Summaries of BFRL Fire Research In-House Projects and Grants, 1992

Nora H. Jason, Editor

Building and Fire Research Laboratory
Gaithersburg, Maryland 20899
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September 1992
PREFACE

This report describes the fire research projects performed in the Building and Fire Research Laboratory (BFRL) and under its extramural grants program during Fiscal Year 1992. BFRL is one of the eight major technical units of the National Institute of Standards and Technology (NIST).

The BFRL Fire Research Program is nationally recognized as the focal point for fire research in the United States of America. 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 community as they relate to all three of the Institute's goals: public health and safety, fundamental research, and assistance to industry. The BFRL fire program combines careful attention to the fire safety community's needs for advances in fire safety technology with its mandated role as the focal point for fire research in the United States. BFRL staff then 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.

In addition to its in-house programs, the BFRL maintains a fire research grants program that supplements its in-house programs and through which 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.

Third, BFRL responds to the needs of other Federal agencies and private sector organizations. This publication summarizes work 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 three program thrusts. The in-house priority projects, grants, and externally-funded efforts thus form an integrated, focussed ensemble. This publication is organized along those lines:

**Fire Risk and Hazard Prediction**
- Carbon Monoxide Prediction
- Turbulent Combustion
- Soot
- Engineering Analysis
- Fire Hazard Assessment
- Large Fires

**Fire Safety of Products and Materials**
- Materials Combustion
- Furniture Flammability
- Wall Fires
Advanced Technologies for Fire and Fire Risk Sensing and Control
Fire Detection
Fire Suppression

For the convenience of the reader, an alphabetical listing of all grants is contained in the Part 2.0.
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Part 1.0 BFRL/NIST Fire Program projects (in-house projects, associated grants funded by NIST, and projects funded by other agencies and private sector organizations)
A. Fire Risk and Hazard Prediction

A1. Carbon Monoxide Prediction
CARBON MONOXIDE PRODUCTION AND PREDICTION

Professional Personnel

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George W. Mulholland, Research Chemist
William J. Parker, Guest Worker
William H. Twilley, Engineering Technician

Project Objective

To provide the HAZARD team with an understanding of the mechanisms of carbon monoxide (CO) formation and sufficient algorithms to allow the development of tools which engineers and material designers can utilize to make accurate predictions of the quantity of CO produced under specified conditions.

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 FY92 work has focused on four (discussed below) components 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]. All of these components are designed to allow 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 situations. 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.

1. Investigation of CO Formation in a Reduced-Scale Enclosure (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
zero. For high HRR fires, temperatures in the upper layer were 200-300 K higher in the front of the RSE than in the rear.

The experiments for which the concentration of CO was mapped within the RSE showed that the distribution in the rear of the enclosure was fairly uniform, but that increasing concentrations of CO were observed when moving from the fire position towards the doorway. The latter finding suggests that reactions within the upper layer away from the fire plume lead to the formation of CO.

A short series of experiments were done to determine whether the pyrolysis of oxygen-containing polymers in a highly vitiated upper layer of a fire could contribute to the generation CO. The ceiling and upper wall areas (within the upper layer) of the RSE were lined with plywood. Natural gas fires similar to those described above were burned. Significantly higher concentrations of CO were observed in the upper layer than when the wood was absent. CO levels as high as 14% were observed in the rear of RSE while levels in the front were on the order of 4.5%. While preliminary, these findings demonstrate that extremely high concentrations of CO can be generated in enclosure fires by the pyrolysis of oxygen-containing polymers in a high temperature vitiated environment. Such a mechanism is consistent with the very high concentrations of CO which have been observed in some previous full-scale fire tests at NIST.

2. Field Modeling of the Reduced-Scale Enclosure Fires (Davis)

A commercial field modeling code, FLOW3D, has been used to simulate experiments within the RSE. Predicted velocity flow fields and distributions of combustion products (assuming simple combustion which generates only water and carbon dioxide as products) are the model outputs. The results provide plausible explanations for the observations of the RSE experiments.

The calculations show that a large recirculation zone develops within the upper layer in the rear of the RSE which tends to recirculate combustion products generated by the fire plume. Measurements of concentrations in this region should yield results similar to those of the idealized hood experiments. As noted above, CO concentrations measured at the rear of the RSE for high $\phi$ are similar to those observed by Morehart.

In the front region of the enclosure there is a significant "upwelling" of gas from the lower layer (which is found both experimentally and calculationally to consist of nearly clean air entrained through the doorway) near the enclosure walls and that this gas is rapidly mixed throughout the front region of the upper layer. The calculations suggest that the air which is entrained directly into the upper layer by this mechanism reacts rapidly with the fuel-rich gases flowing from the region of the fire plume. This is consistent with the higher temperature readings recorded in the front upper layer of the RSE. The experimental observation of an increasing CO concentration towards the doorway suggests that the air entering the upper layer is mixed with the hot rich gases coming from the plume and reacts to generate primarily CO and hydrogen. The idealized full-kinetic calculations discussed in the next section predict just such a result.

3. Chemical Stability of Upper Layers in Fires (Pitts)

During the past year an investigation of the reactivity of the combustion gases observed in the idealized hood experiments was completed. This work is described in detail in last year's project summary. The major conclusion of this work is that the combustion mixtures generated in the hood
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 here at NIST has been used to characterize CO formation for a variety of test conditions using natural gas as fuel.

Dimensional scaling has been used in the design of the RSE. The relative dimensions are based on those for a standard ISO fire test ["Fire Tests-Full Scale Room Test for Surface Products", ISO/Dis 9705]. The RSE uses a 2/5 scale factor with the doorway scaled such that $Ah^{1/5} = 2/5$.

The RSE was instrumented with thermocouple trees located in the front and rear of the enclosure. Cooled and uncooled probes were positioned at different locations to sample the upper combustion layer. Grab-bag samples were analyzed for $H_2$ for several fires. The RSE was located under a furniture calorimeter exhaust hood which allowed oxygen calorimetry and gas analysis to be performed on the exhaust gases from the fire. An attempt was made to measure air influx through the door with a pressure probe and aspirated thermocouples located in the doorway. The air flow in conjunction with fuel flow data was used to estimate a global equivalence ratio, phi ($\phi$), for the enclosure.

Natural gas was used as fuel for over 140 test fires with heat release rates (HRR) ranging from 7 to 650 kW. Fires of greater than 150 kW HRR were judged to create post-flashover conditions within the RSE. CO and CO$_2$ (NDIR detectors) and O$_2$ (paramagnetic detector) concentrations inside and outside of the RSE were measured. Since water interferes with NDIR measurements, sampled gases were dried before measurement. An approximation based on simple chemical considerations allows the concentration of water which is trapped to be estimated. Typical experiments ranged from 15 to 20 minutes in duration. Generally, concentration measurements were recorded for well defined positions located at the front and/or rear of the RSE. Several burns were made during which a sample probe was moved in order to characterize the spatial distributions of fire gases. Different burner positions and a narrow door configuration (1 cm width, HRR of 7-25 kW) were employed in a limited fires to investigate the effects of fire configuration and transient fire development, respectively.

Figure 1 shows a plot of measured steady-state CO concentrations (volume percent) versus the calculated HRR. The CO concentration begins to rise for HRR greater than 100 kW and levels off for HRR greater than 400 kW. CO concentrations at large HRR are found to be higher in the front (near the doorway) of the RSE ($\approx 3\%$) than in the rear ($\approx 2\%$). For comparison purposes, Morehart et al. ["Species Produced in Fires Burning in Two-Layered and Homogeneous Vitiated Environments," NIST GCR 90-585] observed $\approx 2\%$ CO at high $\phi$ in their idealized two-layer configuration. The measurements show that CO$_2$ concentrations within the RSE are inversely correlated with CO, being higher in the rear. For $\phi > 2$ oxygen concentrations in both the front and rear approach
experiments become reactive for temperatures typical of enclosure fires and that reaction of rich combustion gases generates CO in preference to CO₂.

4. Development of an Instrument for Measuring the Global Equivalence Ratios in Fire Gases (Mulholland and Babrauskas)

At the present time the techniques employed for GER measurements in earlier idealized laboratory investigations of underventilated burning cannot be implemented in our reduced- or full-scale experiments. As a result, an instrument for such measurements has been under development at NIST. The project summary for last year discusses the development of a prototype instrument, dubbed the phi-meter (ϕ-meter).

During the past year the ϕ-meter was developed further to allow testing on realistic fires. A number of measurements were carried out on gases extracted from the upper layer of fires within the RSE. The local measurements of ϕ were in excellent agreement with the expected fire behavior. For instance, a linear relationship was noted between HRR and measured ϕ. Significantly, values of ϕ near one were measured for fires having HRR such that the oxygen concentration in the upper layer just approached very low values. This is the expected result for these high temperature upper layers. On the basis of these findings it is concluded that the ϕ-meter provides an accurate measurement of the local ϕ within a fire environment.

Reports and Publications

Reports describing the RSE experiments, the field modeling effort, and the development of the ϕ-meter are in preparation and will be available shortly. In addition, a manuscript is being prepared which uses the findings of all of these studies as well as others to assess the validity of utilizing the global equivalence ratio concept to predict CO generation in enclosure fires.


Related Grants


"Radiation From Turbulent Luminous Fires," Gerard M. Faeth, University of Michigan.


The goals of the three year investigation are to (1) quantify the efficiency of external flames in destroying toxic gases produced in two-layer compartment fires, (2) measure and correlate yields of secondary toxicants over a wide range of equivalence ratios, and (3) evaluate the robustness of existing CO yield correlations for forced ventilation compartment fires designed to include poorly defined two-layer environments.

The production and spread of carbon monoxide in compartment fires is a primary fire hazard. Combustion dynamics in a compartment fire differs markedly from the combustion of the same fuel source in the open. It has long been recognized that the fuel burning rate in a compartment can be as much as an order of magnitude greater than the rate for the same fuel source in the open. This results primarily from the enhanced radiative feedback from the hot layer to the fuel source. The combustion of the fuel volatiles is also strongly affected by compartment effects. The flow of air to the flame may be seriously restricted by the limited ventilation areas present in most compartments and the height over which air may be entrained into the flame may be seriously limited by the hot gas layer formed in the upper part of the compartment.

The limited air availability has been shown to increase the yield of carbon monoxide by an order of magnitude over the CO yield for open burning. While limited ventilation has a definite effect on CO generation, there may be additional effects which relate to the quality of combustion air as well. Most compartment fire experiments are conducted under conditions which lead to a well defined two layer environment in the compartment. CO yield correlations as a function of equivalence ratio seem to be quite robust. It remains to be seen if this robustness will be observed in poorly defined 2-layer environments. The spread of CO from a compartment fire is significantly effected by the occurrence of flames outside the compartment. In the case of underventilated fires, external burning reduces the quantity of CO spreading from the fire.
External Burning

Experiments were completed in the past year which evaluate the efficiency of external flames in destroying CO generated in the compartment with a window-style vent. These experiments are restricted to simple vertical flames extending from the vent opening. This orientation is most like flames outside buildings. Additional work continues to include two important interior geometries: flames issuing into corridors from end and side rooms.

