characterized.

Technical Accomplishments

A representative electronics cabinet and room geometry, fuel load, and ignition source was identified after reviewing the literature and having conversations with those familiar with the application. A scaled-down, mock electronics package was designed and a chamber built to contain the spray to emulate the physical system of interest. The test chamber is 1.68 m wide, 0.91 m deep, and 2.13 m high, with an exhaust fan at the center of the top to remove products of combustion after each test has been run. Two walls are glass to allow visual observation of the entire process. The mock electronics cabinet is 0.5 m wide by 0.2 m deep and 0.4 m high, and is shown in Figure 1. The fuel

cabinet to simulate the flow of cooling air. Ignition is by an electrically heated nichrome wire.

The influence on extinguishing efficiency of the nozzle geometry, location relative to the fire, water application rate, and the depth to which the fire is buried within the simulated cabinet are all parameters which have been examined. A phase-Doppler particle analyzer (PDPA) is being used to determine the droplet size distribution and two components of velocity at locations internally near the fire in the circuit board and external to the cabinet. These data are key to relating the extinguishment event to conditions adjacent to the fire, and indicate the fate of the droplets as a function of different initial conditions in the spray. A baseline study is to be performed to determine the amount of a gaseous agent ( $CF_3H$ ) necessary to extinguish fires as a function of the extent to which the fire is buried within the simulated electronics cabinet. Trifluoromethane was used rather than halon 1301 because it is a proposed gaseous alternative total flooding agent, and is significantly less effective than halon 1301.

A minimum enclosure situation corresponds to a PMMA circuit board totally exposed to the air and water spray. This arrangement is the easiest to extinguish, and identifies the locations within the test chamber where there is the greatest likelihood of suppression. Figure 2 indicates the time required to suppress the PMMA sample following a 30 second preburn time as a function of position below the pressure jet nozzle. The pressure is 2.1 MPa and the flow rate is 2.1 l/min. The affect of increasing water pressure (and flow) was is to greatly expand the region in which extinguishment is possible in under 60 s. This is due partly to the greater flux of water and partly due to the increased momentum of the water spray.

### Reports and Publications

Reports have been in the form of monthly letters to the sponsor. A comprehensive report on the first year of research will be available by October 1, 1994.

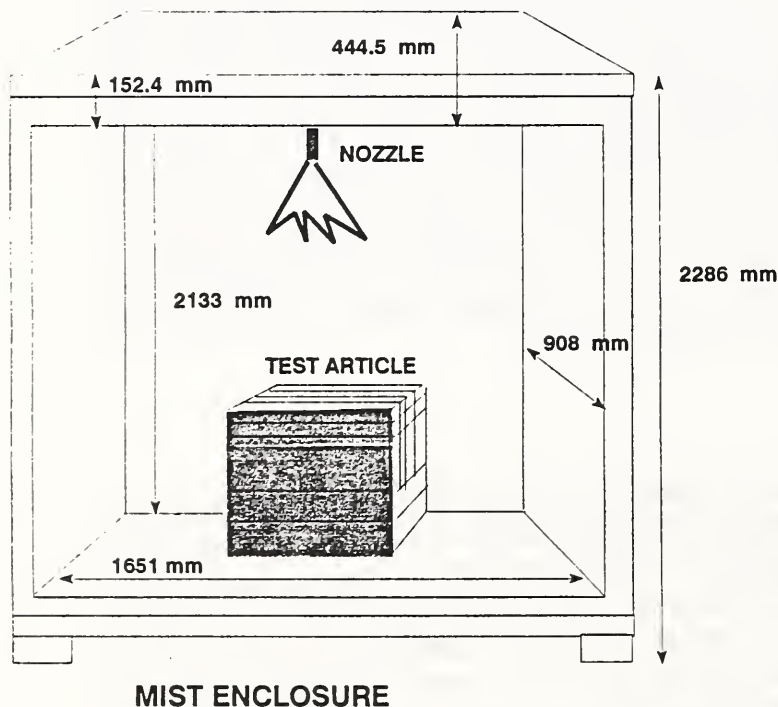


Figure 1. Schematic of test article

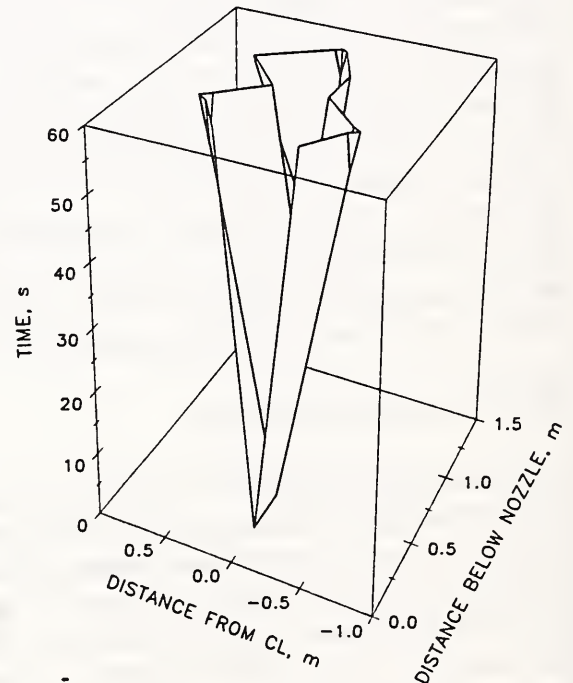


Figure 2. Time to extinguishment

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

SUPPRESSION OF SIMULATED ENGINE NACELLE FIRES

Funding Agency

U.S. Air Force, U.S. Army, U.S. Navy, and the Federal Aviation Administration

Professional Personnel

Anthony Hamins, Project Leader  
William Grosshandler, Mechanical Engineer  
Glenn Forney, Applied Mathematician  
Thomas Cleary, Mechanical Engineer  
Darren Lowe, Computer Specialist  
Michael Glover, Technician  
Cary Presser, Aerospace Engineer

Project Objective

Document guidelines for fire suppression system performance based on improved understanding of the influence of various parameters on fire suppression in an engine nacelle.

Technical Accomplishments

The project extends the range of parameters studied in FY93 to a broader range of suppression and re-ignition conditions, typical of in-flight engine nacelles. The project is composed of two parts. Part 1 consists of flame suppression measurements conducted in a coaxial turbulent jet spray burner with JP8 as the fuel.

The spray burner uses JP8 jet fuel and the agents tested are  $CF_3I$ , HFC-125, and HFC-227. The amount and rate of application of agent needed to suppress the spray flame is being measured. A broad range of suppression and re-ignition conditions are being tested and the influence of a number of flow parameters on flame stability are being investigated including the fuel and air flow, air and agent temperature, system pressure, rate of agent application, and agent injection interval. Preliminary results show that as the agent delivery interval decreases, the mass of agent required to suppress the flame increases. Measurements also show that the air velocity has little impact on the required mass or agent delivery rate (see Fig. 1). The agent delivery rate is defined as the ratio of the mass of agent delivered to the delivery interval.

Part 2 of the study consists of computational fluid dynamic modeling (using FLOW3D) of conditions in the engine nacelle. Information regarding criticality of the number, placement, and orientation of agent injection nozzles as well as the rate of gaseous agent injection will be determined. To demonstrate the capability of computational fluid dynamics in this application, the flow field model will be experimentally validated using a mock engine nacelle that is being constructed.



The knowledge gained through this project will be used to develop guidance tools to assist suppression system designers.

#### Reports and Publications

"A Turbulent Spray Burner for Assessing Halon Alternative Fire Suppressants", Grosshandler, W., Lowe, D., Rinkinen, B., Presser, C., ASME Paper No 93-WA/HT-23, 1993.

"Assessing Halon Alternatives for Aircraft Engine Nacelle Fire Suppression", Grosshandler, W., Presser, C., Lowe, D., and Rinkinen, W., to appear in J. Heat Transfer (1994).

"Suppression of Elevated Temperature Hydraulic Fluid and JP8 Spray Flames", Vazquez, I., Grosshandler, W., Rinkinen, W., Glover, M., and Presser, C., to appear in the Proceedings of the Fourth International Symposium on Fire Safety Science, 1994.

#### Related Grants

None

## **D. LARGE/INDUSTRIAL FIRES**





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT- FY94

SMOKE MOVEMENT AND SMOKE LAYER DEVELOPMENT IN HIGH BAY AREAS

Funding Agency

National Aeronautics and Space Administration

Professional Staff

Kathy A. Notarianni, Project Leader

William D. Davis, Physicist

Margaret Jackson, Mechanical Engineer

Project Objective

To provide NASA with data on smoke movement and smoke layer development in high bay areas to enable NASA to make decisions on fire detection and suppression in their high bay spaces.

Technical Accomplishments

There is a special need to address fire protection issues for high ceiling height large spaces. NASA has numerous high bay spaces that are used to perform a variety of functions. Examples of high bay spaces at NASA include those used for clean rooms, shuttle simulators, assembly/storage, vacuum and vibration chambers, vehicle assembly, and/or testing facilities with payloads. These spaces represent some of the most difficult fire protection challenges in that detection of a fire in a large space may be delayed due to the distance smoke and products of combustion must travel to reach the detector, the large amount of ambient air for smoke dilution, the high dollar value of these spaces, and the low damage threshold of a clean room. Some of these spaces also involve forced airflow.

In year one of this project, use of a field model for a high space was investigated using NIST measurements of fire gas temperatures and disk temperatures taken along the ceiling of a 30.4 m aircraft hanger during live fire tests. Measurements were compared to predictions of a NIST field model. NIST field modeling was then used to model a NASA high bay space to predict smoke movement and smoke layer development. A final report was delivered to NASA fully documenting the modeling procedure, inputs, and results. During FY94, a survey of NASA high bay spaces was conducted in order to quantify materials and fire sizes. Existing detection and suppression systems were documented as well as forced air flows. A matrix of NASA spaces was produced. In the second part of FY94 and FY95, modeling will be used to determine the appropriateness of available detection and suppression systems to each type of NASA space. A final applications matrix will be produced so that NASA can make decisions on type and location of fire detection and suppression equipment for its high bay spaces.

Reports and Publications

"The Use of Computer Models to Predict Temperature and Smoke Movement in High Bay Spaces,"  
K.A. Notarianni and W.D. Davis, NISTIR 5304, 1993.

Related Grants

None

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

ANALYSIS OF INDUSTRIAL FACILITY FIRES

Professional Personnel

David Evans, Acting Division Chief  
William Walton, Acting Group Leader

Project Objective

To develop by the year 2000 a collection of engineering methods for analysis of large fire events in industrial facilities.

Scope

This project included interactions with a broad range of professionals in the fire safety community for the purpose of discovering the important problems that could be addressed by increased analytical capabilities and understanding of fire. As a result of this investigation, the problem of combined installation of sprinklers with draft curtains in large plan area facilities was chosen for further technical investigation. In connection with post-earthquake fire events, an investigation of fire that occurred as a result of the Northridge, California earthquake was conducted.

Technical Accomplishments

During FY94, input from fire safety professionals indicated that possible interactions between sprinklers, draft curtains, and vents needed to be understood better to optimize design. In addition, data was needed on all types of industrial fire sources so that many of the models being developed by BFRL could be utilized better for industrial fire problems. The Northridge earthquake provided an opportunity to investigate individual fires, fire fighting, and building to building fire spread in an residential area.

Reports and Publications

Todd, D., Carino, N., Chung, R.M., Lew, H.S., Taylor, A.W., Walton, W.D., Cooper, J.D., Nimis, R., 1994 Northridge Earthquake: Performance of Structures, Lifelines, and Fire Protection Systems, NISTSP 862, May, 1994.

Related Grants

"An Investigation of Oil and Gas Well Fires and Flares," Professor Jay Gore, Purdue University





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

SMOKE PLUME SAMPLING

Professional Personnel

William D. Walton, Project Leader

Funding Agency

U.S. Coast Guard, Research and Development Center

Objective

The objective of this project is to design and test two smoke plume sampling packages, one that can be suspended from a helicopter and one that can be suspended from a miniblump for use in monitoring of in situ crude oil burns.

Technical Accomplishments

Although laboratory and mesoscale test burns have demonstrated the effectiveness of in situ burning as an oil spill mitigation technique, questions remain concerning the composition of the smoke in the plume downwind of the fire. In order to provide information for decision makers, measurements of the smoke composition are necessary. For measurement of the composition of smoke in the plume it desirable to take samples over an extended period of time. The only means for maintaining a sampling package in the plume for an extended period of time appear to be helium filled miniblumps and helicopters. The blimps provide a good measurement platform near the fire but may not be capable of obtaining the altitude required to make downwind measurements. Helicopters can fill this need although they are more expensive to operate.

NIST has used smoke sampling packages suspended from miniblumps for several years during mesoscale burns in Norfolk, Virginia and Mobile, Alabama. The design of these packages has been improved several times to reduce the weight and increase the reliability. Improvements to the package design have been developed after the most recent mesoscale burns and a new package has been constructed for use in burns of opportunity. The basic package consists of an aluminum box with overall dimensions 305 by 311 by 127 mm and weighs 0.6 kg. It is designed to be disassembled into the six component sides so it can be transported in a compact fashion. The package can accommodate up to three battery operated sampling pumps. Figure 2 is a schematic drawing of the package identifying the principal components. The total weight of the package in this configuration is 3.4 kg. Normally the package is located 60 m below the blimp so the blimp can be kept above the plume with the package in the smoke. The tether line from the blimp is connected to the top of the package and the line to the ground is connected to the bottom allowing the package to orient itself into the wind.