In the end room configuration, the flame extends directly along the corridor while the side room case involves deflection of flame on the opposite corridor wall and turning of the flame to proceed along the corridor. In both cases the products exit the corridor into an exhaust hood where species flow rates are measured and compared to the species flow rates from the compartment.

Forced Ventilation

The natural ventilation experiments performed to date have been quite valuable and have shown that the previous hood based CO yield correlations do work in compartments [1]. Further, those natural ventilation experiments have demonstrated a previously unrecognized temperature dependence of the CO yield correlations.

The major weakness of the prior work is the very excellent two layer environments created in the experiments. While this was originally sought in the experimental design, it has been quite difficult to degrade the two layer nature of the compartment environment in the present configuration. The compartment used for the previous work [1] will be modified to be a forced ventilation system to allow maximum control and measurement accuracy, Figure 1. During the current grant period, experiments will be performed with forced ventilation inlets both high and low in the compartment, with exhaust from the existing variable size exhaust vent. Air supply will be varied in amount and inlet location, allowing ventilation from below, from above, and mixed below and above configurations. This will allow us to make direct measurements of air supply rate, fuel mass loss rate, and control the degree of stratification in the compartment. Experiments will be conducted with the same fuels used in the natural ventilation experiments: hexane, PMMA, wood and polyurethane foam.

An important adjunct to this experiment is the opportunity to simultaneously explore the effect of ventilation rate and inlet position on the extent of stratification (2-layer formation) in forced ventilation fires. It has been demonstrated that fires ventilated from above via forced ventilation can lead to much reduced stratification and poorly defined 2-layer environments [2]. Quantification of this phenomena is very important for future developments in fire modeling. Fire extinction in fires with forced ventilation from above has been observed for methane fires [3]. No increase in CO generation was noted as extinction was approached. No investigations of these phenomena for condensed fuels have been performed to date. Given the wide use of HVAC systems with air supply in the ceiling, it is important that we begin to deal with forced ventilation fires.

Summary of First Year's Accomplishments

The ignition and burning of fuel-rich upper layer gases outside of a fire compartment (external burning) was observed experimentally. Hexane fires were burned in a 2.2 m³ compartment with a window-style exhaust vent to study the effects of external burning on carbon monoxide and smoke yields downstream of the fire compartment. External burning was observed to occur in several modes: 1) intermittent flashes, 2) bursts that lasted for only a few seconds and 3) sustained external burning. Results showed that the flammability of the compartment fire effluent was a function of the equivalence ratio and that distinguishable equivalence ratios exist that determine which mode of external burning can be obtained for a given compartment fire. Results also showed that the reduction of carbon monoxide and smoke only occurs when sustained external burning occurs. At plume equivalence ratios above 2.1, sustained external burning always occurred and downstream carbon monoxide yields were reduced to 10 to 25 percent of the upper layer yields, Figure 2. For equivalence ratios below 2.1, carbon monoxide yields downstream of a compartment fire were the same as upper layer yields even when flashes or short bursts of external burning occurred. During the course of a fire, including times with and without external
burning, the production and consumption of smoke downstream of a fire compartment qualitatively followed that of carbon monoxide. For plume equivalence ratios above 2.1, the downstream smoke yield was reduced to 0 to 50 percent of the level observed prior to sustained external burning

Beyler's ignition criterion for layer burning was applied to the mixing of the hot fuel-rich, upper layer gases and ambient air outside of the fire compartment. The results show that the ignition index predicts the potential for external burning at equivalence ratios of 1.2 and greater, and experiments support this prediction quite well. However, the occurrence of external burning is dependent on the presence of an ignition source which is dictated by the vent geometry and fire size.

Also during the current year, the hallway apparatus was designed and constructed. To allow for the hallway setup, necessary modifications of the existing gas sampling system and measurement system were completed. The test procedure and experimental setup were outlined for the experiments investigating compartment fires with external burning under varying exterior geometries. Experiments of the end room design were begun. Preliminary results show that external burning occurs down the entire 3.65 m length of ceiling. Initial results indicate that CO is not burned as efficiently with this hallway configuration as with the window-style vent.

The upper layer of the hexane-fueled compartment fires were further characterized. Temperature measurements show that there is on average a 20 C temperature rise from front to back in the upper layer. This rise is attributed to the flow dynamics which cause the fire plume to be slightly deflected towards the back of the compartment. Species concentration measurements show a relatively uniform upper layer composition.

Utilization of Results:

This project provides direct support to the development of toxic hazard analysis techniques by providing basic data for the modeling of toxic gas production. In addition, through the experiments involving external flames, it provides information about the spread of toxic species from the compartment of fire origin. Since the spread of toxic gases is frequently involved in fire deaths remote from the compartment of origin, this data is crucial to modeling the overall fire hazard in a building. The development of these models and this data will markedly improve the ability to assess the impact of different building materials and building designs on the fire safety provided.

References

Papers:
Figure 1. Modified compartment with forced ventilation

Figure 2. CO Yield Verse Equivalence Ratio
Introduction: Since CO inhalation is one of the major causes of fire fatalities, significant effort has been directed towards obtaining an understanding of the increased 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].

Our earlier work [3] sought to obtain a fundamental understanding of the relationship between the production rates of CO and soot in diffusion flames. The effects on the CO depletion rates of lower temperatures (due to radiation heat loss from the soot particles) and competition between CO and soot for the oxidizer species OH· were examined using equilibrium estimates of the OH· concentration. Based on the rates of CO and soot oxidation due to OH·, competition between these species for OH· was found to be plausible in both fuel lean and fuel rich regions of the flames studied. While radiation quenching (through reduction of OH· radicals) seemed important in the fuel lean regions, the equilibrium concentrations of OH· did not correlate with the observed CO destruction rates in the fuel rich regions.

Our recent work [4] has shown that equilibrium estimates of OH· concentrations are not reliable, with the departure from equilibrium depending upon the soot loading. Therefore, in order to carefully evaluate the interaction between CO and soot, OH· concentration measurements were extended to the flames of our earlier study [3]. Additionally, these overventilated diffusion flame studies have been supplemented by an investigation of underventilated diffusion flames. Underventilated flames offer the opportunity to study much richer fuel conditions, but previous studies of this flame configuration are lacking. In the present study, a series of underventilated laminar diffusion flames have been investigated with respect to the CO and soot yields as a function of fuel and oxidizer ratio and flow rate. Based on the analysis of soot samples collected on filters, information on the organic carbon content of the soot...
Experimental Approach: For the overventilated flame studies, laminar diffusion flames burning fuel mixtures were used to vary the soot concentration while keeping the total carbon flow rate constant. Flames burning methane (9.8 cm³/s) and methanone (5.6 cm³/s) doped with either butane (1.05 cm³/s) or 1-butene (1.05 cm³/s) were studied. The OH⁻ concentrations were measured in the soot oxidation region of these flames using laser-induced fluorescence. The experimental arrangement and the measurement procedures are described in detail elsewhere [4].

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 ration, $\Phi$, 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 2.88 cm i.d. Both methane (CH₄) and ethene (C₂H₄) fuels were studied. For the methane flames, fuel flow rates of 10 and 20 cm³/s were examined, while for ethene, flow rates of 3.2 and 6.4 cm³/s were considered. The air flow rates were selected in each case to allow the overall equivalence ration $\Phi$, to be varied between 0.5 and 4.0. Measurements of CO and CO₂ 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.

Results And Analysis: Figure 1 presents the OH⁻ concentration as a function of the axial centerline position in the three flames, with the error bars showing the estimated uncertainty. The pure methane flame and the methane/butane flames have maximum centerline soot volume fractions of 0.76 and 2.55 ppm respectively and completely oxidize all the soot produced within the flame. Consequently these

![Figure 1](image-url)
flames have a closed flame tip at axial locations of 10.7 and 11.7 cm respectively. The methane/1-butene flame has a maximum centerline soot volume fraction of 5.46 ppm and does not have a closed flame tip since it emits smoke. Figure 1 clearly shows that as the soot concentration increases, the centerline OH· concentration decreases. The most noteworthy feature is that the pure methane and the methane/butane flames have approximately the same OH· concentration along the flame centerline once the soot particles are completely oxidized. Thus, the decrease in the OH· concentration in the presence of soot particles can be attributed to chemical consumption by soot particles.

In addition to the soot concentration, the OH· concentration can be expected to depend on the local stoichiometry (φ), temperature (T) and the CO concentration (which may not be uniquely related to φ [3]). Equilibrium calculations reveal that the OH· concentration is not very sensitive to φ for φ ≤ 0.95. Thus, the lean flame region, with the elimination of the φ dependency, is amenable to a simple analysis for the evaluation of the relative contributions of thermal and chemical effects to the observed OH· concentration.

Along the centerline the OH· concentration depends upon the temperature and the concentrations of CO and soot, i.e. [OH·] = f(T, [Soot], [CO]). However, on the lean side of the flame front, where there is no soot and little CO, the OH· concentration depends only on the temperature, i.e. [OH·] = f(T). A comparison for flames with different soot concentrations allows a simple estimate to be made of the relative contributions of thermal and chemical effects on the CO depletion rates. If

\[
F_1 = \frac{f(T)_{\text{Butane}}}{f(T)_{1-\text{Butene}}} \quad F_2 = \frac{f(T, [\text{Soot}], [\text{CO}])_{\text{Butane}}}{f(T, [\text{Soot}], [\text{CO}])_{1-\text{Butene}}}
\]

then the relative contribution of radiative quenching to the observed decrease of the OH· concentration in the methane/1-butene flame is the ratio F_1/F_2. This analysis indicates that radiative quenching makes only a 6% ± 2% contribution to the observed lower OH· concentration along the centerline in the methane/1-butene flame. Thus, the OH· concentration in the presence of soot particles is suppressed

Figure 2. Yield of CO (▲) and soot (♦) for the ethene flame at a fuel flow rate of 6.4 cm³/s. Yield of CO is in grams of CO per gram of fuel (C₂H₄) and yield of soot is in grams of C per gram of fuel. CO Measurements of CO are based on a dry analysis. The lines of the graph are only to indicate trends and are not curve fits.
primarily due to oxidation reactions as opposed to thermal quenching effects.

Figure 2 shows the CO and soot yields obtained in the underventilated diffusion flames as a function of overall equivalence ratio for the ethene flame with a fuel flow rate of 6.4 cm$^3$/s. It should be noted that this fuel flow rate corresponds to conditions well above the smoke point for ethene. For these conditions, the soot yield is observed to initially increase slightly as $\Phi$ is increased from one-half. However, this quantity then is observed to decrease for $\Phi$ greater than one with the soot yield varying by about one order of magnitude, as $\Phi$ is varied from lean to rich conditions. For $\Phi$ greater than one, CO is qualitatively observed to follow a similar, although somewhat smaller, variation. For lean overall equivalence ratios (0.5 $\leq$ $\Phi$ < 1) the yields of CO are observed to be quite low. These trends are consistent with previous observations regarding the behavior of soot and CO in overventilated laminar diffusion flames. Analysis of the elemental and organic carbon content of soot formed in these underventilated flames reveals that for $\Phi$ $\geq$ 2, the organic-to-elemental carbon ratio exceeded one 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 for soot formed in overventilated flames where the organic carbon content is usually much lower.

Future work will emphasize more detailed comparisons with overventilated flame results as well as further analysis of the fuel structure and burner geometry effects.

**Acknowledgement:** The work done at The Pennsylvania State University was supported under grant 60NANBOD1035 from the National Institute of Standards and Technology. Contributions to this work by Drs. Kermit C. Smyth and George W. Mulholland of the Building and Fire Research Laboratory are gratefully acknowledged.

**References:**


**Reports and Papers:**

The George Washington University

60NANB9DO963

Simplifications of Diffusion Flame Chemistry: A Theoretical and Experimental Study of the Structure of Laminar Diffusion Flames

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Introduction

It is now possible to argue that a qualitative description of the chemical processes which lead to the formation, oxidation and possible emission of carbon monoxide, polynuclear aromatic hydrocarbons (PAH), and soot from laminar hydrocarbon diffusion flames is within our grasp. Unfortunately, the list of caveats associated with this claim is somewhat daunting. First the good news: a number of models have been developed which predict soot volume fraction by integrating soot concentrations along convective streamlines using rate parameters for inception, growth, and oxidation as a function of mixture fraction. The rate data is empirical (Kennedy's work) or semi-empirical (our work) in origin. These models are reasonably successful at predicting soot volume fractions when appropriate experimental data are available. Thus, one of the limitations to further application of them is the deficiency of either accurate profiles of soot particulate concentrations (for the empirical models) or chemical species (for the semi-empirical models) for a variety of fuels. A second deficiency is our understanding of the subtle interaction between the presence of soot particles and the concentrations of chemical species in their local environment. For example, Puri et al. [1] have shown that hydroxyl radical is depleted in the presence of large soot volume fractions. It is not clear whether this is a result of direct chemical reaction or due to an indirect chemical effect, i.e. from increased rates of third body recombination reactions due to the lower temperatures that result from radiative heat loss. Carbon monoxide concentrations will also show a dependence on large soot volume fractions: its oxidation will decrease because of the depleted hydroxyl radical and it will be produced when the soot particles themselves are oxidized.

Our research during the past year has followed two paths: the development of a model for PAH growth in axially-symmetric, laminar methane/air diffusion flames and the development of
tunable diode laser diagnostics for combustion systems. To address the deficiencies in the soot models highlighted above, we have begun to combine the knowledge gained in these two tracks in an experimental and theoretical study of the tip of axially-symmetric methane/air and ethylene/air diffusion flames. In the next section of this report, brief summaries of current work will be presented.

Summary of Current Research Status

Over the last year a number of research problems which have engaged us over the past several years have been concluded and research articles have been submitted for publication. This work is summarized briefly below. We have recently initiated some new directions for this research which is also discussed.

Tunable Diode Laser Measurement of Carbon Monoxide Concentration and Temperature in a Laminar Methane/Air Diffusion Flame

In each of the last two years, a component of the research proposed to NIST has been the development of Tunable Diode Laser Absorption Spectroscopy (TDLAS) Diagnostics. The first study using our laser system was the measurement of carbon monoxide concentration and the flame temperature in a methane/air flame supported on a Wolfhard-Parker burner system. Details of the experimental configuration and the absorption theory were provided in last year’s annual report as well as in a manuscript in press [2].

Figure 1 shows simultaneous fits of the CO P(4) (1→0, 2127.68 cm\(^{-1}\)) and R(2) (2→1, 2128.01 cm\(^{-1}\)) lines at 9 mm HAB and -3.8 mm from the burner centerline. For this calculation, it was assumed that both lines had the same room temperature collision halfwidth. Thermocouple measurements gave 1367 K for the temperature at this flame location (after a radiation correction had been applied [3]), in excellent agreement with the temperature from the fit of this data: 1356 K.

Modeling Polynuclear Aromatic Hydrocarbon Growth in Hydrocarbon Diffusion Flames

During the last two years, we have constructed a model for PAH growth in axially-symmetric diffusion flames. Initial results for its application to methane/air flames were presented in last year’s annual report. The model is described in detail in references 4 and 5. We are currently extending the model’s application to ethylene/air diffusion flames, for which considerably more data on the soot particle concentrations are available [6].
Development of a PC-based Infrared Spectral Synthesis Program for Combustion systems.

A key impediment to the development of reliable quantitative diagnostics with infrared absorption is the requirement for reliable data for transition linestrengths, collision halfwidths, and spectral assignments (which is necessary to accurately compute the temperature dependance of the line strengths). Further, spectra collected in reference cells, which can provide some of this data, will not provide insight into potential interferences which may be encountered in actual combustion systems (notably from hot carbon dioxide and water vapor). The atmospheric chemistry community also requires an accurate knowledge of infrared spectral data, not only for diagnostic development, but also for use in models of global climatic change. In response to this need the HITRAN data base of infrared transitions has been assembled. The data base is typically distributed on a 9 track ASCII tape and includes a FORTRAN program for low-level manipulation of the data. We have acquired this data base and are in the process of reconstructing it in a more "user friendly" form.

We envisage a PC-based spectral data analysis program which will allow a user to input the concentrations for dominant combustion species, a temperature, beginning and ending points of a spectral window, and the pathlength. The program will then generate a simulated spectrum, which will be the sum of contributions from the collisionally broadened lines within the window. This program will not only be a valuable resource in our own research, but would be would also be of use in FTIR diagnostics of combustion systems. For this latter application, the spectral data would be passed through a secondary data filter corresponding to instrument broadening of the spectral features.

Figure 2 shows a simulation of a two wavenumber portion of the infrared absorption spectrum through the Wolfhard Parker flame. This spectral window includes the P(4) (1-0) and R(2) (2-1) lines of carbon monoxide (see Figure 1). For this simulation only HITRAN spectral parameters were used. These include air broadened collisional halfwidths, the temperature dependencies of these halfwidths, and line strengths. Experimentally determined concentrations and temperature were also used. Comparison of the absorbances for the two CO lines in Figures 1 and 2 shows excellent agreement between the two.
References


Publications during this reporting period:

3) "\( \pi \rightarrow n \) Transitions of Mono Halo Substituted Phenyl Radicals in Solid Argon at 12 K." P. Hassanzadeh and J.H. Miller, J. Phys. Chem., in press.
A2. Turbulent Combustion
Introduction. The overall goal of this project is to develop chemical, physical, and mathematical models of the detailed combustion phenomena which control a fire's growth. Our emphasis recently has been on the October 20, 1991 Oakland Hills Fire, unsteady pool fire plumes and backdrafts, i.e., the combustion of accumulated excess pyrolyzates.

October 20, 1991 Oakland Hills Fire. Three projects are underway which will provide insight into why this conflagration was so severe and what can be done to prevent a recurrence: 1.) Double pane windows as urban/wildland fire protection, 2.) Weather analysis as an early warning system, and 3.) Fire induced flow fields calculated by the Baum-McCaffrey method to predict spotting.

Double pane windows. BREAK1, for calculating the unsteady temperature fields in a window subject to heating by fire, is readily available on the NIST Building and Fire Research Laboratory Computer Bulletin Board. We are extending this analysis to double pane windows since examination of houses at the boundary of the October 20, 1991 fire indicated that double pane windows may provide fire protection as well as enhanced energy conservation. The simplest way to accomplish the two-pane extension is to allow the convection coefficient on the unheated side of the exposed pane to vary with time rather than treat it as a constant as is currently done in BREAK1. Then model the radiative and convective transport across the gap for use both as a loss for the exposed pane and as a gain for the unexposed pane. The calculation of the the time to breakage of the first pane is otherwise unchanged. Once the first pane breaks, the second pane time to breakage will be calculated as was the first pane time to breakage. The second pane will last longer because of the longer time available for conductive heating of the shielded edge glass. Due to precursor heating, when the first pane was intact, the temperature difference between the frame-shielded glass and the heated glass will be reduced.

Weather. Figure 1 shows wind direction and velocity, temperature and relative humidity on October 19 and 20, 1991 as measured at Chabot Observatory near the fire site. Between 5 and 11
a.m., these hot, dry winds dessicated any remaining moisture from the already dry vegetation and structural fuel and set the stage for the catastrophic conflagration that occurred. Because of the dessication time lag, an early warning system which would alert local fire departments when such hazardous weather conditions exist is possible. Long term weather data suggest that such a warning would be broadcast an average of four times per year. The components of this system could be: 1.) initial fuel moisture (< 10%), 2.) relative humidity (< 20%), 3.) temperature (> 75°F), 4.) mean wind speed (> 10 mph) and 5.) direction (from the NE quadrant). We are examining the weather data during past conflagrations, as well as on October 20, 1991, to determine whether or not a consistent weather pattern can be identified as existing whenever a conflagration occurs. From these data the criteria for issuing an alert status will be determined. Local fire service officers, Berkeley Fire Chief Cates and Oakland Deputy Chief Matthews, are very supportive of these efforts.

Fire Induced Flows. In their award winning paper, Baum and McCaffrey described in detail a rigorous method for predicting the flow field induced by a large number of simultaneously burning large pool fires. We are applying that method to the Oakland Hills fire. The high velocity convective column produced by many houses burning provides a highway along which burning debris can travel to meet high velocity atmospheric crosswinds. This debris becomes flaming brands that create fire spotting behind defense lines constructed by the fire service. This mechanism of spread was significant in the Oakland conflagration.

Backdrafts. A summary of successful half-scale backdraft experiments by C. M. Fleischmann is presented in Papers 4 and 5. During this grant period salt-water model flow experiments were performed to quantify the fluid mechanics occurring in these backdraft experiments. The resulting data are shown in Fig. 2. While gravity currents have been extensively studied for flow in pipes or ducts, little is known about gravity currents initiated through partial openings such as windows or doors or the mid-third section used in the half-scale experiments. In the salt-water experiments, a pH indicator, phenolphthalein, has been used along with standard dyes to identify the fluid interface. The "hot" fluid is blue-dyed fresh water with up to $10^{-3}$ M phenolphthalein. The "cold" fluid is salt-water, specific gravity up to 1.1, with up to $10^{-2}$ M sodium hydroxide as a base to provide an initial pH of 11.5. The mixing region where the two fluids come together is marked by the bright red color the phenolphthalein assumes when in contact with a highly alkaline solution. A wide variety of opening shapes and sizes are being studied both experimentally and analytically in cooperation with Howard Baum and Kevin McGrattan, an NIST post-doctoral fellow in Applied Mathematics. A definitive set of half-scale backdraft experiments is being planned based on comparisons among the current half-scale combustion experiments, salt-water modeling experiments and NIST calculations.

Reports and Papers:


Fig. 1. Wind velocity vectors are plotted here for October 19 and 20, 1991 from the weather station closest to the Oakland Hills conflagration. The 19th data show a typical coastal pattern with light on-shore winds midday and light off-shore winds morning and evening. Hot, dry, fast "Diablo Winds" began pouring over the coast range, out of the NE, before 6 a.m. on the 20th and continued unabated until 9 p.m. (These arrows are red on the color version of this figure.) The fire began at ~ 11 a.m. near the center of Fig. 1, and reached its final perimeter by 6 p.m. The 5 hr. dessication period between 6 a.m. and 11 a.m. on the 20th may indicate that an early warning interval exists during which local fire services can prepare for the consequences of those rare weather conditions.