One of the pumps is connected to an 8 stage cascade impactor which segregates smoke particulate from 0 to 10  $\mu\text{m}$ . The intakes of the other two pumps are connected to 37 mm smoke particulate sampling filters. Other types of filters can be used in place of the smoke particulate filters to permit analysis of the smoke for other chemical components.

The two pumps with filters have a control valve on the discharge which proportions part of the discharge to a tedlar gas sample bag and the rest to the atmosphere. This permits the pumps to be operated at the

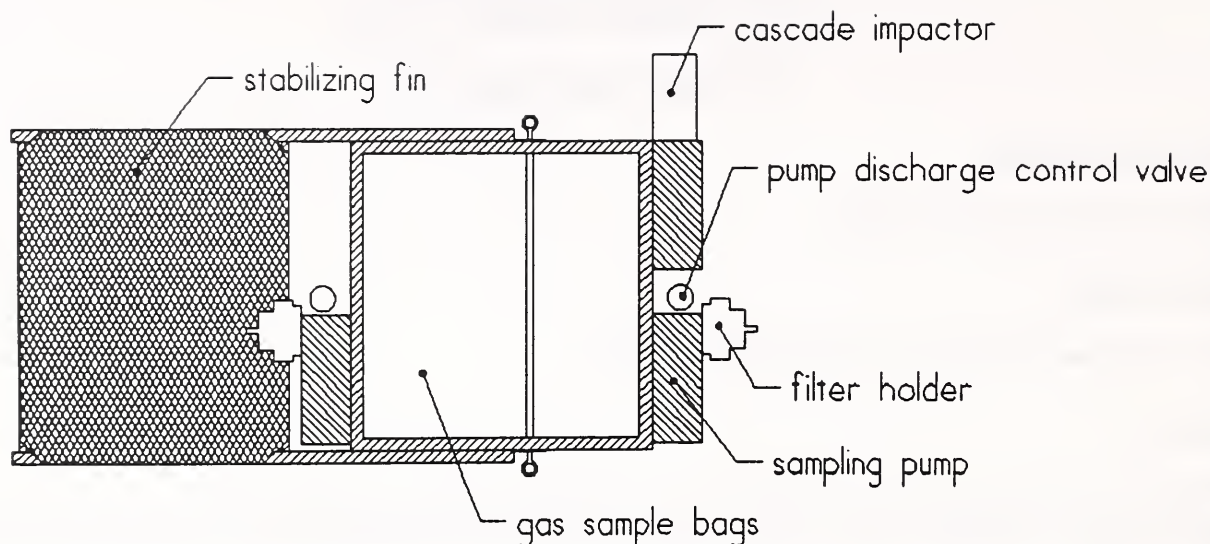


Figure 6. Schematic of miniblimp transported smoke sampling package

maximum flow rate and collect the maximum particulate sample while not over-filling the gas sample bag. The gas collected in the sample bags is typically analyzed with a gas chromatograph.

A helicopter transported instrumentation package, which is about the size of a suitcase, was developed. It contains air sampling pumps, collection media, and sample bags to provide time averaged measurements of smoke yield, smoke particle size distribution, PAH concentration, and volatile organic compounds. In addition, the package has basic metrology measurement of temperature, relative humidity, wind speed and direction, and barometric pressure. The package includes the capability to turn all of the sampling pumps on and off by remote control and a strobe light to indicate that the pumps are operating. The package is designed to be suspended from the winch on a Coast Guard HH-65A helicopter that has a cable with a working length of 75 m. The package can be held in a specific relative location in the plume for approximately 15 minutes in order to obtain an adequate quantity of sample for analysis.

The package has a flat top and bottom, a rounded front end, and tapers toward the rear. It is 370 mm high, 180 mm wide, and 1000 mm long. The stabilizing fin is 340 mm high and 770 mm long. Figure 2 is a schematic drawing of the package identifying the principal components. The total weight of the package in this configuration is 25 kg. Quick connect fasteners are used on one side of the package to allow easy access to the interior. In addition, the entire front of the package which contains the smoke particulate filters can be quickly removed. The package has been designed to separate into three pieces and the fin, each of which can fit into an inexpensive but rugged suitcase size shipping container.

Three pumps are used to collect the samples. The intakes of two pumps are connected to 37 mm smoke particulate sampling filters. Other types of filters can be used in place of the smoke particulate filters to permit analysis of the smoke for other chemical components. One of the pumps can be connect to either a sampling filter or, as for the test burns, an 8 stage cascade impactor which segregates smoke particulate from 0 to 10  $\mu\text{m}$  in effective aerodynamic diameter. The two pumps with filters have a valve on the discharge which proportions part of the discharge to a tedlar gas sample bag and the rest to the atmosphere. The gas collected in the sample bags is typically analyzed with a gas chromatograph.



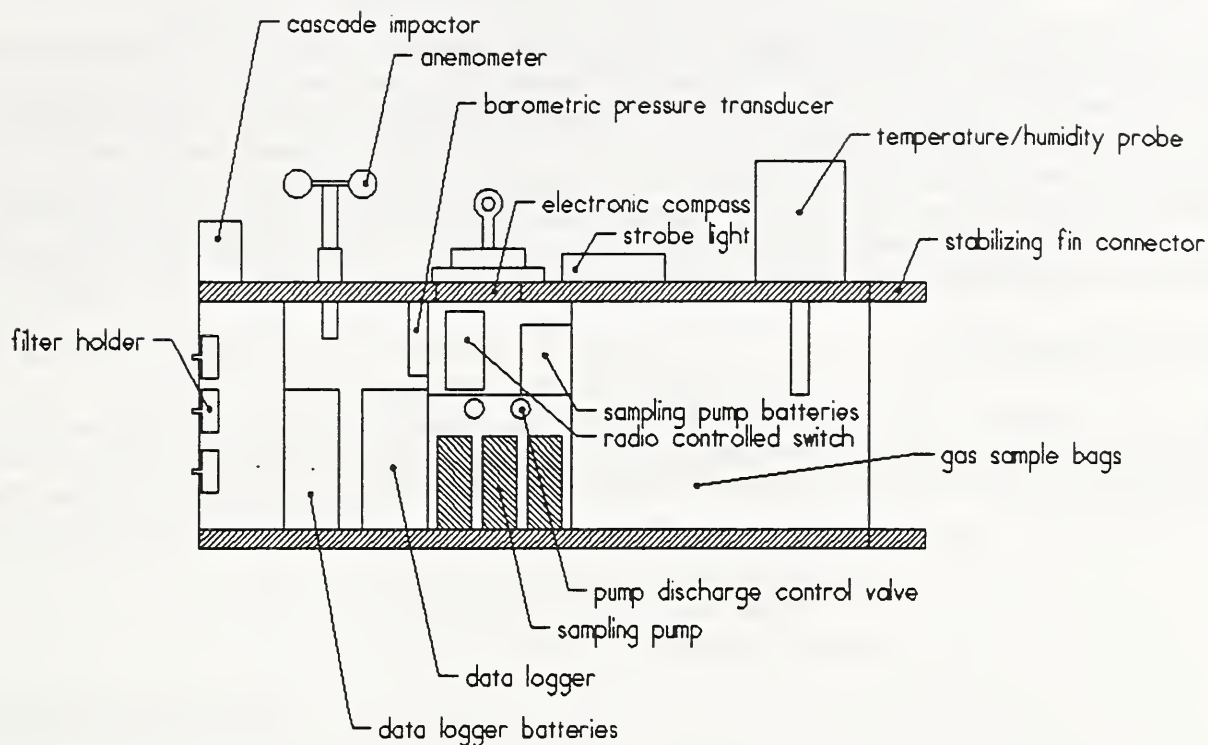


Figure 7. Schematic of Helicopter transported smoke sampling package

The weather instruments include a temperature and relative humidity probe, a barometric pressure sensor, an anemometer, and electronic compass. Data from the weather instruments is collected every 10 seconds on a data acquisition system and stored in a solid state digital storage module for later computer retrieval. The system acquires data during the entire flight without operator intervention. The system can be used to record conditions inside the smoke plume as well as provide an atmospheric profile. From the barometric pressure the relative height of the package above the initial starting point can be determined. The electronic compass determines the orientation of the package and thus the direction of the wind if the helicopter is stationary or the helicopter's direction if it is moving.

The package was tested beneath a U.S Coast Guard HH-65A helicopter from the Coast Guard Aviation Training Center in Mobile, Alabama without a fire. During that test it was learned that the package could be easily deployed through the door of the helicopter on the winch cable. A forward speed of about 10 m/s would prevent the package from spinning during deployment and retrieval. The package was tested with cable lengths of 30 and 60 m and was found to be stable. There was occasionally a slight fluttering of the package with 60 m of cable, no forward helicopter motion, and near calm winds. The package was also tested with the helicopter in forward motion and it appeared that the package would be completely stable when operated with at least light winds.

Both the helicopter and miniblump transported packages were evaluated during three mesoscale fuel oil burns at the Fire and Safety Test Detachment in Mobile, Alabama. The burns were conducted in a 15 m square steel burn pan constructed specifically for oil spill burning. The improved miniblump transported smoke sampling and the helicopter transported smoke sampling package were both shown to be effective means for collecting

smoke samples for in situ burning. There was no visible interference in the smoke sampling from the helicopter downwash.

Measurements from the mesoscale burns showed the average burning rate for the diesel fuel fires on water was  $0.062 \pm 0.001 \text{ kg/s/m}^2$ . The values for smoke yield measured for diesel fuel (from 9.4 to 13.7 % on a mass basis) were within the range of values previously measured for crude oil. The values measured closer to the fire and near the combustion region tended to be lower than those measured further away. The size distributions of aerodynamic effective diameters for the smoke particulate were nearly identical for the diesel fuel burns and the previous crude oil burn. Measurements made using the helicopter transported sampling package closer to the fire showed a slight increase in larger particles. The average value for the three burns was 78 % of the particulate mass was below  $9.8 \mu\text{m}$  in diameter as measured with a cascade impactor.

#### Reports and Publications

Walton, W., McElroy, J., Twilley, W., and Hiltabrand, R., "Smoke Measurements Using a Helicopter Transported Sampling Package," Proceedings of the Seventeenth Arctic and Marine Oil Spill Program Technical Seminar, June 8-10, 1994, Vancouver, British Columbia, Ministry of Supply and Services Canada, pp. 735-764, 1994.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT- FY94

Institution Purdue University

Grant No. 60NANB3D1441

Grant Title A Study of Two Phase High Liquid Loading Jet Fires

Principal Investigator Professor J. P. Gore  
School of Mechanical Engineering  
Purdue University  
West Lafayette, IN 47907-1077

Other Personnel Professor P. E. Sojka, Co-Principal Investigator  
Dr. Y. R. Sivathanu, Research Professor  
Mr. Robert Wade, Graduate Student  
Mr. W. E. Swan, Undergraduate Student

NIST Scientific Officers Dr. David D. Evans

Technical Abstract

Introduction Large scale industrial spray fires may result from rupture of liquid storage tanks, transport pipelines and oil well blowouts. These fires represent a serious hazard to personnel and may result in a large cost penalty in terms of insurance, litigation, loss of service and sales, and replacement of plant and equipment. Well head fires after the liberation of Kuwait serve as a high visibility reminder of the possibility of the stabilization of high liquid loading jet flames. Effective atomization of liquid fuel with minimal amount of dissolved gases occurs when a two phase mixture expands from a high pressure source into the atmosphere. In the presence of appropriate means of flame stabilization, in addition to the effective atomization, a jet fire occurs. Previous NIST sponsored research in this laboratory (Dutta et al., 1994) demonstrated the stabilization of high liquid loading crude oil+methane flames with a hydrogen pilot flame. Measurements of flame length, radiative heat loss fractions, and soot transmittance and temperature were completed. The results showed that two phase flow effects affected the flame lengths and radiation properties significantly and that existing correlations could not be used effectively.

It was conjectured that visible flame lengths could be affected by changes in: (1) evaporation length, (2) air entrainment rate, (3) exit momentum, and (4) fuel and sooting properties, resulting from two phase flow effects in spray fires. The objective of the present project is to conduct measurements of each of these effects using small and intermediate scale laboratory jet fires and delineate the importance of each in determining the visible flame size and radiation properties.

Operating Conditions In addition to the 7 flames studied by Dutta et al. (1994), 19 toluene+methane+hydrogen flames summarized in Table 1 were considered. As seen from Table 1, the first five flames are designed to study the effects of changing the methane to liquid ratio (MLR). Therefore, these flames have a fixed hydrogen to liquid mass flow rate (HLR) and a fixed total heat release rate of 10 kW including the heat release of toluene, methane and hydrogen. The next five flames will show the effect of MLR for identical HLR for flames with a fixed heat release rate of 15 kW. The



Table 1: A Summary of Operating Conditions for the toluene+methane+hydrogen flames.