Salt Water Results

V* Into Compartment

Fig. 2. These preliminary gravity current velocity data were obtained from salt-water experiments in a 15 cm x 15 cm x 30 cm long compartment. The dimensionless velocity, $V^* = (V/(gH\Delta \rho/\rho))^{1/2}$ with $H = 15$ cm here, is independent of $\Delta \rho/\rho$, the horizontal ordinate in Fig. 1, and therefore independent of Reynolds No. $V^*$ does depend on the geometry of the opening between the dyed fresh water in the compartment and the salt-water in the surrounding tank. Four openings are indicated: # completely open $V^* = 0.43$, ▼ a vertical door $H/3$ wide and $2H/3$ high $V^* = 0.35$, □ a centered horizontal slot $H/3$ wide $V^* = 0.33$, and a centered window $H/3 \times H/3$ $V^* = 0.22$. $V^* = 0.5$ is predicted for an ideal fluid with a completely open connection.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
GRANTEE PROJECT - FY92

Institution: University of California, Berkeley
Grant No.: 60NANB1D1174
Grant Title: Fire Propagation in Concurrent Flows
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Technical Abstract:

An experimental study is being conducted of the effect of gas flow velocity, turbulence intensity, and oxygen concentration on the concurrent spread of flames over the surface of a solid combustible. Tasks completed include studies of the effects of air flow velocity and turbulence intensity on the burning of thick PMMA sheets in a floor and ceiling configuration. These studies address the transport mechanisms controlling the flame spread process. Currently underway are experiments to determine the effect of flow oxygen concentration, particularly vitiation, on the concurrent flame spread for both ceiling and floor geometries. The experiments include measurements of the flame spread rate, mass burning rate, flame length, surface heat fluxes, and combustion completion (CO, CO₂, HC), as a function of the flow conditions. The tests are conducted in a combustion wind tunnel with the fuel mounted in the ceiling or the floor of the tunnel test section to observe, by comparison, the effect of buoyancy and geometry. All the tests are conducted with PMMA sheets 76 mm long, 37 mm wide and 12.7 mm thick. The tests are conducted with air flow velocities ranging from 0.25 to 4.5 m/s, grid induced turbulence intensities from 1% to 15%, and oxygen mass fractions from 0.19 to 0.4.

The measurements show that the flow parameters affect significantly both the rate of flame spread and of mass burning, particularly at high flow velocities. The former increases with the flow velocity but decreases with the turbulence intensity, and the latter increases with both the flow velocity and the turbulence intensity. These trends are the result of the combined effect of the flow parameters on the surface heat flux and on the flame length. The flame spread rate measurements are correlated well with a simple expression derived from a heat transfer analysis of the problem. The mass burning rate data show that flat plate boundary layer analyses describe well the process, and a correlation of the data is obtained in terms of a nondimensional burning rate, and a flow parameter that includes the Reynolds number and the turbulent intensity. Comparison of the measurements for the floor and ceiling geometries show that buoyancy has an important influence in these process at least up to flow velocities of 5 m/s. The results indicate that buoyancy introduces two main competing effects, one is the variation of the heat transfer to the wall due to the changes in the flame stand-off distance, and the other is the changes in the combustion reaction completeness due to wall quenching and mixing of the pyrolyzate and air effects.

Fuel Burning in a Turbulent Air Flow: The Effect of Buoyancy

Concurrent Ceiling and Floor Flame Spread. The measured flame spread rates over the PMMA surface show that the flame spread rate increases with the flow velocity, in qualitative agreement with
boundary layer analyses of the process. The turbulence effect can be divided into two regions based on the magnitude of the flow velocity. For low flow velocities, the flame spread rate decreases with the flow turbulence due to a smaller flame length. At low flow velocities, however, the turbulence effect becomes less pronounced, and for flows with velocities less than 0.75 m/sec, the flame spread rate shows only a slight increase with the turbulence intensity. The buoyancy effect on the flame spread can be observed by comparing the experimental data for ceiling and floor flame spread under the same flow conditions, as shown in Fig. 1. It is seen that for flows larger than 1 m/sec, the flame propagates faster in the ceiling configuration than in the floor case. For flows slower than 1 m/sec, however, the ceiling flame spread rate is observed to be smaller than the floor one. From the flame spread rate data and the measurements of major species in the exhaust gas flow, it is concluded that the buoyancy has two opposite effects on the ceiling flame spread. It can increase the surface heat flux by pushing the flame closer to the solid surface, which will tend to increase the flame spread rate. However, the shortening of the flame stand-off distance also greatly enhances the flame quenching at the cold wall, which reduces the chemical reaction completeness and consequently lowers the flame temperature and length, thus decreasing the flame spread rate. The overall buoyancy effect depends on which of the two mechanisms is more dominant. The experimental data suggest that at low flow velocities the flame quenching is more important in the ceiling flame spread. In flows with relatively large flow velocities, the enhancing of heat transfer from the flame to the solid surface becomes the dominant effect.

The mechanisms by which turbulence affects the flame spread rate can be inferred from the theoretical analysis of the spread process. A simplified heat transfer model of the flame spread provides the following expression for the rate of spread:

\[
V_p = \frac{4 q_f^2 l_f}{\pi \kappa \rho c(T_p - T_i)}
\]

where \( q_f \) is the surface heat flux, \( l_f \) the flame length, \( \kappa \) and \( \rho c \) the thermal inertia of the solid, and \( T_p \) and \( T_i \) are the solid pyrolysis and initial temperatures, respectively. The flow velocity and turbulence intensity can affect both \( q_f \) and \( l_f \) and through them the flame spread rate. Thus, it is important to determine how turbulence affects these parameters. From the measured variation of the flame length and surface heat flux with the pyrolysis length it is found that the \( q_f^2 l_f \) is approximately a constant for a given flow condition. With this relation between the flame length and the surface heat flux, it is possible to combine all the results to produce a non-dimensional flame spread rate deduced from Eq. 1. It is found that the non-dimensional flame spread rate is independent of the flow velocity and turbulence intensity, which verifies the validity of Eq. 1 and confirms our previous finding that the effect of the flow turbulence on the flame spread rate takes place primarily through the flame length and heat flux.

Ceiling and Floor Mass Burning. Experiments have been conducted to measure the PMMA ceiling and floor surface regression rate as a function of the flow velocity and turbulence intensity. This information will help in understanding the mechanisms controlling the flame spread process since both processes are closely related. The results show that for all the flow conditions tested, the surface regression rate decreases with the downstream distance from the flame leading edge, agreeing qualitatively with the theoretical predictions of flat plate boundary layer mass burning. As the flow velocity increases the flame gets closer to the surface, which results in the enhancement of the heat transfer from the flame to the solid surface, and consequently of the burning rate. The turbulence also increases the regression rate significantly by wrinkling the flame and bringing parts of it closer to the surface. The buoyancy effect on the mass burning can be seen in Fig. 2 which compares the floor and ceiling regression rates under the same flow conditions. It is found that the ceiling mass burning is stronger than the floor one in low turbulent flows and weaker in high turbulent flows. These observations are the result of the combined effect of reduced flame stand-off distance and incomplete gas phase chemical reactions.

The experimental data can be correlated in terms of nondimensional parameters related to the convective heat transfer from the flame to the fuel surface. The correlation between the non-dimensional parameters gives the following correlations for ceiling and floor burning.
\[ \frac{\dot{m}''_x}{\alpha PB} = 0.32 \text{Re}_x^{0.5} \left[ 1 + 1.72 \left( \frac{u'}{U} \right)^{0.5} \right] \] (2)

\[ \frac{\dot{m}''_x}{\alpha PB} = 0.28 \text{Re}_x^{0.5} \left[ 1 + 3.04 \left( \frac{u'}{U} \right)^{0.5} \right] \] (3)

Concurrent Flame Spread in a Vitiated Flow. Experiments are being conducted to study the effects of gas flow velocity, turbulence and oxygen concentration on the concurrent spread of flames over thick PMMA sheets. A series of experiments with laminar flow have been completed during this reporting period, and we are currently conducting tests in turbulent flow. Most of the experiments are conducted under vitiation conditions, and with the PMMA sheets in a ceiling configuration. A few characteristic cases are conducted at oxygen concentrations above air to have a broader data range.

Experimental results of the variation with the oxygen concentration of the ceiling flame spread rate over PMMA sheets in a concurrent laminar flow are presented in Fig. 3, for several flow velocities. No data for oxygen mass fraction lower than 0.19 was obtained because the spread of the flame could not be initiated or flame extinction occurred after the flame had propagated for a short distance. The results indicate that flame spread rate varies approximately linearly with the flow velocity and with the oxygen mass fraction. Similar results are observed for the floor configuration. We are currently conducting a few tests at higher oxygen concentration to verify the above trends for a larger range of oxygen concentrations. Other data obtained in these tests include the variation of the flame length and surface heat flux with the flow properties. These data has been normalized using Eq. 1, and the results, which are presented in Fig. 4, provide validation for a model of flame spread based on an energy analysis of the process. To further investigate the controlling mechanisms of flame spread, major species concentrations were measured in the exhaust gas. The results show that at low flow velocities and oxygen concentrations, the combustion reaction is quite incomplete, which affects the rate of heat released and consequently the flame spread rate.

Publications and Presentations

Flow Velocity, $U$ (m/s)

**FIGURE 3.**

**FIGURE 4.**

**FIGURE 5.**

**FIGURE 6.**
Technical Abstract:
Massive fires resulting from the burning of oil spills, uncontrolled oil wells, forest fires, and large-scale explosions produce large smoke plumes which rise, in the wind direction, several hundred meters before they become buoyantly stable due to entrainment and atmospheric stratification. After reaching their maximum altitude, plumes may continue to flow horizontally (coning, fanning or lofting), oscillate around a horizontal plane (looping), or descend if their temperature reaches equilibrium with the local conditions (fumigating or trapping). The trajectories of these plumes, which determine their impact on the local, and possibly global environment, are governed by the interaction between the wind pattern, atmospheric turbulences, and stratification, ground terrain, and smoke plume properties. The purpose of this work is to develop an efficient and accurate computational simulation model for the prediction of the smoke plume trajectory, dispersion, and ground distribution as a function of all the parameters mentioned above. The computational model is designed to run on an engineering workstation and to produce data required for assessing the impact of fires on the environment. The intention is to have the model act as a risk assessment tool in cases when fires may be used in an oil spill clean-up and as a predictive tool for uncontrolled fires.