$Q_f$ , kW	MLR %	HLR %	Toluene, mg/s	$H_f$ , cm
10	5	13	172	45
10	10	13	165	44
10	15	13	158	40
10	20	13	152	38
10	25	13	147	34
15	5	13	258	54
15	10	13	247	50
15	15	13	238	45
15	20	13	228	42
15	25	13	220	38
20	5	13	344	59
20	10	13	330	52
20	15	13	317	49
25	5	13	430	64
25	10	13	412	55
10	5	5	206	40
10	10	5	196	39
15	5	5	310	48
20	5	5	413	54

next three flames have identical HLR as the first two sets with increasing MLR at a fixed heat release rate of 20 kW. The next two flames have a total heat release rate of 25 kW and can be studied for two different MLRs with identical HLRs. The last four flames are selected to study the effects of a much lower hydrogen flow rate on the flame properties by fixing the HLR at 5% and selecting the four flames that are stable at this low HLR.

#### Results and Discussion

Measurements of evaporation lengths in the crude oil+ methane flames were obtained using Mie scattering from drops since the interference due to scattering by soot particles could be separated. The evaporation lengths increased with increasing liquid loading and also with increasing firing rates. However, the evaporation lengths for the present atomizer-burner combination were found to be much smaller than the flame lengths showing that changes in these can not account for the flame length variations observed by Dutta et al. (1994). The global properties of the toluene+methane+hydrogen flames are discussed next.

Figure 1 shows the flame height " $H_f$ " normalized by the external orifice diameter " $d$ " (4.76 mm) plotted as a function of total heat release rate for the 19 flames in Table 1. As seen in Fig. 1, the flame heights increase with increasing heat release rate for all the conditions studied. For the lowest MLR of 5%, the flame height increases by approximately 40% with an increase in heat release rate from 10 to 25 kW. For flames with higher MLR, the increase in flame height with increase in heat release rate is less than that for MLR=5%. At a fixed heat release rate, the flame height decreases with increasing MLR for all of the conditions studied. The filled symbols in Fig. 1 show that the flame height decreases with decreasing HLR. This result is somewhat contrary to expectation but has been observed consistently. Measurements of emission temperature and transmittance shed some light on this issue and highlight the importance of radiative cooling in the reduction of the visible flame height. Similar to the finding of Dutta et al. (1994), the correlation for flame height from the literature are not capable of predicting the experimental results shown in Fig. 1.

The radiative heat loss fractions ( $X_R$ ) for the 19 flames were measured using the single point technique of Sivathanu and Gore (1993). The radial distance of the radiometer from the flame axis was selected to be equal to flame height  $H_f$  and the height of the radiometer from the burner exit was selected to be  $H_f/2$  in accordance with the single point technique. The  $X_R$  data for the 19 flames are plotted as a function of the heat release rate in Fig. 2. These measurements show some very interesting trends. For the lowest MLR, the radiant loss fractions are highest for the higher HLR. The  $X_R$  for these flames increase from 32% at a heat release rate of 10 kW to approximately 40% at a heat release rate of 25 kW. This result is completely opposite the conventional observations in gas fired jet flames for which the  $X_R$  remain independent of firing rate in a range of firing rates and then decrease with further increase. For intermediate MLRs, the  $X_R$  do remain relatively constant with increasing heat release rates. For the highest MLR studied, the  $X_R$  decrease with increasing heat release rate. The flames with the highest MLR (25%) and higher HLR (13%) show  $X_R$  values of approximately 10% which are lower than buoyant methane air flames studied in the past. Thus the present spray flame configuration leads to a substantial decrease in  $X_R$  with approximately 40% gaseous fuels added to the aromatic toluene.

Figure 3 shows measurements of average emission temperatures as a function of distance from the burner exit obtained using two wavelength emission pyrometry for 5 flames selected for detailed study. The flames represent a factor of 2 change in heat release rate, a factor of five change in MLR at a fixed heat release rate and a fixed HLR, and a factor of 2.6 change in the HLR at a fixed heat release rate and a fixed MLR. Measurements of average transmittance as a function of axial distance based on extinction of a He-Ne laser beam at 632 nm wavelength are also shown in Fig. 3. The emission temperature instruments record a temperature only if soot particles with a sufficient volume fraction (greater than 0.1 PPM) at temperatures above 1100 K are present along the diametric path. If these conditions are not satisfied the temperature is automatically set to 300 K. Thus the present instrument is not capable of measuring temperatures of nonluminous flames.

For the high MLR flame, the absence of soot particles in the near injector and the far field regions leads to the low average emission temperature data. The reduction in soot formation due to the high MLR is of significance. The remaining four flames have an MLR of 5% and show the effects of varying the HLR and the heat release rates. For a fixed heat release rate, an increase in HLR leads to a reduction in sooting tendency as shown by the increase in the transmittance. The temperature increases due to higher adiabatic flame temperature of hydrogen and remains higher for a longer distance due to slower radiative cooling. This leads to a longer visible flame with increasing HLR as seen in Fig. 1. The increase in temperature and flame size more than compensate for the reduction in the sooting tendency leading to a higher radiative loss fraction with increasing HLR. The increase in heat release rate at fixed HLR also has a similar effect on flame size and radiative loss fraction. The path integrated measurements are being deconvoluted to improve our understanding of these processes.

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Y. R. Sivathanu and J. P. Gore, 1993, "Total Radiative Heat Loss in Jet Flames from Single Point Radiative Flux Measurements," *Combustion and Flame*, Vol. 94, pp. 265-270.

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P. Dutta, Y. R. Sivathanu, and J. P. Gore, "Global Properties of High Liquid Loading Crude-Oil +Methane/Air Diffusion Flames," *Heat Transfer in Fire and Combustion Systems*, B. Farouk et al., Eds., ASME, New York, pp. 37-42.; also 1993, *Proceedings of the Joint Meeting of the Eastern and Central States Sections of the Combustion Institute*, pp. 635-639.



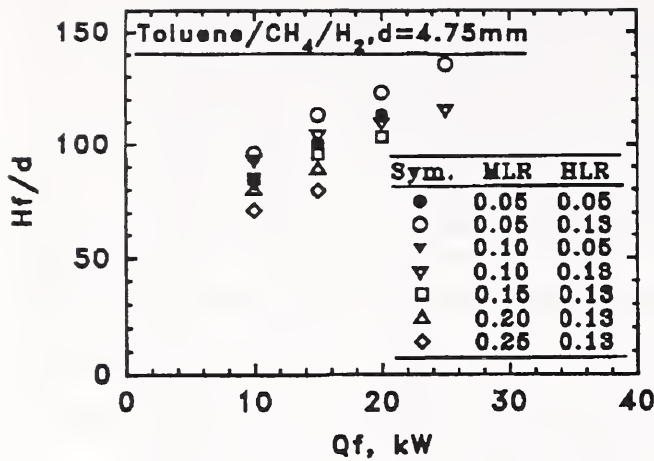


Figure 1. Flame height measurements for 19 toluene+methane+hydrogen spray fires.

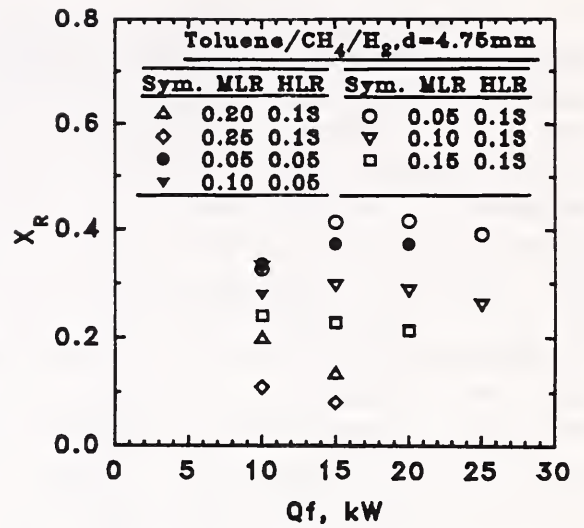


Figure 2. Radiative heat loss fraction measurements for 19 toluene+methane+hydrogen spray flames.

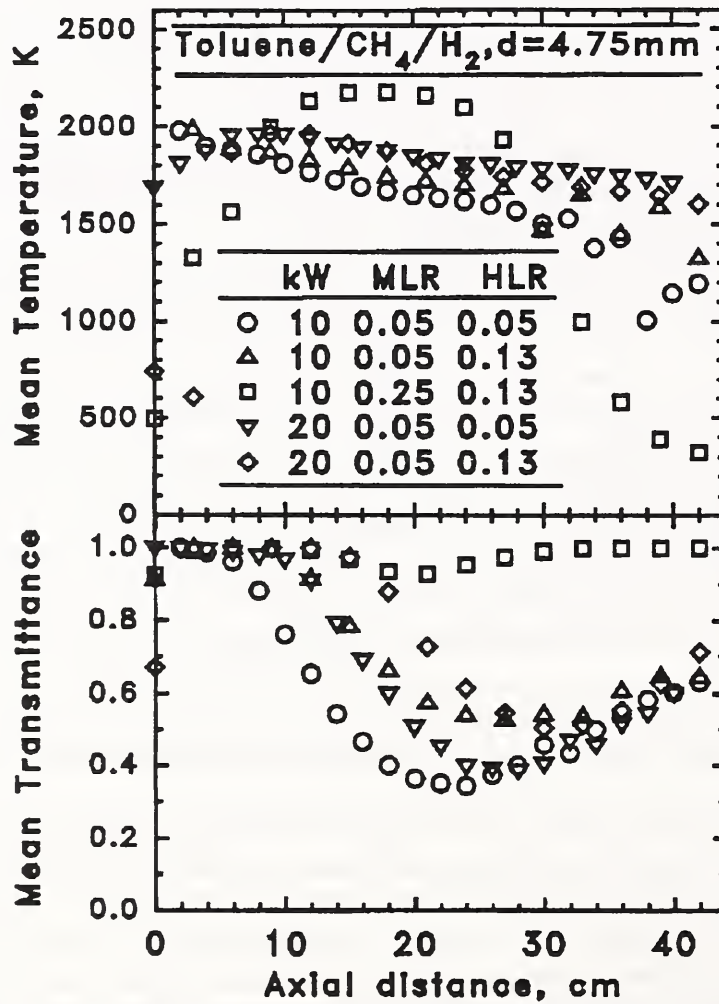


Figure 3. Effective temperature and transmittance measurements for toluene+methane+hydrogen flames using multi wavelength emission and absorption.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY94

Institution University of Maryland

Grant No. 70NANB1H1173,3

Grant Title Transient Cooling of a Hot Surface by Droplet Evaporation

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Technical Abstract

Introduction The modeling of the cooling effect of a sparse spray impinging on a low thermal conductivity semi-infinite solid is proposed. The results of the single droplet evaporative cooling model for the case of radiant heat input from above the surface are used to modify a closed form solution available in the literature. This solution describes the surface behavior for a semi-infinite solid with a circular portion of its surface at constant uniform flux where the rest of the surface is insulated. Three inputs are provided by the full model to modify this closed form solution: a) the heat flux due to conduction (as a portion of the total evaporative flux due also to the direct heat input by radiation); b) the evaporation time; and c) a constant multiplier which incorporates the effects of shrinkage observed when the droplet reaches the receding contact angle (White et al., 1994).

Experimental Data-Base The sparse spray used by Dawson and diMarzo (1993) is characterized by a distribution function which can be expressed as a polynomial of the sixth order. The distribution function represent the fraction of droplets deposited on the surface of radius  $r$ . This distribution function represents very closely the measured droplet distribution. The arguments used to derived this distribution are based on physical measurements and on the kinematic analysis of the droplet generator positioner.

The droplets are equal in size and are delivered with similar kinetic energy to the surface. Previous investigations concerning the single droplet behavior under radiant heat input (diMarzo et al., 1992)

have shown that the effect of impact are not significant since a gently deposited droplet tends to spread on the solid surface to a large extent due to radiant heat input effect on the surface tension at the liquid vapor interface.

Single Droplet Model The study of the effect of the droplet transient geometrical configuration reveals that a simple model based on a segment of a sphere approximation with the proper consideration for the receding angle condition provided good agreement with the data.

The hypotheses of one-dimensionality of the heat flux in the liquid and of flatness of the liquid vapor interface both tend to increase the calculated evaporation time. The one-dimensional computation is performed by neglecting the water motion towards the edge of the droplet during the last stages of the evaporative process thus underestimating the amount of water that can be evaporated at any given time step. The hypothesis of flatness of the liquid-vapor interface leads to underestimating the radiant input by direct radiation by increasing the reflected portion of the incoming radiant flux. These two effects are compensated in the single droplet model by introducing a constant multiplier which is evaluated by matching the experimental evaporation time at a single condition. The value of the multiplier is within the expected bounds which are dictated by physical considerations.

Multi Droplet Model The model is based on the closed form solution previously described which is used in the close field (i.e. for distances up to 5 radii from the droplet deposition location). In the far field, the droplet is represented by an instantaneous point sink which is time delayed by 60 percent of the evaporation time as described by Tartarini et al. (1993).

The results of the computations are qualitatively compared with the data in Fig. 1. Great care is taken in selecting a computational field that matches the same portion of the data collection field. The two top contour plots are obtained via infrared thermography, while the two bottom plots are the results of the code computations. The droplet deposition sites are random generated in accordance with the distribution function previously discussed. Note the similar extent of the isothermal at 129 °C and at 130 °C in the snapshots at 600 seconds and the similar correlation for the 116 °C and 120 °C isothermals at 50 seconds.