To endow the model with universality and flexibility, it is based on a reduction of the three-dimensional Navier-Stokes equations which describe the motion of an incompressible inviscid flow in a gravitational field into their parabolized form using the wind direction as the primary flow direction. The equations are then solved numerically using a grid-free Lagrangian method which is based on the extension of the vortex method to variable density flow. The equations are then normalized to determine the independent parameters of the problem. In a homogeneous field, these are found to be: $\varepsilon = \frac{\dot{m}_p}{\rho_o U A}$ where $\dot{m}_p$ is the smoke mass flow rate, $\rho_o$ is the atmospheric density, $U$ is the wind speed and $A$ is the plume cross-sectional area; and the initial height, $HT$, and aspect ratio, $Ry/Rz$ of the plume cross section. In a density-stratified atmosphere, which was the focus of our studies during the 91-92 academic year, two more parameters are used to describe the environment in which the plume rises. This is because the most important type of atmospheric stratification takes the form of an inversion layer which can be characterized by the magnitude and elevation of a density jump. The effect of both will be described later.
We have developed a moving plane formulation for the problem of buoyant plume dispersion in a stratified atmosphere, (Ghoniea et al., 1992). The solution, including the plume trajectory, and cross sections, and the plume-induced flow is obtained using the transport element method. This is a Lagrangian vortex method extended to include the dynamic effects of density stratification. Our computational plume model thus is an efficient large-eddy simulation, in which small-scale atmospheric turbulence is modeled using a new interpretation of the classical K-theory. The model is flexible enough to accommodate other physically relevant processes such as chemical reactions between the plume material and the atmosphere. Solutions are compared with experimental measurement whenever possible. In the 92-93 effort we plan to extend the model to include the effect of large-scale atmospheric turbulence, which act in the plane of the plume trajectory, on the dispersion of the plume material.

During the past year, we focused on three projects: (1) simulating plume rise in a uniform atmosphere and comparing the results with experimental measurements; (2) investigating the effect of the Reynolds number on the plume trajectory and dispersion; and, (3) analyzing, using the computational results, the influence of an inversion layer on the plume trajectory and dispersion. A sample of the results obtained in each project with a brief discussion of its current status are shown next.

Figure 1 shows plume trajectory data obtained for Reynolds numbers, \( R_e = \frac{VR_*}{\nu} = 10^3 \) - \( 10^5 \) where \( V = \sqrt{\rho R g} \) is the buoyancy induced velocity, \( g \) is the positional acceleration, and \( \nu = \frac{1}{3} \) is the total diffusivity which accounts for the molecular diffusivity augmented by a small-scale turbulent diffusivity. Clearly the plume trajectory is not influenced by small-scale turbulence diffusion, and is in very good agreement with the experimentally derived \( 2/3 \) power law (Briggs, 1975 and Weil, 1988). Note that this agreement was obtained without adjustable parameters and is based on a careful simulation of the buoyancy dynamics of the plume.

The shape of the rising plume cross section is shown in Fig. 2 for three values of the Reynolds number. The figure shows the density contours at the same distance downstream the plume source. The large-scale structure of the plume is not affected by the small-scale diffusivity, consistent with the trajectory results. Instead, the structure, which consists of two counter-rotating vortices that form due to the roll-up of the baroclinically generated vorticity layer, takes the form of the experimentally observed horse-shoe, independent of the Reynolds number (Fanaki, 1975). The latter, however, is found to affect the local concentration of the plume material since mixing with entrained air is augmented as small-scale turbulent diffusivity is increased.

The high temperature of the plume material enables it to penetrate deep into the atmosphere. The depth of penetration is determined by the density gradient of the atmosphere. One important manifestation of atmospheric density stratification is plume material inversion layers which form due to the radiative heating of a thin layer which caps the convective boundary layer. The presence of inversion layer can modify the plume trajectory in a substantial way and thus affects the dispersion of the plume material (Manins, 1979). Figure 3 shows three cases for which (a) the plume penetrates a relatively low, weak inversion layer, \( HT = 14 R_z \) and \( \Delta \rho = \rho_{\text{above}} - \rho_{\text{below}} = -1/2 \pi \) where \( \rho_{\text{below}} = 0 \); (b) the plume partially penetrates a relatively high, weak inversion layer, \( HT = 10 R_z \) and \( \Delta \rho = -1/2 \pi \), and, (c) the plume is reflected off a relatively low strong layer, \( HT = 14 R_z \) and \( \Delta \rho = -2/\pi \). In all cases, \( \rho_{\text{plume}} - \rho_{\text{below}} = -1/\pi \), normalized with respect to \( \rho_{\text{below}} \), and \( HI = 16 R_z \) where \( HI \) is the height of the inversion layer. In case (b), only the middle part of the plume cross section, which maintains the strongest buoyancy, can penetrate the inversion layer while the sides are reflected back downwards. The plume trajectory in these three cases are shown in Fig. 1. The stabilizing effect of an inversion layer is clearly shown.
During the 93-94 year, we plan to extend the computational model to include the effect of atmospheric turbulence on the plume motion and the dispersion of its material. This will be done in the spirit of large-eddy simulation, i.e., by including the small-scale effect via the diffusion coefficient and the large-scale effect through direct computations.

Acknowledgement:

Computer support for this project is provided by the Illinois National Center for Supercomputer Applications.

Reports and Papers


References


Figure 1. The rising plume trajectories for various buoyancy Reynolds number. The solid line is the extended "two-thirds" law which includes the effect of the finite initial plume size. Plume trajectories corresponding to cases (a), (b) and (c) in Figure 3 are also included.
Figure 2. The density contours in the plume cross wind section at $x=5$ for different buoyancy Reynolds numbers. Only half of the cross-section is shown due to the symmetry about the center line.

Figure 3. The density contours at successive downwind location for a plume approaching an inversion layer when: (a) the plume is initially close to a weak inversion layer (penetration); (b) the plume is initially far from a weak inversion layer (partial penetration); and (c) the plume is initially close to a strong inversion layer (reflection).
SIMULATION OF TURBULENT COMBUSTION AND TRANSPORT IN FIRES

Professional Personnel

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Project Objective

To develop a fundamental understanding of the mechanisms which control the gas phase combustion and transport processes in fires and develop a predictive capability which will allow the computer simulation of these processes to be based on the mathematical expression of underlying physical principles.

Scope

A theoretical and computational approach to the study of the transport, mixing, diffusion, reaction, and radiation processes occurring in both enclosure and exterior fires. Emphasis is placed on gaining an understanding both of the individual phenomena, which occur on widely differing length and time scales, and on the interaction between them. Analyses and computer simulations of separate phenomena are combined and applied to problems of general interest.

Technical Accomplishments

Activities in FY 1992 consisted of three areas: the generalization of the two dimensional enclosure fire induced flow model to handle a wide variety of geometries, the development of a "thermal element" combustion and radiation model to be used in conjunction with large-eddy combustion and fire simulations, and the adaption of the methodology used in the enclosure fire model to predict the smoke transport and deposition by wind blown plumes in a prescribed atmosphere. Each of these will be discussed in more detail below.

The enclosure fire model contains a hydodynamics calculation based on two-dimensional time dependent solutions of the Navier-Stokes equations in the Boussinesq limit. The calculations are performed using a conformal transformation of the spatial variables allowing the equations to be solved in an arbitrary polygonal domain. The conformal map transforms the physical geometry into a rectangular domain in which the transformed equations are solved using finite difference techniques. The flows are driven by a combustion model in which the heat is released on Lagrangian fuel elements which are convected by the large scale fluid motion. This is the high Reynolds number limit of diffusion controlled combustion on discrete fuel elements. The model permits computations of smoke and hot gas transport at Reynolds numbers of order $10^5$ in enclosures of complex shape without employing empirical turbulence models.

The "thermal element" model contains a local scale diffusion controlled combustion model which consists of a small sphere (or cylinder in two dimensions) of gasified fuel being consumed by a transient flame. A prescribed fraction of the fuel is converted to soot which can
emit radiation to its surroundings or absorb radiation from other thermal elements. At large scales which characterize the overall geometry of the scenario under investigation the model consists of a large number of point sources of energy and volume. The large and small scale pictures are coupled together both hydrodynamically and thermally. The location in space and time of each thermal element is determined by a particle tracking computation of its thermal elements. The local asymptotic expansion velocity, together with the chemical and net radiative heat sources are fed back into the computational mesh used to calculate the large scale flow. Thus, the overall fire induced flow is decomposed into an irrotational expansion flow and a solenoidal buoyancy generated flow. The Navier–Stokes equation simulations described above determine the solenoidal flow while the thermal elements determine the expansion field and generate the thermal sources for the large scale buoyancy field.

The smoke transport and deposition model is designed to predict the ground level footprint of particulate matter generated downwind of a large pool fire. The work is part of a larger project (described elsewhere) sponsored by the Minerals Management Service of DOI investigating the feasibility of cleaning up oil spills by burning the spill material. The plume is described in terms of the steady state physical location of the hot gas and particulate matter introduced by the continuously burning fire into the atmosphere. It is assumed that the overall heat release rate and the particulate mass generation rate are known, and that the initial plume structure within a few flame lengths of the fire is not of interest. The atmosphere is taken to be linearly stratified with a uniform wind. The subgrid (less than 10 meters) mixing due to the natural turbulence in the atmosphere is represented by a constant eddy viscosity. All scales above this are calculated directly from the governing equations, which take the form of two dimensional Navier–Stokes equations in a cross-flow plane moving with the wind. The particulate matter is represented by a large number of Lagrangian elements which are convected by the combined effects of the atmospheric and plume induced motion. The model predicts the rise and stabilization of the thermal plume, the separation of the particulate plume, and its descent to ground level. When the particulate is within one computational cell of the ground, it is removed from the atmosphere and its position in the ground plane recorded. The totality of final ground level positions is the particulate deposition pattern.

Publications


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.
A3. Soot
GROUND-BASED SMOKE SAMPLING TECHNIQUES TRAINING COURSE
AND COLLABORATIVE LOCAL SMOKE SAMPLING IN SAUDI ARABIA

Funding Agency: Ministry of Defence and Aviation, Kingdom of Saudi Arabia

Professional Staff:
Nelson Bryner, Project Leader
Bruce A. Benner, Jr., Research Chemist (CSTL)
Robert A. Fletcher, Research Chemist (CSTL)
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J. Randall Lawson, Research Physicist

Project Objective:
Train three Saudi operators in smoke sampling techniques, collect samples in Saudi Arabia, and jointly analyze smoke samples. Visit facilities in Riyadh, Saudi Arabia.

Technical Accomplishments:
Operator Training - NIST will train three Saudis to operate portable gas and particulate sampling instrumentation. This training which is scheduled to take place at NIST on August 17-28, 1992 will involve lectures and demonstrations of gravimetric measurements, light scattering cells, portable size classifiers, battery-powered gas analyzers and filter sampling trains. NIST's organic analytical group will demonstrate sample preparation and illustrate the use of gas and liquid chromatography instrumentation.

Local Sampling in Saudi Arabia - In order to demonstrate the operation of portable gas and particulate sampling instrumentation, a team of Saudi and NIST researchers in October 1992 will collect smoke, and gas samples in Saudi Arabia for analysis. Analysis of smoke and gas samples may include determination of PAH, CO, CO2 and total particulate concentrations. Split-sample analysis will be conducted with some samples being locally analyzed and other samples returned to NIST for more specialized analysis, such as laser microprobe analysis.
MATHEMATICAL MODELING OF INTUMESCENT MATERIALS

Professional Personnel

Takashi Kashiwagi, Project Leader
Howard R. Baum

Project Objective

To develop a mathematical model of the thermal response of intumescent materials that incorporates the basic physical and chemical mechanisms which govern the behavior of these materials in fire situations.

Scope

A theoretical and computational study that incorporates the hydrodynamics, thermal conduction, and thermal degradation of the material in a way that permits the effectiveness of their thermal and chemical properties in protecting the substrate material to be assessed.

Technical Accomplishments

A review of the technical literature revealed only one attempt to develop a theory of intumescent materials. The existing model assumes a one dimensional continuous medium with an empirically determined density-temperature relationship to describe the material. Such a model is intrinsically unable to describe the observed structure and swelling behavior as determined from cone calorimeter tests. A two phase model has been developed that seems capable of explaining the observed behavior.

The model consists of a liquid-like polymer melt phase which represents the original material above the "glass transition temperature". The liquid contains a number of initially randomly distributed sites containing a chemical that can gasify upon heating. The gaseous bubbles that form at each site deform the material by their expansion, thus producing the observed void structure and swelling. The gasification rate at each site is governed by a chemical rate equation whose parameters permit a crude dependence on chemical properties to be assessed. Finally, the temperature distribution in the material is formulated in a Lagrangian coordinate system that permits the thermal retardation to be explained in terms of a reduced "effective conductivity" that arises from the swelling induced by the gasification process.
Introduction. Thermal radiation from fires is an important aspect of fire spread and ignition. Fires are usually highly luminous i.e., much of the radiation is due to the presence of particles of carbonaceous soot in the flames. The prediction of luminous radiation continues to be a difficult problem in combustion research because of the inherent difficulty in predicting the amount of soot that is present in a flame. Several approaches to the prediction of soot and its radiation have been explored over the last decade. Some methods rely on scaling approaches or on empirical correlations of radiation while others attempt to solve conservation equations for the amount of soot in a flame. Among the latter approaches there are two methods. One method attempts to predict the production of soot with detailed chemical kinetics from acetylene to the first aromatic ring and upwards in molecular weight. This approach is strictly a research tool; it will not be possible to implement the complex kinetics in an engineering prediction in the near future. The other possible method is a semi-empirical approach in which knowledge of the soot process that is derived from experiments is used to develop a correlation of soot production and oxidation rates. The rates are then used in conservation equations that are solved numerically. This semi-empirical approach to soot formation and oxidation has been explored in this project.

Model for Soot Formation and Oxidation. The basis for the model of soot that we have developed is a correlation between soot surface growth rates and the local equivalence ratio in a flame i.e., the mixture fraction. This correlation was obtained from experiments in a counterflow diffusion flame. An Arrhenius dependence on temperature is also assumed for the surface growth rate. The rate of growth is assumed to be depend on the total surface area of the soot aerosol. It was found that the details of the nucleation step were not necessary in order to achieve satisfactory predictions of soot volume fractions. Rapid coagulation of freshly nucleated particles collapsed the number of particles to low values and there was a resulting insensitivity to the nucleation step when soot volume fractions were high. Therefore, calculations were performed with only the soot volume fraction equation as part of an integrated flow field prediction. The other equations that were solved included the continuity equation, the momentum equation and an energy
equation. The latter equation included a radiative heat loss term to account for the energy lost by luminous radiation from soot.

The equation for the soot volume fraction included the two source terms and two sink terms. The source terms were the contribution to the soot volume fraction due to the nucleation of new material and the formation of soot due to surface growth. The sink terms included oxidation due to attack by OH and by $O_2$. Equilibrium values of OH and $O_2$ at the local mixture fraction and enthalpy were used in the original prediction that are reported in detail in the 24th Symposium on Combustion.

Recent measurements at NIST and Penn State of OH concentrations in a sooty flame have raised doubts about the validity and accuracy of the modeling that has been used for the oxidation step in the soot process. The LIF measurements indicate that OH concentrations are up to an order of magnitude higher than the equilibrium values that have been used in the soot modeling. Furthermore, the model that we have developed has shown that the loss rate of OH on soot is comparable to the estimated net production rate of OH in the flame. Therefore, a goal of the project in this year has been the relaxation of the equilibrium assumption regarding OH (and other radicals such as $O$). The impact of soot burnout on the flame chemistry and the inverse problem of the impact of finite rate OH kinetics on soot oxidation have been investigated.

Calculations with Detailed Chemistry A model has been developed for the co-flow axisymmetric diffusion flame. The governing equations were solved in boundary layer form. Hence, the parabolic system of pde's could be solved with considerably greater speed than can be achieved if the full elliptic problem is solved. For example, the calculations that are presented here were obtained on a UNIX workstation in about 7 hours; the elliptic problem requires many hours on a Cray. Neglecting phenomena such as diffusion in the axial direction is probably not important in the present situation in view of the inaccuracies surrounding the soot model. A detailed kinetic scheme for methane and air has been used. The "short" mechanism from Sandia with forty six reactions was adopted. Seventeen species equations were solved along with the momentum equation, the energy equation and the soot volume fraction equation with the same source terms as before. However, in the present treatment of oxidation, the actual predicted OH and $O_2$ mole fractions are used. In addition, a sink term in the equation for OH has been included in order to model the loss of OH on soot particles. In a sense, the model as it stands at present is a hybrid model with detailed chemistry for methane but surface growth rates that apply to an ethylene flame. In the near future, $C_2$ chemistry will be incorporated into the model so that true ethylene-air chemistry can be treated. In the mean time, however, we can learn about the effect of finite rate kinetics on OH and O in luminous flames with the methane kinetics. The thermochemistry (temperatures and densities) is not sufficiently different to ethylene-air to affect the flow field and the predictions of soot volume fractions.

Predictions of Soot, OH and O with Finite Rate Kinetics The axisymmetric ethylene diffusion flame of Santoro et al has been calculated. Figures 1 to 5 show results that were obtained for conditions that pertain to a non-sooting flame (flame 3 in the original paper, flow rate of fuel of 3.85 cc s$^{-1}$). Figure 1 presents the computed radial profile of temperatures at two axial stations in this flame viz., at $X/D$ of 2 and 5. It apparent from the figure that the latter figure is close to the end of the flame (although not quite at the very end). The impact of radiative heat loss on the calculated temperatures is apparent when the maximum temperatures are compared at $X/D = 2$ and $X/D = 5$. 
The soot volume fractions across the flame are shown in Fig. 2 at X/D = 2 and 5. The amount of soot increases along the flame until oxidation becomes important towards the end and the soot volume fractions begin to decrease. The soot layer lies within the flame envelope. The peak soot distribution is in reasonable agreement with the levels that were reported by Santoro et al from laser extinction measurements. In our earlier model we found that we could not obtain the amount of soot on the centerline of the flame that the experimentalists reported. This phenomenon is also observed in the present results. It most probably results from inadequacies in the correlation of soot growth rates with mixture fraction i.e., inaccuracies in the flamelet model for these processes in which the Shvab-Zeldovich assumptions are inappropriate.

Calculated OH mole fractions are compared with equilibrium mole fractions in Figs. 3 and 4 at two axial locations. The equilibrium values of OH were obtained by running STANJAN with the calculated temperature at each radial point and the calculated N, O, C, and H atom ratios. It is immediately apparent that large superequilibrium values for OH are predicted. At the peak OH location the calculated OH mole fraction can exceed the equilibrium value by as much as a factor of 10. This value confirms the measurements of Puri, Moser, Santoro and Smyth in an ethylene flame. Further work needs to be done with ethylene kinetics to be certain of this result but it is not likely to be greatly different. It can be seen that the peak OH mole fraction decreases along the flame, primarily as a result of the drop in temperature due to radiation.

Another potentially important oxidant of soot is the O atom. A radial profile of the O atom is shown in Fig. 5 at X/D = 5. The equilibrium mole fractions are also shown. Again, it is apparent that large superequilibrium concentrations are obtained, in this case up to a factor of 60 larger than equilibrium. The soot model does not include O as an oxidant at present. These results suggest that it may be potentially important. The assumption of equilibrium concentrations for OH are also inaccurate. It is not clear at present how these non-equilibrium effects can be incorporated into the basic soot model while retaining it potential for use in turbulent flame calculations.

Reports and Papers:


![Temperature Profiles At X/D = 2.0, 5.0](image)
Soot Volume Fractions At X/D = 2.0, 5.0

Figure 2

Mole Fraction of OH At X/D = 2.0

Figure 3

Mole Fraction Of OH at X/D = 5.0

Figure 4

Mole Fraction Of O at X/D = 5.0

Figure 5
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
The University of Michigan
Ann Arbor, MI 48109-2140
Other Personnel: Ü. Ö. Köylü, Doctoral Candidate
Z. Dai, Graduate Student
L.-K. Tseng, Postdoctoral Fellow
NIST Scientific Officer: Dr. Howard R. Baum

Technical Abstract:

Introduction. This investigation is considering two aspects of unwanted fires: (1) the physical and optical properties of soot in diffusion flame environments, and (2) the scalar properties of turbulent buoyant plumes. The findings of the research have applications to modeling fires in structures, developing materials test codes, and developing fire detectors.

Soot Properties. The physical and optical properties of soot were measured within the fuel-lean (overfire) region of buoyant turbulent diffusion flames in still air, and the results were used to develop and evaluate methods for predicting soot optical properties. The findings have applications to nonintrusive measurements of soot concentrations and structure within flame environments as well as the prediction of continuum radiation from soot in flames.

The study was limited to pool-like fires in still air in the long residence-time regime, where soot and carbon monoxide emission factors are independent of flame size and position in the overfire region for a particular fuel. Both gas and liquid fuels (acetylene, propylene, ethylene, propane, toluene, benzene, n-heptane and isopropanol) were studied to provide information for a range of H/C ratios (1-2.67) and fuel types. Measurements included thermophoretic sampling and TEM to find soot structure, ultimate analysis to find soot composition, and laser scattering and extinction to find soot optical properties.

Soot aggregate properties varied with the fuel but not with position in the overfire region or residence time in the long residence time regime. Primary particle diameters were 30-51 nm with average numbers of primary particles per aggregate of 255-552 — both increasing with increasing propensity of the fuel to soot. Aggregate size distributions were unusually broad (typically 30-1800 primary particles per aggregate) but could be represented reasonably well using a log-normal function. The aggregates were made
fractal-like, with fractal dimensions of 1.7-1.8. Elemental mole ratios of soot composition were variable, suggesting potential for variable refractive indices, e.g., C/H = 8-18, C/O = 58-109 and C/N = 242-976.

Soot structure and laser scattering measurements were used to develop predictions for soot optical properties. These predictions were based on existing Rayleigh-Debye-Gans (RDG) fractal aggregate optical theories (Martin, J.E. and Hurd, A.J., J. Appl. Cryst. 20, 61, 1978; Dobbins, R.A. and Megaridis, C.M., Appl. Optics 30, 4747, 1992), extended to consider the broad size distributions of overfire aggregates. Predicted and measured angular scattering patterns (scattering crosssections for various polarization states) are illustrated in Fig. 1 for acetylene soot at a wavelength of 514.5 nm. The results indicate large departures from the small particle (Rayleigh) scattering approximation (e.g., forward scattering is 100-1000 times larger than wide angle scattering), with excellent agreement between RDG predictions and measurements over the accessible range of scattering angles. The performance of the theory for soot from other fuels was similar.