In Fig. 2 the overall transient is represented for the data available from Dawson and diMarzo (1993). The temperatures are normalized with respect to the initial solid surface temperature,  $T_{so}$ , and with respect to the steady state temperature,  $T_{ss}$ . The steady state temperatures are obtained from the code computations after validation against the data in terms of actual temperatures. Note that the experimental data and the results of the computations are in good agreement and that all the points are within  $\pm 20$  percent of the asymptotic value at steady state. The data set for  $T_{so} = 162$  °C and for a water mass flux  $G = 0.5$  g/m<sup>2</sup>-s is not within this bound. Further, note that this data set shows a stronger cooling effect than the data set at the same initial temperature but at twice the water mass flux. This apparent inconsistency can be explained since the initial portion of the transient for the data set at  $G = 0.5$  g/m<sup>2</sup>-s happens to be in nucleate boiling. The onset of nucleate boiling condition for water and Macor (i.e. the surface material) is observed for temperatures slightly above 162 °C. At lower water mass flux, nucleate boiling is observed in this data set and this occurrence causes a very rapid cooling of the surface within the first three minutes of the transient. Thereafter, evaporative cooling is observed. However, the initial portion of the transient has depleted the internal energy of the solid which then cools to a lower temperature. A slow upward trends in the surface temperatures is observed after the first ten minutes which suggests a recovery toward the steady state temperature.

The most notable result is that the temperature normalization is able to collapse the data and the computations. Note that the water mass flux is used to compute the steady state solid surface temperature. The time constant of the process yields a characteristic length of about one centimeter (i.e. penetration depth). This is comparable with the radius influence associated with the cooling effect of the single droplet (diMarzo et al., 1993).

#### Acknowledgements

The authors are indebted to Dr. H. Baum for his guidance in the development of the single and multi-droplet codes and to Dr. D. Evans for his continuous support and advice.

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P. Tartarini, M. diMarzo, "Dropwise Evaporative Cooling in a Radiative Field" *Proceedings of the 10th International Heat Transfer Conference*, Brighton, UK, in press, 1994

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G. White, S. Tinker, M. diMarzo, "Modelling of Dropwise Evaporative Cooling on a Semi-Infinite Solid Subjected to Radiant Heat Input" *Proceedings of the 4th International Symposium on Fire Safety Science*, Ottawa, Canada, in press, 1994

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BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT - FY94

LARGE SCALE TEST FACILITY

Professional Personnel

Emil Braun, Physicist

Project Objective

To perform large scale fire tests and provide data to support other fire research projects. To apply, refine, and develop methods and equipment that contribute to the successful conduct of large scale fire tests. To develop plans for the expansion and modernization of the facility.

Scope

Improve the utilization of the current facility, upgrade existing hardware, develop calibration techniques for primary fire test equipment, and introduce new measurement techniques to measure critical fire parameters. Development of a laboratory for the calibration and repair of measurement tools such as heat flux meters, pressure transducers, gas analyzers, etc. Provide a testbed for the evaluation of new measurement equipment, such as the Open Path FTIR, and new developments in computer fire modeling, such as model verification tests for HAZARD, wind aided plume flow, etc. Investigate and measure new fire phenomena in a large scale environment.

Technical Accomplishments

Activities in FY 1993:

- With removal of floor/wall furnace, new exhaust system was installed for the furniture calorimeter. This included the installation of new gas analysis equipment.
- Stand alone data acquisition equipment was installed to allow for the conduct of concurrent experiments.
- Rejuvenation and reuse of steel structure for the evaluation of complex floor assemblies. Successful test performed on an interstitial space assembly.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

IN SITU BURNING OF OIL SPILLS

Funding Agency: Minerals Management Service, DoI

Professional Staff: David D. Evans, Project Leader  
William D. Walton, Fire Protection Engineer  
Howard R. Baum, NIST Fellow  
Kevin McGrattan, Mathematician  
Anthony D. Putorti Jr., Fire Protection Engineer  
Nora H. Jason, Technical Information Specialist

Project Objective:

To determine the ignition and burning characteristics of crude oil on water using laboratory, mesoscale, and fields experiments to support the use of burning as an oil spill response technology.

Technical Accomplishments:

Smoke particulate emissions were measured during the 1993 Newfoundland Offshore Oil Burn Experiment (NOBE) conducted by a group of over 25 agencies from the United States and Canada off the coast of Newfoundland, Canada. Measurements were conducted using a helium filled miniblomp tethered to a vessel operated approximately 300 m downwind of the fire. The smoke sampling package suspended from the miniblomp consisted of sampling pumps which drew smoke through either a cascade impactor or filter and discharged gas samples into collection bags. The smoke yield and smoke particle size distribution were found to be similar to previous measurements made for mesoscale crude oil fires in Mobile, Alabama. For the Newfoundland burns the smoke yields was found to be 14.8 to 15.5 % of the mass of the fuel burned. Measurement with the cascade impactor showed that 83 percent of the smoke particulate mass was below 9.8  $\mu\text{m}$  in effective diameter.

Laboratory experiments were conducted to measure the ignition times for both oils and water-in-oil emulsions when heated by thermal radiation. Measurements of thermal radiation for diesel fuel sources of various sizes likely to be used as oil spill igniters were combined with the laboratory measurements of ignition times to provide a guide for ignition of spills of weathered and emulsified oils under no wind conditions.

Calculation of the smoke plume trajectory and smoke particle deposition from the in situ burning of oil spills were performed using a Large Eddy Simulation (LES) model. The LES model was applied to a number of scenarios of interest including: a study of Alaskan in situ burns, a comparison with data collected at the NOBE burns, and an investigation of the feasibility of using in situ burning during the Tampa Bay spill of 1993. Several improvements to the model were made, mainly to accommodate vertical shifts in wind speed and direction (wind shear).

NIST hosted, at the request of the Minerals Management Service, a workshop on in situ burning of oil spills in Orlando, Florida. The goals of the workshop were: 1. To present the state of knowledge

to representatives of industry, government, and research organizations, 2. To review the present status guidelines for the use of in situ burning as an oil spill response method, 3. To prioritize research and information needs to support decisions on the use of in situ burning of oil spills. The conclusions of the conference are included in the proceedings.

Publications:

"1993 Spill Off Tampa Bay, A Candidate for Burning?" R.P. LaBelle, E.J. Tennyson, J.A. Galt, K.B. McGrattan, Proceedings of the Seventeenth Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, June 8-10, 1994, Vancouver, British Columbia, pp. 635-649, (1994).

"Ignition of Weathered and Emulsified Oils," A.D. Putorti Jr., D.D. Evans, E.J. Tennyson, Proceedings of the Seventeenth Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, June 8-10, 1994, Vancouver, British Columbia, pp. 657-667, (1994).

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"Simulations of Smoke Plumes from Large Pool Fires," H.R. Baum, K.B. McGrattan, R.G. Rehm, Proceedings of the Twenty-Fifth International Symposium on Combustion, The Combustion Institute, Irvine, CA, August 1994.

"Smoke Measurements Using a Tethered Miniblimp at the Newfoundland Offshore Oil Burn Experiment," W.D. Walton, W.H. Twilley, J. McElroy, D.D. Evans, E.J. Tennyson, Proceedings of the Seventeenth Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, June 8-10, 1994, Vancouver, British Columbia, pp. 1083-1098, (1994).

"Smoke Plume Trajectory from In Situ Burning of Crude Oil in Alaska," K.B. McGrattan, H.R. Baum, R.G. Rehm, Proceedings of the Seventeenth Arctic and Marine Oil Spill Program (AMOP) Technical Seminar, June 8-10, 1994, Vancouver, British Columbia, pp. 725-733, (1994).

Related Grants:

Numerical Modeling of Plume Dispersal and Smoke Deposition from Large Scale Fires, Ahmed F. Ghoniem, Massachusetts Institute of Technology.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT - FY93-94

Institution Massachusetts Institute of Technology  
Grant No. 60NANB3D1439  
Grant Title: Development of a Computational Model for Large Fire Plumes  
Principal Investigator: Professor Ahmed F. Ghoniem  
Department of Mechanical Engineering  
Massachusetts Institute of Technology  
Cambridge, MA 0239  
Other Personnel: Hong Zhou, Graduate Research Assistant  
NIST Scientific Officer: Dr. Howard Baum

Technical Abstract:

Massive fires, whether they are natural (forest) or man made (oil spill or oil well), have substantial impacts on the environment. They may lead to measurable change in the local weather condition through their heat release and wind generation, and can cause severe air, and potentially ground pollution problems due to the injection of large quantities of hazardous gases into the atmosphere. The ultimate goal of this work is to develop computational models which can predict large fire dynamics and can be used to assess the impact of massive fires, in terms of the amount and composition of the fire combustion products, on the environment. In a previous effort, we developed smoke plume rise, dispersion and deposition computational models. In work, we are working on extending these models to include the fire zone as well.

Large fires have been modeled experimentally as pool fires, which while maintaining the major characteristics of massive fires, can be studied in the laboratory. In the experimental studies, three zones have been observed in a fire plume[1,2]: the continuous flame zone, the intermittent zone, and the plume zone. The continuous flame zone is located near the base of the pool, where the combustion between the fuel vapor and the entrained air causes a luminous, sooty, oscillating flame envelope to evolve. Above the continuous flame zone is the intermittent zone, where the flame surface fluctuates in a more irregular, turbulent, intermittent form, and chemistry becomes less important. In this zone, the products of combustion are further diluted by the entrained air. The plume zone lies above the top of the intermittent zone. The flow in this region, which we have modeled in our previous work [3-5] is non-reacting, turbulent and its dynamics can be predicted on the basis of a wind blown buoyant flow analysis.

This project is focused on the structure of the continuous, oscillating flame zone, which is of utmost importance to the heat release rate and combustion products composition. In this zone, the fuel is evaporated from the pool, and may be pyrolyzed by the thermal radiation from the luminous sooty diffusion flame. The fuel vapor is convected upwards by buoyancy, diffused into the reaction zone where it mixes and reacts with the entrained air. This, in turn, determines the structure and the luminosity of the flame which defines the radiation flux back to the pool, thus by controlling the rate of fuel evaporation. Within this continuous flame zone, periodic oscillations, speculated to occur due to the shedding of large vortical structures, have been observed in the laboratory and in real fires. This phenomenon has been called "fire puffing." Experimental investigations have shown that puffing is critical to the entrainment rate of the ambient air into the flame zone, and thus to the overall rate of burning (see, e.g., Refs. 6,7).



Figure 1 summarizes the experimental results [7] of pool fires of different sizes and various fuel types, including gaseous, liquid and solid fuels, as well as those obtained for nonreacting buoyant plumes. It can be observed that the puffing frequency is largely dependent on the size of the pool and almost independent of the fuel type. The solid line represents a correlation which can conveniently be expressed as  $St = 0.5$ , where  $St$  is the Strouhal number defined as  $f\sqrt{D/g}$ , the units for the puffing frequency,  $f$ , the pool diameter,  $D$ , and the gravity acceleration,  $g$ , are, respectively,  $Hz$ ,  $m$ , and  $m/s^2$ . Clearly, the puffing frequency is mainly controlled by the fluid mechanics rather than chemistry. Numerical results from our simulations of isothermal, axisymmetric helium plumes are also presented in Figure 1. The predicted frequencies fall well within the experiment data, confirming that puffing is consistent with the buoyant dynamics of the hot plume rising above the flame zone.

The objective of this work is to develop a computational methodology which can be used to describe the dynamics of fire plumes produced during the combustion of oil spills, forest fires, wild and urban fires, etc. The methodology is designed to predict the burning rate, concentration of smoke and other environmentally hazardous materials, fire intensity, plume rise and dispersion rate above the fuel pool. The modeling approach is constructed around a set of computational algorithms which are efficient enough to run, when coarse discretization is sufficient, on powerful engineering workstations. To achieve this efficiency, a set of Lagrangian computational schemes based on the vortex method, which limits the computational effort to the combustion and plume zone only, are used. The Lagrangian treatment will be extended to the computation of the radiative transport and smoke dynamics using recently developed fundamentally based simplifications [8]. The Lagrangian particle schemes for the dynamics, transport and radiation are also compatible with massive parallel computations when accurate detailed simulations are desired. The results of the model will be used to develop a better understanding of the mechanisms controlling fire spread and its dependence of the fuel characteristics, local wind conditions and ground terrain, the burning rate and the formation of environmentally hazardous material in each fire scenario.

During the first year of this effort, we focused on the simulation of the fluid dynamics and mixing in a buoyant plumes produced from a finite size source immediately above the fire. To validate the models, we focused on attempting to predict the puffing, qualitatively and quantitatively, and explain its origin. As shown in figure 1, the approach can indeed predict the puffing frequency and its dependence on the pool diameter. Since in this example, only non reacting flow is treated, we assume that the light fluid is injected at the plume source at a rate proportional to the buoyancy velocity. The computational method traces the material surfaces between the light fluid and the heavy fluid, and generates vorticity due the action of the baroclinic torque supported by the gravity and the density gradient. Vorticity is convected with the fluid particles and diffuses due to molecular diffusion. The latter is very small at high Reynolds number typical of fire problems and the overall dynamics is dominated by convection. Under these conditions, the vorticity sheet generated along the vertical interface is unstable, and rolls up to form large coherent vortical structures. The shedding of these structures is essentially what leads to the observed puffing phenomenon, as shown by the results of figure 2.