Strong scattering from soot aggregates affects both laser extinction measurements of soot concentrations and predictions of continuum radiation from soot. This is illustrated in Fig. 2, where present predictions of mean scattering to absorption crosssections, $p_{sa}$, are plotted as a function of wavelength. $p_{sa}$ is significantly greater than unity for wavelengths in the visible, which implies a corresponding overestimation of soot concentrations from laser extinction measurements interpreted using the Rayleigh scattering approximation. Additionally, $p_{sa}$ remains large for heavily sooting materials in the near infrared, where continuum radiation from soot is most important. Thus, past measurements of soot concentrations in flames, as well as determinations of the refractive indices of soot in flame environments, should be reviewed because they generally are based on the assumption of the small particle (Rayleigh) scattering limit which clearly is questionable for the overfire region of large-scale turbulent flames.

Current work is focussing on the physical and optical properties of soot in the fuel-rich (underfire) region of laminar diffusion flames. This work has two main objectives: (1) to evaluate predictions of the RDG theory in the small angle (Guinier) regime which is more accessible for underfire soot aggregates than for overfire soot in the long residence time regime, and (2) to develop information needed to evaluate continuum radiation predictions in flames.

Scalar Mixing in Turbulent Plumes. The scalar mixing properties of round buoyant turbulent plumes were measured in still air. This is an important fundamental problem that has attracted significant attention since the classical work of Rouse et al. (Tellus 4, 201, 1952), see List (Ann. Rev. Fluid Mech. 14, 199, 1984) and references cited therein for discussion of research during the intervening years. However, recent work in this laboratory has highlighted the need for additional information concerning the turbulence properties of scalar quantities within buoyant plumes, in order to address turbulence/radiation interactions in fire environments. In particular, the response of flame radiation to turbulent fluctuations is unusually sensitive to the moments, probability density functions, and spatial and temporal correlations of mixture fraction fluctuations. While the classical work of Pitts and Kashiwagi (J. Fluid Mech. 141, 391, 1984) provides information of this type for nonbuoyant turbulent jets, surprisingly, comparable information is not available for buoyant turbulent plumes. Thus, the objective of the present investigation was to complete measurements of mixture fraction statistics in round buoyant turbulent plumes, and to interpret and correlate the results as a first step toward treating turbulence/radiation interactions in flames.
The experiments employed techniques developed earlier in this laboratory. This involved using mixtures of carbon dioxide and air, and observing the resulting negatively-buoyant plumes. Initial conditions consisted of fully-developed turbulent pipe flow, with mean velocities adjusted so that the flow corresponded to the asymptotic Froude number of round turbulent plumes, in order to enhance rates of development toward fully-developed turbulent plume conditions. Effects of room disturbances were controlled by observing the flow in a screened enclosure surrounded by a plastic enclosure, all within a windowless room, with the plume exhausted using a distributed collection system located in the corners of the plastic enclosure. The mixture fraction measurements were made using laser-induced iodine fluorescence (LIF) based on the 514.5 nm line of a cw argon-ion laser (with roughly 1500 mW of optical power). The laser beam passed horizontally across the flow and was not focussed, so that two traversible detectors could be used to measure the radial spatial correlations of mixture fraction fluctuations — a rarely measured property of turbulent mixing that is crucial for understanding turbulence/radiation interactions. Various positions in the flow could be studied by traversing the plume generator.

We expected the measurements of mean mixture fractions in the plumes to serve primarily as a check of the operation of the present apparatus, however, this was not entirely the case and these measurements were pursued more thoroughly than planned. In particular, while existing measurements are seemingly in the fully-developed portions of the plumes, based on a Monin number criterion, they all are actually at relatively low \((x-x_0)/d\), ca. 20-30, where \(x\) and \(x_0\) are the streamwise distance of the position of interest and the virtual origin and \(d\) is the plume generator diameter. Thus, past flows generally are not fully developed and present measurements indicate somewhat narrower plume widths in fully-developed portions of the flow, for \((x-x_0)/d = O(100)\). Within this regime, however, the classical similarity behavior proposed by Rouse et al. is observed and entrainment rates agree with results in the literature within experimental uncertainties.

Radial profiles of mixture fraction fluctuations confirmed our findings concerning the development of mean property distributions with streamwise distance. Near the plume generator, mixture fraction fluctuations are relatively low and exhibit a dip to a local minimum near the axis. With increasing distance, however, the dip disappears and fluctuation intensities near the axis stabilize at roughly 40\%, which is higher than existing results in the literature. Probability density functions of mixture fraction are represented reasonably well by the clipped-Gaussian function, while the behavior of the popular beta function distribution is somewhat less satisfactory. Temporal power spectra exhibited a limited inertial range because present measurements are still at modest Reynolds number; additionally, the results show that effects of signal noise on present measurements are small. Finally, present two-point measurements of radial spatial correlations are in qualitative agreement with earlier results for forced-flow conditions in flames.

Current work is concentrating on measurements at larger \(x/d\), to establish fully-developed behavior more firmly, and at larger plume Reynolds numbers, to assess effects of the extent of the inertial range of the spectrum. We also are seeking information on streamwise spatial correlations and temporal and spatial integral scales, as well as simple correlations of all flow mixing properties for fully-developed plume conditions.

**Reports and Papers**


Fig. 1  Angular scattering pattern of overfire acetylene soot.

Fig. 2  Mean ratios of scattering-to-absorption crossections for overfire soot.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - FY92

SOOT FORMATION AND EVOLUTION

Professional Personnel

Kermit C. Smyth, Project Leader
George W. Mulholland, Project Leader
Joel E. Harrington, NRC-NIST Postdoctoral Research Associate
Nelson P. Bryner, Chemical Engineer
J. Houston Miller, Visiting Scientist

Project Objectives

Develop scientifically sound principles, metrology, and data which contribute to a predictive model for the formation and evolution of smoke components in flames based upon the best available information for use in understanding fire phenomena. This work embraces broad areas underpinning the BFRL Fire Research Programs, with focussed study of hot gas chemistry and physics. Efforts are directed toward improved understanding of the chemical and physical processes which underlie macroscopic fire phenomena and include development of new techniques and methods for studying these processes.

Technical Accomplishments

During hydrocarbon combustion the exothermic chemical reactions which lead to the formation of water and carbon dioxide consume most of the fuel. However, in many cases a significant fraction of the fuel is converted into species which participate in chemical growth reactions. These processes lead to dramatic consequences in numerous combustion environments. For example, the formation of intermediate hydrocarbons, such as polycyclic aromatic hydrocarbons (PAH), occurs under fuel-rich conditions and poses a potential long term health hazard since many PAH are carcinogenic. In addition, such compounds are also involved in further growth reactions to form soot particles. Radiation from soot dominates energy transfer from large fires, and thus soot formation plays a key role for flame spread. In turn, particle formation and radiative energy transfer control the amount of smoke produced, which is important in fire detection and pollutant emission. In contrast to the oxidation of simple hydrocarbons, which is reasonably well understood, the detailed mechanisms for producing large hydrocarbons during combustion have not been established. The elucidation of chemical growth mechanisms continues to be one of the most challenging research problems in combustion science today.

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 Formation

This project is part of a long-term study of the fundamental chemistry of soot formation. We have investigated the detailed chemical composition of laminar, hydrocarbon diffusion flames using a variety of laser-based optical techniques as well as mass spectrometric sampling. Our recent emphasis has been to make accurate quantitative and relative profile measurements of the radical species. Two studies have been completed this year:

(1) We have undertaken a detailed comparison of our experimental species and temperature data with the flame structure calculations of Mitch Smooke at Yale. To this point few studies have addressed the question of how well flame structure calculations reproduce experimental results. The experimental data were obtained using a rectangular Wolfhard-Parker burner with a flame height of approximately 33 cm, while the computation has been carried out for a 3.8 cm tall axisymmetric flame. Comparisons of temperature and species concentrations have been made by basing the analysis on the local flame conditions, specifically the mixture fraction and the scalar dissipation rate. The best method for establishing a basis of comparison for the scalar dissipation rate involves using a least-squares procedure over a range of mixture fraction, rather than matching at a specific point which corresponds to the stoichiometric surface or the temperature maximum.

Good agreement is found for the major radical species OH*, H atom, and O atom, while for the hydrocarbon radicals CH* and CH3* some features of the profiles agree well but significant areas of disagreement exist. Overall, the calculated positions of the peak radical concentrations are slightly more compressed in terms of the mixture fraction compared to the experimental results. The predicted concentration profiles for the major species agree with the experimental measurements as well as found in investigations on premixed flames, for example in acetylene combustion (Westmoreland et al., 1986). The model results are somewhat more sensitive to the scalar dissipation rate than are the experimental profiles.

The most serious areas of disagreement concern the comparison of the temperature profiles and the much larger degree of O2 penetration in the computed flame structure. The influence of the latter, particularly in rich flame regions, is likely to be small and can be further investigated by carrying out one-dimensional counterflow calculations with and without a small amount of O2 added to the fuel stream and then comparing species profiles. Given the importance of the temperature field in determining the chemical structure of a diffusion flame, the disagreement between the computed and the experimental temperature profiles certainly deserves further study before one can be satisfied with the generally excellent agreement for the individual species profiles.

(2) Recent measurements have also been made of absolute OH* concentrations in the soot oxidation region of laminar, hydrocarbon diffusion flames with Bob Santoro and his students. In the oxidation region there exists a competition for OH* between CO and soot particles, since OH* is a key oxidizer for each. Furthermore, the oxidation of soot itself leads to enhanced levels of CO. Previous work has shown that the emission of CO from diffusion flames is closely related to the observed soot concentrations within the flame, which in turn control smoke emission levels.
OH· concentrations have been measured in four coannular diffusion flames, burning methane at a single fuel flow rate and ethene at fuel flow rates which produce non-smoking, incipient smoking, and smoking conditions. Laser-induced fluorescence was used to make point profile, line image, and two-dimensional image measurements. These data have been placed on an absolute basis by reference to earlier absorption data obtained in our Wolfhard-Parker burner. As the soot concentration increases, both the OH· concentration and the flame temperature are found to decrease. Estimates of the superequilibrium levels of OH· increase as the measured concentrations decrease, which makes accurate a priori prediction of OH· concentrations problematic.

These experimental results should both test and guide the development of soot production models which include oxidation processes, since current soot models must utilize either assumed or estimated OH· concentrations. It is especially noteworthy in this regard that equilibrium and partial equilibrium approaches may not even be a reasonable starting points for estimating OH· concentrations in the region where soot oxidation rates are expected to be largest.