The results in figure 2 were obtained for a plume whose density, normalized by the ambient density is  $\rho f = 0.1413$ , initial velocity normalized by the buoyant velocity  $v f = 0.1644$ , Reynolds number based on pool diameter,  $Re = 700$ , and Richardson number  $Ri = 225$ . The figure shows the density distribution above the plume source. Large material puffs, composed of the plume material mixed with the entrained air and associated with vortical structures are shed periodically near the pool. In the structure nearest to the pool, there exists a region where the density is almost equal to that at the pool, i.e., the "fuel rich" region. The boundary of the puff is blurred due to the mixing between the plume gas and the ambient air by the combined action of convection and diffusion. In figure 2a, a new puff is rolled up near the pool. In figure 2b and 2c, this puff moves upwards, propelled by buoyancy, while entraining the fresh air from the ambient. This leads to the overall increase of the density of this puff. Meanwhile, a new bulge appears in figure 2b and 2c, leading to the formation of a third puff in figure 2d, thus completing an entire cycle. All of these phenomena are qualitatively similar to those observed in the experiments. The power spectral density for the radial velocity at  $r = 0.4$ ,  $z = 0.8$ , both normalized

with respect to the plume diameter, shows a distinct peak at 7.7 Hz, corresponding to a Strouhal number of 0.5, as mentioned earlier.

The vorticity field associated with these results shows that the concentration of vorticity, which is generated along the diffuse interface between the plume fluid and its surrounding, is indeed highest within the same rounded structures shown by the density distribution shown in figure 2 [9]. The large structures, i.e. the "puffs," can be clearly observed as well in the plots of the vorticity distribution and the convoluted material surfaces. Both confirm the speculation that fire puffing is connected with the shedding of large vortices forming as the vorticity sheet between the hot gases and the ambient atmosphere roll up due to an intrinsic instability. We still need to confirm the survival of these structures under reacting flow conditions.

In future work, we will obtain the field of the Shvab-Zeldovich variables using the assumption of infinite chemistry, to compute the species distribution, the temperature profile, etc. The temperature and species distribution will then be used to estimate the radiation flux to the pool and the fuel evaporation rate. The numerical method will then be extended to account for the dynamics of the volumetric expansion near the fire front.

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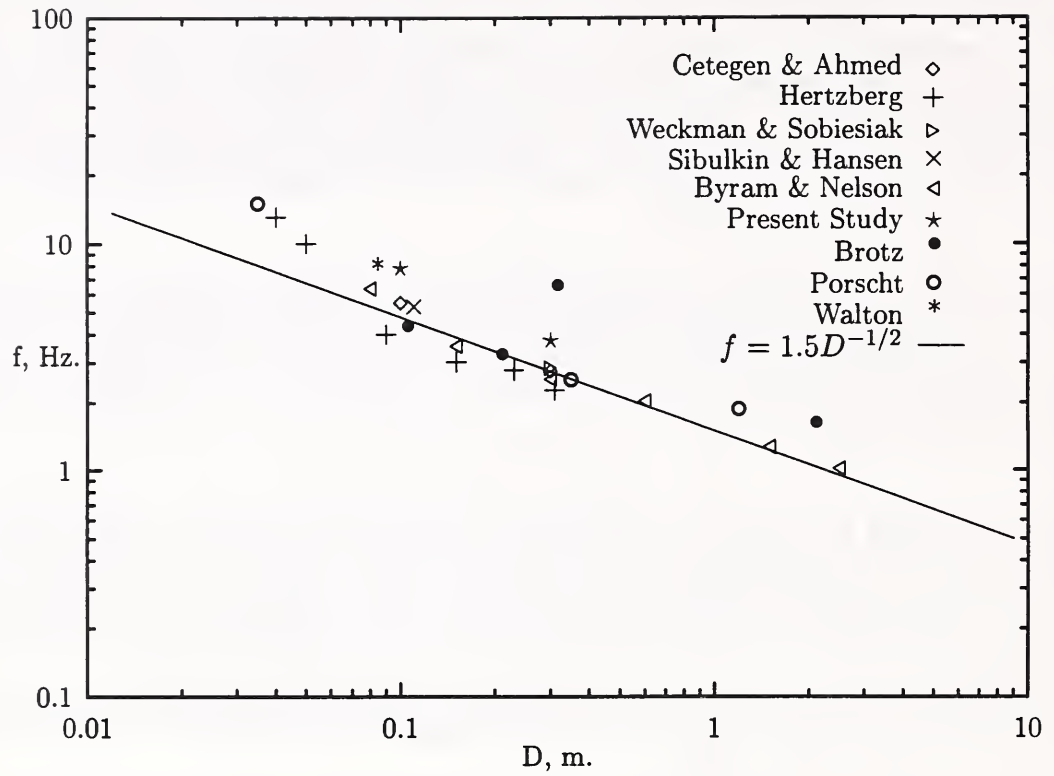


Figure 1: Comparison between the numerical prediction and experimentally measured puffing frequency of buoyant and fire plumes and its dependence on the pool diameter.

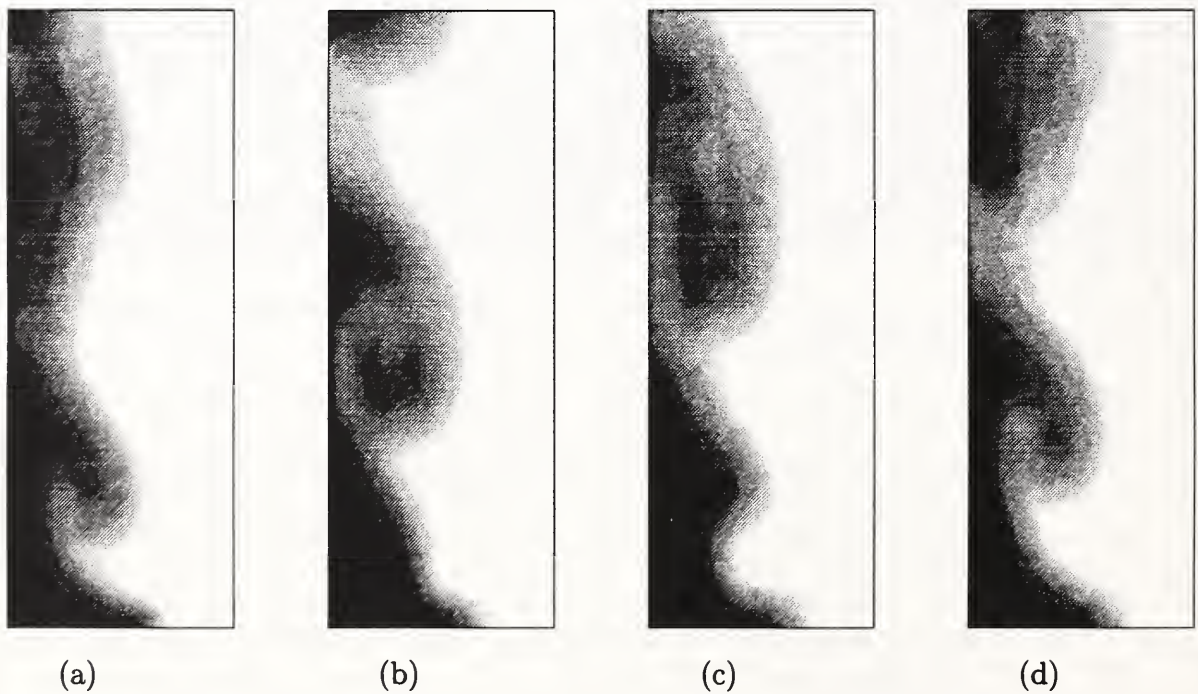


Figure 2: The density field of the buoyant plume at  $t = 26.4(a), 27.0(b), 27.4(c), 27.8(d)$ , nondimensionalized with respect to the pool diameter and the buoyancy velocity. The pool diameter is 0.1m, while the Reynolds and Richardson number are, respectively, 700 and 225.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT – FY94

SIMULATION OF TURBULENT COMBUSTION AND TRANSPORT IN FIRES

Professional Personnel

Howard R. Baum, NIST Fellow  
Kevin B. McGrattan, Mathematician  
Ronald G. Rehm, NIST Fellow (CAML)

Project Objective

Develop a fundamental understanding of the mechanisms which control the gas phase combustion and transport processes in fires and a predictive capability which will allow the computer simulation of these processes to be based on the mathematical expression of underlying physical principles.

Scope

The interaction of a fire with its environment, whether that environment is an individual room in a building or the atmosphere in the vicinity of a large outdoor fire is the problem under consideration. Theoretical and computational techniques are applied to the study of transport, mixing, diffusion, radiation, and reaction processes occurring at widely different length and time scales. Detailed studies of individual phenomena are carried out in a manner that permits them to be assessed individually and later combined into overall simulations of problems of interest.

Technical Accomplishments

The study of gas phase combustion and convection processes in fires using a combination of mathematical analysis and computer simulation is continuing. The approach is to solve the governing equations directly (if approximately) by decomposing the fire into a large scale convective and radiative transport problem coupled to a small scale "thermal element" model of combustion and radiative emission. The thermal element model solves the combustion equations in a local Lagrangian coordinate system convected by the large scale motion, which in turn is driven by the heat released by the combustion processes. The large scale flow is studied using finite difference techniques to solve large eddy simulations of the Navier-Stokes equations. The application of this methodology to enclosure fires is described in the priority project, "Development of Large Eddy Enclosure Fire Model".

The work on the Large Eddy Simulation (LES) plume trajectory model (see Figure 1) continued with the development of certain refinements to the existing methodology. These refinements are meant to address certain atmospheric and geographical phenomena such as wind shear and terrain effects. As yet these refinements have not been implemented in the general purpose predictive code because the issues that are addressed are scenario specific. The model is usually used to address a wide variety of meteorological conditions and fire sizes. Adding terrain and wind shear to the parameter space makes this predictive process even more complicated. It is foreseen that the scenario specific refinements will be used either when comparing the model with actual experiments or when addressing a very specific situation. An example of the terrain capability is shown in Figure 2, where the streamlines of a flow of stratified air over a large obstacle is simulated. This flow field could be incorporated into the LES model to account for a rising shore

line, for example.

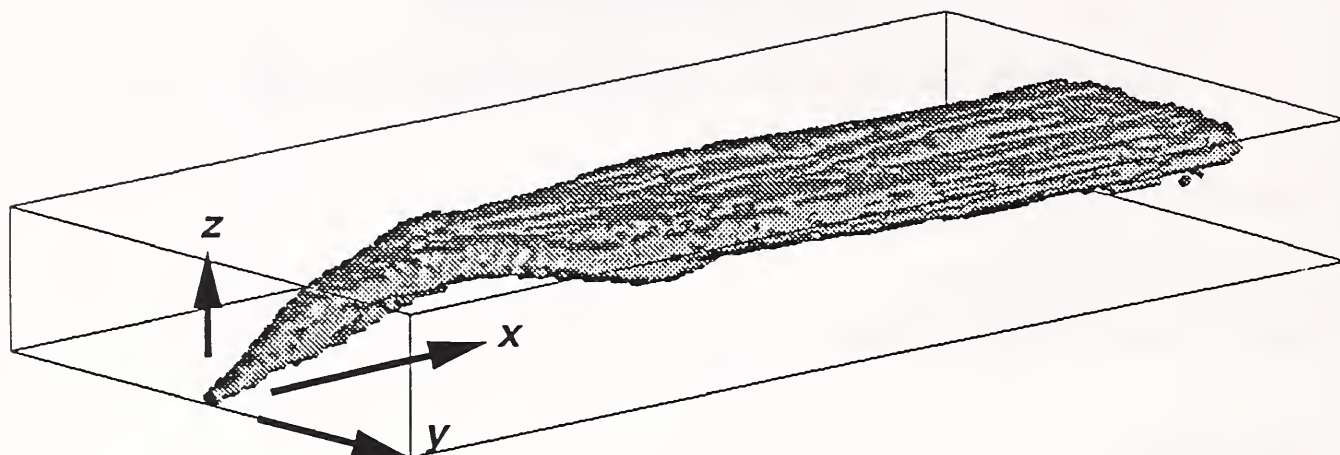


Figure 1: Numerical simulation of a smoke plume from a large outdoor fire. The viewing space is 1 km high, 8 km long and 4 km wide. The wind speed is roughly 6 m/s. The fire size is about 200 MW.

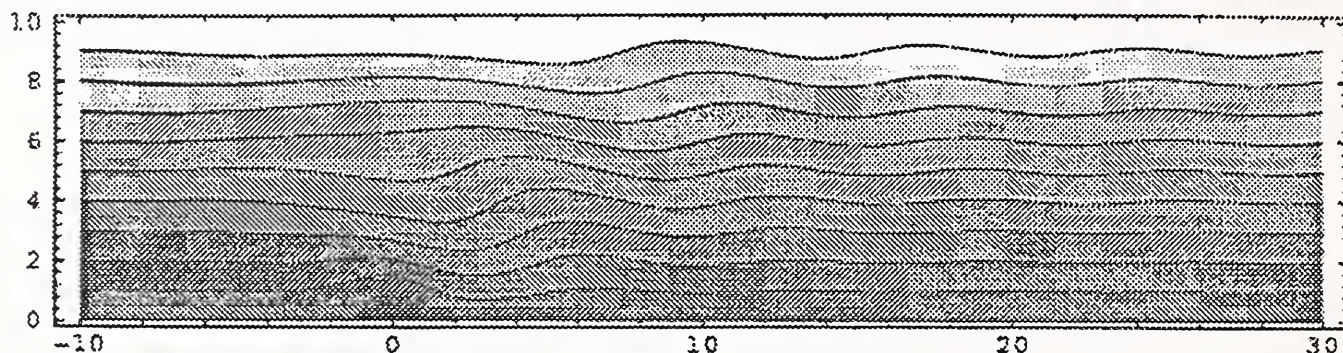


Figure 2: Streamlines of flow over an obstacle. The length scale is in units of kilometers. This obstacle might be considered a shoreline or mountain range, for example.

A missing piece in the assessment of large outdoor fire plumes is the dynamics of the fire itself. It is virtually impossible with any type of numerical model to simultaneously track the smoke plume for tens of kilometers while at the same time resolve the fine scales of the fire itself. Instead, a numerical model of the fire and the initial segment of the smoke plume is modeled separately. This model of the fire itself will utilize the methodology put forth above. Preliminary two and three dimensional pool fire simulations have been performed to assess the practicality of the computations. The resolution of the numerical grids must be fine enough to adequately describe the entrainment of air into the fire plume. The puffing frequency of the simulated fires has been checked against the well known correlation in which the frequency is proportional to the reciprocal of the square root of the diameter. Figure 3 shows the nondimensionalized temperature contours of an axisymmetric fire plume. Evidence of the puffing can be seen in terms of periodic shedding of vortices at the base of the fire. The results of these calculations are checked against experimental correlations.

#### Reports and Publications

Baum, H.R., Ezekoye, O.A., McGrattan, K.B. and Rehm, R.G., "Mathematical Modeling and Computer Simulation of Fire Phenomenon", *Theoretical and Computational Fluid Dynamics* 6:125-139 (1994).

Baum, H.R., McGrattan, K.B., and Rehm, R.G., "Simulations of Smoke Plumes from Large Pool Fires", *Proceedings of the 25th International Symposium on Combustion*, The Combustion Institute, Irvine, CA,



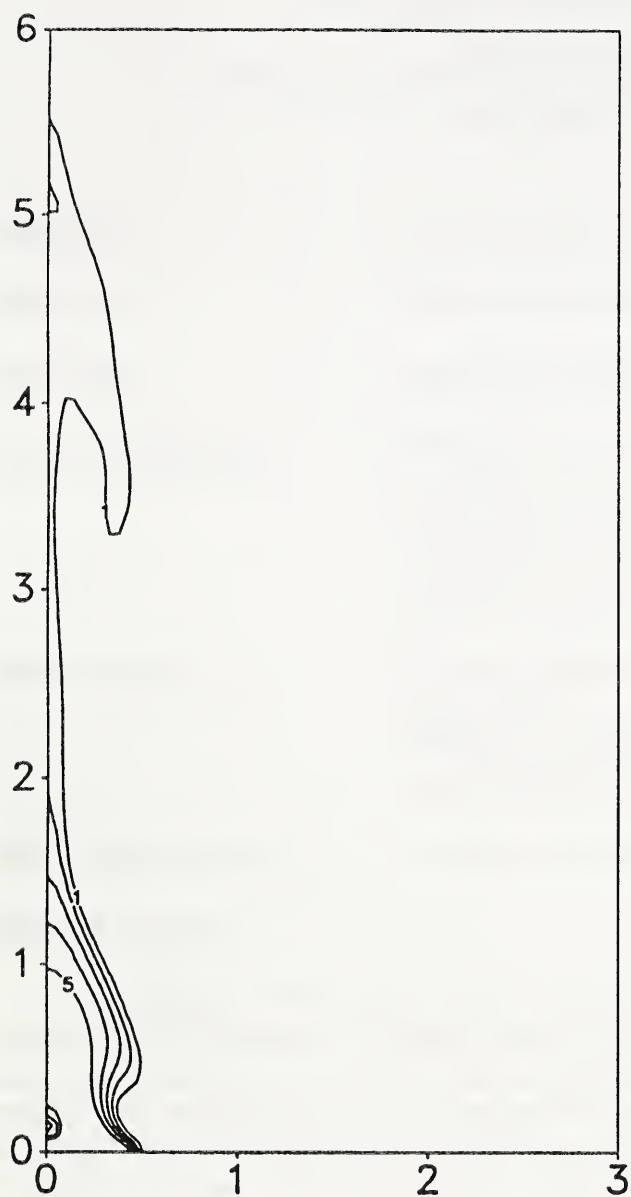


Figure 3: Nondimensionalized temperature profile ( $\Delta T/T_0$ ) for an axisymmetric plume. The shedding vortices are manifested by the appendages of the contours.

August 1994.

Related Grants

“Radiation from Turbulent Luminous Flames,” Prof. G.M. Faeth, University of Michigan.

“Fire Modeling,” Prof. P.J. Pagni, University of California, Berkeley.

“Numerical Modeling of Plume Dispersion and Smoke Deposition from Large Scale Fires,” Prof. A.F. Ghoniem, Massachusetts Institute of Technology.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT-FY94

Institution The University of California at Berkeley

Grant No. GDOC 60NANB3D1438

Grant Title Large Fire Analyses

Principal Investigator Professor Patrick J. Pagni  
Mechanical Engineering Department  
5131 Etcheverry Hall  
University of California  
Berkeley, CA 94720

Other Personnel Professor Charles M. Fleischmann  
Javier Trelles  
Nicholas A. Dempsey  
Robert Schoerder

NIST Scientific Officer Dr. Howard R. Baum

Technical Abstract

Introduction This abstract describes our research program on large fires for 1994. Our eventual goal is to develop a modular urban/wildland interface fire growth model. During the coming year we will focus on two of the principal problems: 1.) The fire-induced flow field generated from multiple fire sources and its role in lofting burning brands which are recognized as one of the most important and least understood fire spread mechanisms; and 2.) The consequences of those brands as they land on or near individual structures, i.e. we will attempt to quantify a building's response to typical wildland fire exposures. Through our connection with Berkeley's College of Natural Resources the rich forest fire literature is being fully utilized. Our direct experience with the third worst fire in U.S. history, the 20 October 1991 Oakland Hills Fire, and the 1993 Los Angeles fires provides specific case studies for the application of our models.

The very successful backdraft experimental program conducted at the Richmond field Station over the last several grant periods has been completed by Professor Charles M. Fleischmann. He is continuing this research while conducting Fire Protection Engineering classes in the Civil Engineering Department at the University of Canterbury, New Zealand. His well-characterized backdraft apparatus has also provided valuable compartment fire model validation data. This work was presented at the Fourth International Symposium on Fire Safety Science at Ottawa, Canada. Finally, Professor Howard Emmons and I continue to collaborate on a text aimed at fire protection students and professionals entitled *Case Studies in Fire Safety Engineering Science* which will be published by Wiley.

Backdrafts A backdraft is defined as the rapid deflagration of accumulated excess pyrolyzates

mixed with fresh air by a gravity current formed by the sudden opening of a vent, e.g., a thermally compromised window, a door opened by fleeing fire victim or a structural failure. Ignition occurs by a smoldering brand or a small surviving flame. Dr. Fleischmann's experiments showed that our initial idea of a thin mixed layer riding at the edge of the gravity current was wrong. His salt-water and model backdraft experiments proved that the entire gravity current is mixed. This is important since a larger region is flammable and therefore backdrafts are more easily produced than previously thought. Dr. McGrattan at NIST demonstrated, with elegant numerical simulations, that large scale vortical structures, providing ignitable mixtures throughout, fill the gravity current. Their joint paper will be published shortly.

Urban/Wildland Interface Fire Growth Model Each physical phenomenon is separately modeled so that improvements can be incorporated as they occur. This approach also allows the overall model to be specialized to particular applications. Twenty phenomena have been identified for separate modules so far. Two graduate students will be addressing modules at opposite ends of the spread process during the coming grant period. One will focus on the initial brand lofting that occurs in the flow fields produced by many large fires using the Baum-McCaffery mass fire model. Brand distributions expected from different types of vegetation and structures will be determined from the literature. A critical question is how does the brand weight and shape change during flight due to combustion. The pioneering work of Tarifa on wooden spheres and cylinders representing vegetative brands, reported in the Tenth International Symposium on Combustion proceedings( pp 1021-1037 ), will be extended to thin wedges representing shakes and shingles from structures. The distribution of landing sites and the condition of the brands upon landing determine the potential ignition sites of new spot fires. The second student will explore the final stage of the spread process, i.e., what is the response of a structure and the vegetation surrounding it to the deposited brands. To model the urban/wildland fire spread rate, it will be necessary to know the time lapsed between initial structural ignition and eventual brand production by that structure. So it will be necessary to properly incorporate existing compartment fire models into the interface model. Both students intend to complete their doctoral dissertations during the coming grant period.

#### Reports and Papers

1. C. M. Fleischmann, P.J. Pagni, R.B. Williamson, "Exploratory Backdraft Experiments", *Fire Technology*, 29:4,298-316, 1993.
2. P. J. Pagni, "Causes of the 20 October 1991 Oakland Hills Conflagration," *Fire Safety Journal*, 21:4,331-340, 1993.
3. A. A. Joshi and P.J. Pagni, "Fire-Induced Thermal Fields in Window Glass I - Theory," *Fire Safety Journal*,22:1,25-44,1994.
4. A. A. Joshi and P.J. Pagni, "Fire-Induced Thermal Fields in Window Glass II - Experiments," *Fire Safety Journal*,22:1,45-66,1994.
5. C. M. Fleischmann, P.J. Pagni, R.B. Williamson, "Salt Water Modeling of Compartment Gravity Currents", *Fire Safety Science - Proceedings of the Fourth International Symposium*, IAFSS, in press.
6. C. M. Fleischmann, P.J. Pagni, R.B. Williamson, "Quantitative Backdraft Experiments", *Fire Safety Science - Proceedings of the Fourth International Symposium*,IAFSS, in press.



BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY  
GRANTEE PROJECT —FY94

Institution: The University of Michigan  
Grant No.: NANB1D1175

Grant Title: Soot, Carbon Monoxide and Radiant Emissions of Luminous Turbulent Flames

Principal Investigator: Professor G. M. Faeth  
Department of Aerospace Engineering  
3000 FXB Building  
The University of Michigan  
Ann Arbor, MI 48109-2118

Other Personnel: Z. Dai, Doctoral Candidate  
Ü. Ö. Köylü, Postdoctoral Fellow  
L.-K. Tseng, Postdoctoral Fellow

NIST Scientific Officer: Dr. Howard R. Baum

Technical Abstract:

Introduction. This investigation is examining two aspects of unwanted fires, as follows: (1) the mean and turbulence structure of self-preserving buoyant turbulent plumes, and (2) the physical and optical properties of soot in diffusion flame environments. The findings of the research have applications to modeling fires in structures, developing materials test codes, and developing fire detectors.

Structure of Turbulent Plumes. Understanding the structure and mixing properties of round buoyant turbulent plumes is an important fundamental problem that has attracted significant attention since the classical work of Rouse et al. (*Tellus* 4, 201, 1952). In particular, the round buoyant turbulent plume has been widely used to develop and evaluate methods for predicting the properties of buoyant turbulent flows. This motivated initial measurements in this laboratory which emphasized conditions where the buoyant turbulent plumes become self-preserving, i.e., where they achieve classical turbulence similarity scaling and disturbances due to effects of the source have been lost (Dai et al., *J. Heat Trans.* 116, 409, 1994; *Ibid.*, in press).

The present initial studies of round buoyant turbulent plumes showed that flow properties approximated self-preserving behavior for streamwise distances larger than 87 source diameters and 12 Morton length scales from the source. This was significantly farther from the source than past observations, and yielded narrower flow widths and larger mean velocities and mixture fractions near the axis, suggesting that earlier results in the literature were representative of transitional rather than self-preserving plumes. This finding helped explain past problems of modeling buoyant turbulent flows using existing data, see Pivovarov et al. (*Combust. Flame* 92, 308, 1992), but also implied that new

measurements of round buoyant turbulent plume properties, properly within the self-preserving region of the flow, are needed. Thus, the objective of this phase of the investigation was to obtain data of this type.

The test plumes consist of dense gas sources (carbon dioxide and sulfur hexafluoride) in order to provide negatively buoyant plumes in still and unstratified air. Measurements of mixture fractions are made using laser-induced fluorescence (LIF) and measurements of velocities are made using laser velocimetry (LV). Measurements in the past year have concentrated on turbulence quantities needed to supplement measurements of mean mixture fractions and velocities mentioned earlier. Properties considered have included fluctuating quantities, probability density functions, temporal power spectra, temporal and spatial integral scales, two-point spatial correlations and single point correlations of turbulence quantities up to fourth order — all in the self-preserving region of the flow.

In the following only a few sample results concerning the properties of round buoyant turbulent plumes will be considered, see papers by Dai et al. summarized at the end of this report for more details. One of the most interesting issues of this work has been the observation of effects of turbulence/buoyancy interactions based on comparing the present measurements in self-preserving round turbulent plumes with recent measurements in self-preserving round turbulent jets, see Panchapakesan and Lumley (*J. Fluid Mech.* 246, 197, 1993) and references cited therein. While turbulence/buoyancy interactions influence most turbulence properties in plumes, they particularly affect mixture fraction fluctuations. In particular, mixture fraction fluctuations near the axis of plumes are nearly twice those in nonbuoyant jets. This behavior is caused by the strong production of mixture fraction fluctuations near the flow axis due to buoyant instability resulting from the rapid decay of mean scalar properties in the streamwise direction in round buoyant turbulent plumes. Notably, due to smaller streamwise decay rates, analogous effects for velocity fluctuations are small in all plumes, and should be much reduced for mixture fraction fluctuations in plane plumes (although the latter behavior has not yet been experimentally confirmed).

Another interesting turbulence/buoyancy interaction was observed in the temporal power spectra of both mixture fraction and velocity fluctuations. In particular, in addition to the conventional inertial/diffusive regime, where the spectra decay according to the  $-5/3$  power of frequency, there is a prominent inertial/diffusive region at higher frequencies where the spectra decay according to the  $-3$  power of frequency that is not seen in nonbuoyant turbulent flows. This behavior should be useful for investigating the effect of the fine-scale features of buoyant turbulent flows that are crucial issues for computationally tractable three-dimensional time-dependent numerical simulations and sub-grid-scale modeling of these flows.

Current work is emphasizing measurements of various correlations and moments of velocity and mixture fraction fluctuations, and using these results to construct scalar and velocity variance budgets and to evaluate existing ideas for predicting the properties of buoyant turbulent flows.

**Soot Properties.** An understanding of the optical properties of soot is needed in order to properly interpret nonintrusive optical measurements of soot concentrations and structure, and to predict the continuum radiation properties of soot. These objectives are somewhat problematical, however, due to the complexities of soot structure. In particular, soot consists of nearly monodisperse spherical primary particles (dia. less than 60 nm) that individually satisfy the Rayleigh scattering approximation, but these primary particles collect into large aggregates (frequently exceeding 1000 nm in size) that approximate



neither Rayleigh nor Mie scattering behavior (Köylü and Faeth, *J. Heat Trans.* 115, 409, 1993). Nevertheless, earlier work in this laboratory, where both the soot structure and scattering properties were measured, suggested that an approximate scattering theory based on the Rayleigh-Debye-Gans scattering approximation, while assuming that soot aggregates are polydisperse mass fractal objects (denoted RDG-PFA theory in the following), was reasonably satisfactory (Köylü and Faeth, *J. Heat Trans.* 116, 152, 1994; *ibid.*, in press). Nevertheless, this evaluation did not reach the small-angle (Guinier) regime where the accuracy of RDG-PFA theory is most questionable. Additionally, accurate evaluation of RDG-PFA theory at all angles requires careful measurements of soot structure based on transmission electron microscopy (TEM) measurements, raising questions about the fractal properties of soot and the relationship between the actual structure properties of soot aggregates and their projected images. Finally, long-standing deficiencies about soot refractive index data limit the successful application of soot optical property theories. Thus, there are three objectives of this phase of the investigation, as follows: (1) to complete an evaluation of RDG-PFA theory in the critical Guinier regime, (2) to complete an investigation of the fractal properties and the relationship between the actual and projected structure properties of soot aggregates, and (3) to initiate an investigation of the refractive indices of soot.

The evaluation of RDG-PFA scattering theory in the Guinier regime is fully described by Farias et al. (*J. Heat Trans.*, in press). This study involved comparing RDG-PFA predictions with results computed using the more exact ICP approach of Iskander et al. (*Appl. Optics* 28, 3083, 1989). These calculations showed that RDG-PFA and ICP predictions in the Guinier regime agreed within experimental uncertainties. Thus, coupled with earlier satisfactory experimental evaluations, RDG-PFA theory appears to be the best available approximate solution for the optical properties of soot and is recommended for applications involving fire environments.

The investigation of the fractal and projected structure properties of soot aggregates is fully described by Köylü et al. (*Combust. Flame*, in press). The experimental work involved analysis of stereoscopic TEM images of soot aggregates in order to find the fractal properties of soot and the relationships between projected and actual soot properties. It was found that both the fractal properties and the relationship between projected and actual properties are durable properties of soot, with current best estimates of the fractal dimension and prefactor of 1.83 and 8.5, respectively. The computational portion of this study generally confirmed the experimental results.

The investigation of the refractive index properties of soot is still in progress. Experiments in this case are considering soot emitted from large buoyant diffusion flames fueled with acetylene, ethylene, propylene and propane. The first evaluation of soot refractive indices is proceeding by measuring the extinction coefficients of this soot for roughly twenty wavelengths in the range 200-5200 nm. This provides one piece of information needed to find the refractive indices but another is needed because there are two unknowns (the real and imaginary parts of the refractive indices) at each wavelength. Thus, the second piece of information is being supplied by the Kramers-Krönig (KK) causality relationships while interpreting all results using RDG-PFA theory in conjunction with earlier measurements of the structure of the soot. A final aspect of analysis involves the development of a dispersion model for the refractive indices of soot; this model is needed in order to estimate the temperature variation of soot refractive indices, which must be known before soot refractive indices can be measured in flames.

Current work is concentrating on measuring and developing appropriate dispersion models, for soot refractive indices, considering a variety of flame environments. The overall goal of this work is to determine the effects of fuel type, state of formation or



oxidation, residence time and temperature on soot refractive indices. Once these issues are resolved, subsequent work can focus on nonintrusive optical diagnostics for soot properties as well as the radiative properties of soot.

### Reports and Paper

1. Z. Dai, L.-K. Tseng and G.M. Faeth, "Structure of Round, Fully-Developed, Buoyant Turbulent Plumes," *J. Heat Trans.*, Vol. 116, No. 2, pp. 409-417, 1994.
2. Z. Dai, L.-K. Tseng and G.M. Faeth, "Velocity Statistics of Round, Fully-Developed Buoyant Turbulent Plumes," *J. Heat Trans.*, in press; also ASME Winter Annual Meeting, Chicago, November 1994, in press.
3. Z. Dai, L.-K. Tseng and G.M. Faeth, "Buoyant Turbulent Plumes Revisited," *Heat and Mass Transfer 94* (A.R. Balakrishnan and S.S. Murthy, ed.), Tata McGraw-Hill Publishing Co., Lmted., New Delhi, pp. 59-66, 1994; also ISHMT/ASME Heat and Mass Transfer Conference, Bombay, India, January 1994.
4. Ü.Ö. Köylü and G.M. Faeth, "Optical Properties of Overfire Soot in Buoyant Turbulent Diffusion Flames at Long Residence Times," *J. Heat Trans.*, Vol. 116, No. 1, pp. 152-159, 1994.
5. Ü.Ö. Köylü and G.M. Faeth, "Optical Properties of Soot in Buoyant Turbulent Diffusion Flames," *J. Heat Trans.*, in press.
6. T.L. Farias, M.G. Carvalho, Ü.Ö. Köylü, and G.M. Faeth, "Computational Evaluation of Approximate Rayleigh-Debye-Gans/Fractal-Aggregate Theory for the Scattering and Extinction Properties of Soot," *J. Heat Trans.*, in press; also 6th AIAA/ASME Thermophysics and Heat Transfer Conference, Colorado Springs, CO, June 1994.
7. Ü.Ö. Köylü, G.M. Faeth, T.L. Farias and M.G. Carvalho, "Fractal and Projected Structure Properties of Soot Aggregates," *Combust. Flame*, in press.
8. Z. Dai, L.-K. Tseng and G.M. Faeth, "Mixture Fraction and Velocity Statistics in Fully-Developed Turbulent Plumes," Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, PA, pp. 173-176, October 1993.
9. T.L. Farias, M.G. Carvalho, Ü.Ö. Köylü, and G.M. Faeth, "A Computational Study of the Absorption and Scattering Properties of Soot," Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, PA, pp. 394-397, October 1993.
10. G.M. Faeth, "Soot Morphology and Optical Properties in Nonpremixed Flame Environments," Proceedings of the Spring Technical Meeting, Canadian Section of the Combustion Institute, Pittsburgh, PA, pp. 2-1 to 2-5, May 1994
11. Z. Dai, L.-K. Tseng, and G.M. Faeth, "Properties of Self-Preserving, Round, Buoyant Turbulent Plumes," 47th Annual Meeting, American Physical Society, Division of Fluid Dynamics, Atlanta, GA, November 1994, in press.
12. Ü.Ö. Köylü, Z. Dai, L.-K. Tseng, and G.M. Faeth, "Radiation and Mixing Properties of Buoyant Turbulent Diffusion Flames," Report No. GDL/GMF-93-01, University of Michigan, Ann Arbor, 1993.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
PRIORITY PROJECT – FY94

DEVELOPMENT OF LARGE EDDY ENCLOSURE FIRE MODEL

Professional Personnel

Howard R. Baum, NIST Fellow  
Kevin B. McGrattan, Mathematician  
Ronald G. Rehm, NIST Fellow (CAML)

Project Objective

Develop by 1997 a three dimensional large eddy simulation capability for heat and smoke movement in mechanically ventilated enclosed commercial and industrial spaces.

Scope

There is an internationally expressed need for an advanced heat and smoke transport simulation capability for fire scenarios in large mechanically controlled environments. Commercial CFD codes cannot offer the required spatial and temporal resolution due to their generality of purpose and turbulence models, while their proprietary nature prevents generally available modification. The present commercial codes depend upon empirical turbulence models for their output, inherently limiting their predictive capability. This restriction leads to an ongoing burden of detailed experimental verification of the computations for each new fire scenario or building geometry.

Technical Accomplishments

A large eddy simulation model of smoke movement in enclosed spaces has been under development for several years. The focus of the work has been to simplify the Navier-Stokes equations which govern the fluid flow to yield high resolution solutions which resolve the flow on lengths scales from centimeters to tens of meters. This enhanced resolution will greatly reduce the dependence on empirical turbulence models which are characteristic of present day field models. The flexibility and efficiency of the methodology combined with the increased speed of modern generation computers now allows for Reynolds numbers<sup>1</sup> on the order of  $10^5$  for two dimensional simulations, and  $10^4$  for three dimensional simulations. These simulations have been performed in a variety of geometrical configurations. In order to preserve the efficiency and high resolution of the computations, a simple masking technique has been implemented which essentially allows for solid wall boundaries which coincide with computational grid cells. This technique allows the user to define a multi-room building element by merely "blocking off" grid cells which correspond to solid walls. This technique is particularly well suited to the fire problem since typical building elements are inherently rectangular. Even in cases which involve cylindrical elements (tunnels, shafts), the numerical code may be easily written in cylindrical coordinates and still make use of the efficient Poisson solvers which are vital to solving the elliptic equation for the pressure.

An example of the methodology is shown in Figure 1. A series of experiments were conducted in Sweden

<sup>1</sup>The Reynolds number is given as  $Re = UH/\nu$ , where  $H$  is the enclosure height,  $U$  is the characteristic buoyant velocity, usually given by  $U = \sqrt{gH\Delta\rho/\rho_0}$ ,  $\rho$  is the density of the gas, and  $\nu$  is an eddy viscosity.



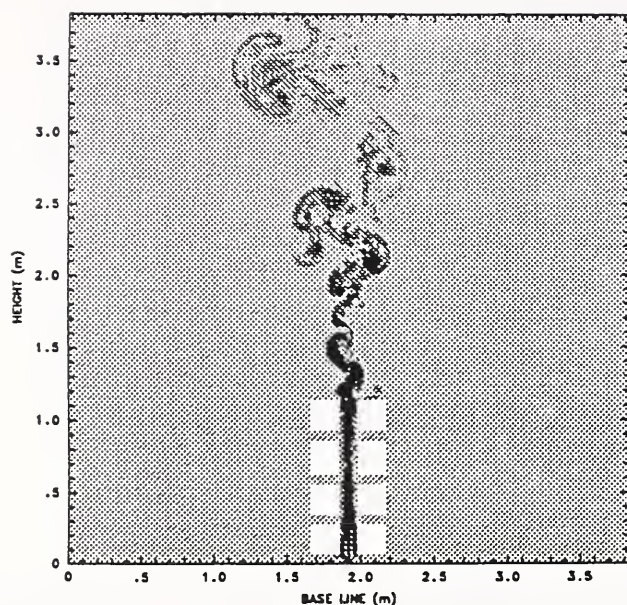


Figure 1: Temperature profiles of the rising smoke column from a rack storage fire simulation. Shown is a cross section of the quasi-2D experiment. The heat release from the line burner is about 30 kW/m. About 10,000 thermal elements released steadily in time and according to a Gaussian distribution in space simulate the heat release. The computational grid is  $384 \times 384$ , yielding 5 mm resolution. The Reynolds number for the simulation is 100,000.

by Haukar Ingason of SP in which various long non-flammable boxes were stacked with spaces in between. The source of the fire was a line burner, and thus the experiment was designed to be two dimensional. The numerical simulation of the experiment required a grid of 384 by 384 cells, yielding a spatial resolution of 5 millimeters. Based on the height of the computational domain, the Reynolds number for this simulation is 100,000. Figure 2 shows a comparison of the numerical solution with the data collected by Ingason.

A second example of the methodology involves a three dimensional simulation of the smoke movement in a large atrium. The actual building of interest here is the FRI large scale fire test facility in Japan, where NIST fire researchers are planning to do tests this fall. Figure 3 displays the building filling up with smoke, which in this case is represented by heated particles. These “thermal elements” of Ezekoye and Baum simulate the heat release due to the fire. This subgrid combustion modeling is needed here due to the unavoidable coarseness of the grid (20 cm resolution in a 20 m high facility).

### Reports and Publications

Baum, H.R., Ezekoye, O.A., McGrattan, K.B. and Rehm, R.G., “Mathematical Modeling and Computer Simulation of Fire Phenomenon”, *Theoretical and Computational Fluid Dynamics* 6:125–139 (1994).

McGrattan, K.B., Rehm, R.G. and Baum, H.R., “Fire-Driven Flows in Enclosures”, *Journal of Computational Physics* 110, No. 2, pp. 285–292, (1994).

McGrattan, K.B., Baum, H.R. and Rehm, R.G., “Mathematical Modeling and Computer Simulation of Fire Phenomenon”, *Proceedings of the 4th International Symposium on Fire Safety Science*, Ottawa, Canada, June, 1994.



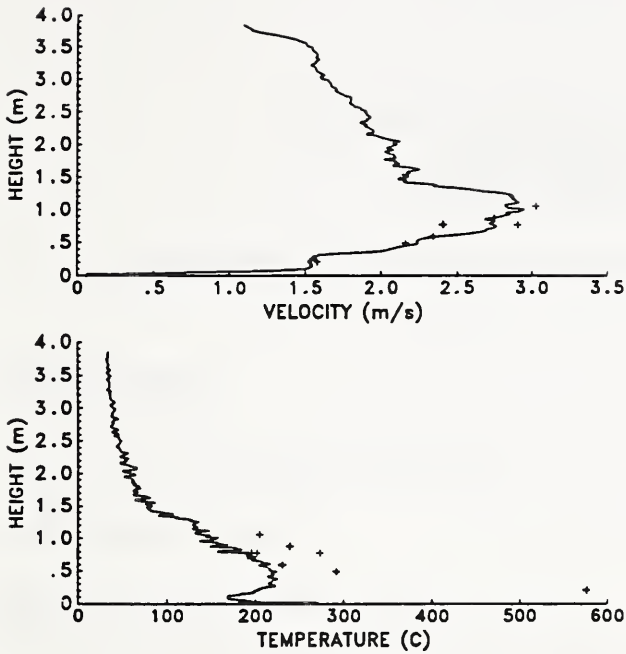


Figure 2: Numerically computed velocity and temperature profiles along the centerline of the rack, compared with the time-averaged experimental data of Ingason.

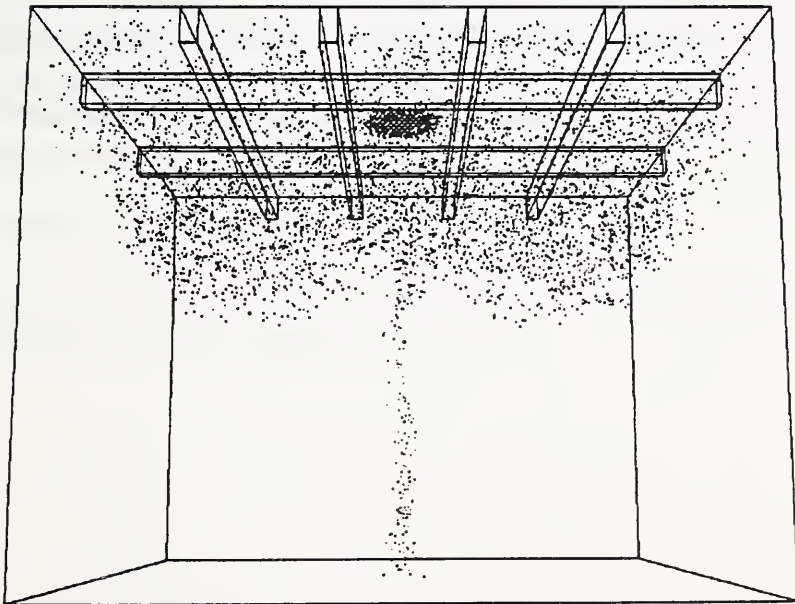


Figure 3: Simulation of smoke movement in the FRI facility. Shown are the thermal elements rising from a 2 MW fire in the center of the building. The actual facility is about 20 m high and 25 m on each side. The grid employed in the simulation has  $96 \times 96 \times 80$  cells. The Reynolds number is 5,000.



BUILDING AND FIRE RESEARCH LABORATORY  
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OTHER AGENCY PROJECT - FY94

MODIFICATION OF FIRE PROTECTION REQUIREMENTS FOR NRC

Funding Agency

U. S. Nuclear Regulatory Commission

Professional Personnel

Robert S. Levine, Project Leader  
W. Doug Walton, Acting Group Leader, Large Fire Research

Objective

Support NRC in developing a new "rule", that will permit the utilities to use performance-based methods to design fire protection provisions for nuclear power plants.

Technical Accomplishments

Reviewed status and problems of utilizing, worldwide, performance-based fire safety regulation in the built environment, and to nuclear power plants in France and Japan. Interface with Brookhaven National Laboratory on Probability Reliability Assessment techniques, which can be used to rate the importance of various intervention strategies. Compared NRC prescriptive fire protection requirements with those in the NFPA and other codes with a view toward reducing the cost of fire safety where a cost saving is justified.

Reports and Publications

Letter reports and memos to the sponsor. The results, after NRC review, will appear in the Federal Register for public comments.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROJECT  
OTHER AGENCY PROJECT - FY94

FIRE AND THERMAL CHARACTERISTICS OF NAVY FIREFIGHTING TRAINERS

Funding Agency

U.S. Navy, Naval Air Warfare Center, Training Systems Division

Professional Personnel

Robert S. Levine, Project Leader  
W. Doug Walton, Acting Group Leader, Large Fire Research

Objective

To support the development and implementation of prototype firefighting trainers at Norfolk, VA., Orlando, FL., Mayport FL., Bangor WA., and Ingleside TX.,

Technical Accomplishments

This program is over 6 years old. Original problems were to insure that the Navy training experience was safe, but realistic. This involved measuring temperatures, gas concentrations, properties of the artificial smoke, and other interior parameters. Due to "Base Closings", some of the original training compartments will no longer be available, so new ones, with inevitable modifications, are being built. This raises new technical development problems, plus interfacing with new environmental agencies.

Reports and Publications

Letter reports and memos to the sponsors.





BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

OFFICE BUILDING FIRE RESEARCH PROGRAM

Funding Agency

U.S. General Services Administration

Professional Staff

Daniel Madrzykowski, Project Leader  
Robert L. Vettori, Fire Protection Engineer  
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Project Objective

Quantify the impact of large fires on buildings and their occupants, and investigate the use of current technology/resources for mitigating the hazards.

Technical Accomplishments

Specific tasks currently being addressed by this program are 1) to analyze smoke flows down a corridor with and without sprinkler intervention and 2) to investigate the extent that materials or geometry effect the fire performance of systems furniture.

If the fire can not be suppressed in the room of origin, the impact of the smoke flow in the corridor (means of egress) with and without sprinkler intervention needs to be quantified. A series of fire tests in the U.S. Coast Guard's full scale corridor fire test facility have been completed. Smoke flows in the 37.5 m long corridor have been measured for fires with heat release rates ranging from 235 to 1600 kW. Results from these tests have been compared with predictions from the existing corridor flow model in FPEtool. The FPEtool sub-model, CORRIDOR, predicts the position, velocity, longitudinal temperature profile and depth of the initial wave front resulting from a steady-state fire. Comparisons with steady fire conditions yield conservative results i.e. faster velocities, higher temperatures and thicker smoke layers than those measured. A computer model of the burn room and corridor experimental facility has been developed using the CFDS-FLOW3D field model. Comparisons of the data with predictions from the field model are currently underway and are expected to continue through FY95.

Due to the wide spread use of systems furniture in open office plan space, the potential fire hazard of these furnishings in "as used" situations needs to be quantified. A combination of laboratory scale and full scale tests will be used to quantify the fire development in open office plan scenarios and address means of mitigating the potential fire hazard. Cone calorimeter tests of office furnishing materials have been conducted at incident heat flux rates of 35, 70 and 105 kW/m<sup>2</sup>. The cone

calorimeter tests yield a peak heat release rate per unit area value for each sample tested. This value is then used to predict the peak heat release rate of the full scale furnishing fuel packages. Eighteen full scale experiments will be conducted for comparison with the bench scale tests. The testing will be completed by September 1994.

#### Reports and Publications

Three reports are in progress:

Corridor Smoke Flow: Experimental vs. Predicted Results

Heat Release Rates of Office Furnishings and Work Stations

Heat Release Rates of Office Work Stations: Bench Scale vs Full Scale Experiments.

#### Related Grants

New Grant - A Study of Occupant Load Factors and Fuel Load in Contemporary Office Buildings, Dr. James A. Milke, Department of Fire Protection Engineering, University of Maryland.

BUILDING AND FIRE RESEARCH LABORATORY  
FIRE RESEARCH PROGRAM  
OTHER AGENCY PROJECT - FY94

FIRE ENDURANCE OF AN INTERSTITIAL SPACE CONSTRUCTION DESIGN FOR  
DEPARTMENT OF DEFENSE HOSPITALS

Funding Agency

United States Army Corps of Engineers, Medical Facilities Design Office

Professional Personnel

James R. Lawson, Project Leader  
Emil Braun, Physicist

Objective

Evaluate the fire endurance of the walk-on deck design incorporated into the integrated building system approach adopted by the Department of Defense for use in hospitals.

Technical Accomplishments

On June 28, 1994, the Building and Fire Research Laboratory of the National Institute of Standards and Technology conducted a National Fire Protection Association NFPA 251 fire endurance test on an interstitial space construction design for hospitals. The 28.8 m<sup>2</sup> (320 ft<sup>2</sup>) test assembly was constructed to be representative of that proposed for a new Elmendorf Air Force Base Hospital. Preliminary analysis of the test data, indicate that the assembly successfully met all criteria for a two hour fire endurance rating. In addition, it is noted that the test was conducted over a period of 2 hrs 30 mins. Initial evaluation of the test data shows that the following maximum temperatures were measured in the construction assembly just prior to test termination.

Functional Floor Surface	-	18° C (35 °F) above ambient
W18x35 Steel Beam	-	119° C (247 °F)
Steel Tube Hangers	-	109° C (229 °F)

No openings were observed in the functional floor, and no hot gases passed through the functional floor which would result in the ignition of cotton waste.

The "NFPA 251, Fire Tests of Building Construction and Materials 1990 Edition" fire test method is intended to evaluate the duration for which a building assembly will contain a fire, or retain its structural integrity or both. The test subjects a construction assembly to a standard time-temperature exposure for determining fire endurance. In the test at NIST, a 4.4 MW (15,000,000 Btu/h) propane gas burner was used to heat the fire compartment below the test floor. NFPA 251 was also used for the evaluation of the Veterans Administration interstitial space designs tested, in 1983. This was reported in NBSIR 85-3158 "Fire Performance of Interstitial Space Construction Systems." In addition with this test, NIST used the same steel test structure and facilities as were reported in the



Veterans Administration tests. The same ignition and temperature acceptance criteria for the VA tests were also applied to the proposed Elmendorf Air Force Base Hospital design.

Passage criteria for this test after a given time are as follows:

The functional floor shall have sustained an applied load of  $20 \text{ kg/m}^2$  ( $100 \text{ lb/ft}^2$ ) without developing surface conditions that will ignite cotton waste.

The average temperature on the top surface of the functional floor shall not rise more than  $121^\circ \text{C}$  ( $250^\circ \text{F}$ ) above ambient conditions.

The temperature of the steel beams or hangers within the interstitial space shall not exceed  $704^\circ \text{C}$  ( $1300^\circ \text{F}$ ) at any location during the test, nor shall the average temperature recorded by four thermocouples at any section have exceeded  $593^\circ \text{C}$  ( $1100^\circ \text{F}$ ) during the test.

#### Reports and Publications

A report for publication is in progress.

**PART 2.0 ALPHABETICAL LISTING OF BFRL FIRE RESEARCH  
GRANTEES AND THEIR GRANTS**

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This report describes the fire research projects performed in the Building and Fire Research Laboratory (BFRL) Fire Research Program and under its grants program from October 1, 1993 through September 30, 1994.

KEY WORDS (MAXIMUM OF 9; 28 CHARACTERS AND SPACES EACH; SEPARATE WITH SEMICOLONS; ALPHABETIC ORDER; CAPITALIZE ONLY PROPER NAMES)

Charring; combustion; fire models; fire research; flame spread; blowout fires; hazards; ignition; polymers; egress; soot; smoke; sprinklers; halons

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