2. Smoke Agglomerates

A combined experimental and theoretical effort is focussed on the characterization of the optical and structural properties of smoke agglomerates. Previous theoretical analysis was based on Rayleigh-Debye scattering theory. This theory does not include multiple scattering within the agglomerate and is limited to primary particle sizes in the agglomerate with dimensionless size parameter $x = \pi D^2/\lambda$ small compared to 1. The Electric/Magnetic Coupled Dipole Method (EMCD) has been developed in collaboration with Craig Bohren at The Pennsylvania State University to overcome these deficiencies of the Rayleigh-Debye method. The coupling in effect allows treatment of multiple scattering and including the magnetic dipole term allows treatment of primary spheres with size parameter up to about 1 (0.2 μm diameter spheres for the HeNe laser wavelength). The following expressions are obtained for the exciting field at the center of each primary sphere:

$$\tilde{E}_i = \tilde{E}_i^0 + \alpha_E^k \sum_{j=1}^{N} \tilde{C}_{ij}\tilde{E}_j + \alpha_H^k \sum_{j=1}^{N} \tilde{F}_{ij}\tilde{H}_j$$

$$\tilde{H}_i = \tilde{H}_i^0 + \alpha_H^k \sum_{j=1}^{N} \tilde{C}_{ij}\tilde{H}_j + \alpha_E^k \sum_{j=1}^{N} \tilde{F}_{ij}\tilde{E}_j$$

The matrices $C_{ij}$ and $F_{ij}$ correspond to the electric dipole and magnetic dipole interaction. In short, the analysis consists of solving these equations by successive approximation for the exciting fields, computing the dipole moments from the exciting fields and the electric and magnetic polarizabilities, $\alpha_E$ and $\alpha_H$, and then computing the differential and total cross sections by making use of the far field expressions for the electric and magnetic dipoles.

The computational code has been validated by comparing with the exactly solvable two sphere problem and calculations have been made on selected low density agglomerates with 17, 52, and 165 primary spheres. These agglomerates were generated by Raymond Mountain using his Brownian dynamics code. The focus of this work has been on comparing results for the Rayleigh-Debye method with the EMCD method. Much insight is being obtained regarding the role of primary sphere size and number of agglomerates on the accuracy of the Rayleigh-Debye approximation, but for some issues such as the effect
on the fractal dimension, we must treat larger agglomerates and include orientation averaging. Such calculations are being planned. One advantage of our new method compared to the Rayleigh-Debye approximation is the prediction of both the polarization and the depolarization ratios. These quantities are not currently measured for agglomerates but may provide insight regarding the agglomerate structure.

Publications


T. Cleary, G.W. Mulholland, L. Ives, R. Fletcher, and J. Gentry, Aerosol Science and Technology 16, 166 (1992)


Related Grants


2. Modelling of Soot Formation in Diffusion Flames, Ian Kennedy, University of California at Davis.

3. Experimental and Modelling Studies of Soot and Carbon Monoxide in an Ethylene/Air Diffusion Flame, J. Houston Miller, George Washington University.

I. Review of Research on Microparticles. The presence of polydisperse, singlet particles low in the diffusion flames of ethene, methane and acetylene (Refs. 1-4) has been reported in the past. These particles were found to be generally circular in cross section and, in opposition to aggregates at found in the higher temperature regions of the flame, they offer a low contrast to the electron beam. These microparticles are similar to those found by Wersborg et al. in 1973 in the lower region of the premixed acetylene flame operating at low pressures. This suggests that these microparticles are a universal precursor of carbonaceous soot in hydrocarbon flames.

This discovery was made possible by our prior development of the thermophoretic sampling technique that is now in use at several universities and at NASA Lewis. This technique affords detailed views of the particle morphology in the various regions of the diffusion flames. This morphology has proven to be highly variable, and it complicates the interpretation of the laser scattering/extinction experiments which have been widely practised during the last decade. In the past year, we have used the thermophoretic sampling in conjunction with HRTEM for the first time to explore internal texture of both microparticles and mature soot particles.

II. High Resolution Transmission Electron Microscopy (HRTEM). A JOEL Model JEM2010 microscope with high resolution capability has become available here, and the initial examination of the flame generated carbon was conducted. This microscope has a point-to-point resolution of 0.19 nm and operates up to 600 kV. The contrasting internal textures of soot particles are made apparent by means of this instrument, see Figs. 1a and 1b.

Mature soot particles sampled from the high temperature regions of the flames are readily examined using our previously developed sampling techniques. The HRTEM micrograph shown in Fig. 1a reveals the development of rudimentary, irregular graphitic layers which are
parallel to the surface of this carbonaceous particle. Within the particle there exist a series of concentric whorls, which are termed as growth centers. Primary particles are strongly bonded in the aggregate shown in Fig. 1a with the concentric layers. The microtexture shown in Fig. 1a is very similar to HRTEM micrographs that originate in carbon black literature.

Microparticles are more difficult to observe in HRTEM because they offer low contrast to the carbon film substrate upon which they are collected. We are experimenting with the use of bare grids as a collection medium to bring out the internal texture of the soot precursor particles. Figure 1b is a micrograph taken of a particle collected without a carbon substrate showing a more amorphous internal structure. This method is more difficult to use because the bare grids have a lower collection efficiency for the microparticles.

The above microscopic information and the literature that documents the role of PAH species in hydrocarbon flames leads us to conclude that the microparticles are likely to be composed mainly of mixtures of these compounds. Howard has explained the role of aryl radicals in promoting the reactive coagulation of large PAH species. This mechanism would account for the growth of the microparticles that we have observed. The microparticles which are converted to carbonaceous soot as a result of exposure to high temperatures portions of the flame. The mature soot particles then undergo cluster-cluster aggregation coexisting with surface growth and partial or total oxidation. The formation of soot is thus portrayed schematically, Fig 2, a graph of species hydrogen mole fraction vs. the logarithm of the particle mass. Here microparticles are portrayed as an intermediate stage formed by reactive coagulation from PAH species and depleted by annealing at higher flame temperatures to form carbonaceous soot.

III. Examination of Improved Laser Scattering/Extinction Tests. Santoro, Puri and Richardson of Pennsylvania State University have generated new laser scattering/extinction data for the nonsooting laminar coanular ethene flame. This data has been analyzed using the optical cross sections we have previously formulated (Ref. 5). The results of this analysis provide strong support our previous description of the partitioning of soot aerosol dynamic processes in the laminar flame. An article has been submitted on this topic (Ref. 6). The above recent results on the presence and significance of microparticles does offer an important understanding of the inception and growth processes in laminar diffusion flames. Thus particle inception takes place in the region of intermediate temperatures usually close to the burner mouth and is accompanied by reactive coagulation. As these particles pass into the higher regions of the flame, they are exposed to the higher temperature which causes dehydrogenation and the formation of mature, partially graphitic soot aggregates. The primary particle concentration that persists in the upper flame is established in the inception zone.

IV. Research Reporting These research results on the presence of soot microparticles were first reported to conferences in Hiedelberg, Travis City, and Ithaca (Ref. 1-3) during the fall of 1991. At these meetings our results were found to be consistent with observations by several European groups. The coexistence of microparticle singlets and carbonaceous aggregates has convinced us that the interactive use of laser scattering/extinction and transmission electron microscopy have great potential in the diagnosis of particles formed in flames. This viewpoint has been promoted in several of our recent presentations (Refs. 3,7,8). Our work confirms the fractal-like nature of soot aggregates and this aspect was discussed at the meeting at Montreal (Refs. 8). A presentation on the atmospheric impact of soot has been accepted (9). Two additional presentations on the soot precursor (microparticles) are impending (4,10).
Acknowledgements - Mr. Alan F. Schwartzman of the Division of Engineering who in charge of the Electron Microscope Facility has conducted the high resolution transmission electron microscopy on soot particles sampled in flames.

Recent and Impending Reports and Publications:


Figure 1. HRTEM of (a) Mature Carbonaceous Aggregate and (b) Young Microparticle

Figure 2. The Representation of the Formation of Carbonaceous Soot From Hydrocarbon Fuels
STUDY OF SMOKE AGGLOMERATES

Funding Agency: National Aeronautic and Space Administration

Professional Staff: George Mulholland, Research Chemist
Raymond Mountain, NIST Fellow
Nelson Bryner, Chemical Engineer
William Pitts, Supervisory Chemist
Eric Steel, Supervisory Microscopist
Dave Bright, Analytical Chemist

Project Objective:

Provide ground base information regarding the study of the optical properties and growth dynamics of large smoke agglomerates in a micro-gravity environment.

Technical Accomplishments:

The project is a combined experimental and theoretical study of the optical properties and growth dynamics of large smoke agglomerates. The light extinction coefficient and total scattering coefficient will be measured by a transmission cell-reciprocal nephelometer, which was recently developed at NIST. Differential scattering measurements will be made to characterize the radius of gyration and fractal dimension as the agglomerates grow. The facility for making these measurements is in the process of being fabricated.

There is a parallel theoretical component of the study. The objective is to compute the optical properties, the fractal dimension, and the radius of gyration of large clusters containing up to 100,000 primary spheres to provide comparison with experiment. We will be generating the agglomerates using a Brownian dynamics code previously developed by Raymond Mountain. Initial light scattering calculations will be made based on Rayleigh-Debye scattering theory, which we have used in the past for smaller agglomerates.

The Rayleigh-Debye has the advantage of being computationally fast; however, this theory does not include multiple scattering within the agglomerate and is limited to primary particle sizes in the agglomerate with dimensionless size parameter $x = \pi D_p/\lambda$ small compared to 1. During the past year, the Electric/Magnetic Coupled Dipole Method (EMCD) has been developed by George Mulholland in collaboration with Craig Bohren at The Pennsylvania State University to overcome these deficiencies of the Rayleigh-Debye method. The computational code has been validated by comparing with the exactly solvable two sphere problem and calculations have been made on selected low density agglomerates with 17, 52, and 165 primary spheres. During the next year, the validity of the Rayleigh-Debye method will be tested over a wide range of agglomerate sizes.
A4. Engineering Analysis
Institution: George Mason University
Grant No.: 50SBNB1C6527
Grant Title: Effectiveness of Staging Areas in Office Buildings
Principal Investigator: Prof. Carl M. Harris, Chairman
Dept. of Operations Research & Applied Statistics
George Mason University
4400 University Drive
Fairfax, VA 22030-4444

Other Professional Personnel: Dr. Bernard M. Levin
Dr. Norman E. Groner

NIST Scientific Officer: Dr. John Klote

Technical Abstract:

Objectives. One approach for assuring the safety of disabled occupants of office buildings, in a fire emergency, is to provide a staging area or an area of refuge where the disabled occupants can wait safely until either they can be assisted out of the building or the fire is extinguished. The General Services Administration (GSA) of the Federal Government has retrofitted six office buildings with staging areas to upgrade the fire safety for disabled occupants: three in Washington, DC; one in Toledo, OH; one in St. Paul, MN; and one in Bemidji, MN. This provided a unique opportunity to evaluate the value of staging areas as an approach for providing a high level of actual safety; to evaluate the perceived safety of the office buildings by the disabled occupants; and to develop guidelines for implementing future systems. The thrust of this project was the human factors aspects of fire protection systems that use staging areas.

Site Visits. During the first year of the project, Drs. Groner and Levin visited the six GSA buildings retrofitted with staging areas. They observed the physical sites and the staging areas, discussed problems and procedures with responsible officials, interviewed building occupants (especially those with disabilities and those who fill emergency roles such as floor wardens), and in some cases observed fire drills.

Final Report. A final report was submitted to the National Institute of Standards and Technology. Revisions were made after review by the project officer, and in April, the report was published as a NIST contractor grant report (NIST-GCR-92-606).

The main body of the report provides technical information that could be used by sponsors in evaluating the advantages and limitations of the use of staging areas to provide safety for occupants with disabilities in office buildings. It discusses the characteristics of the different types of staging areas; the role of the "designated official" in planning and training activities; human factors...
considerations related to such physical features as automatic folding doors, telephone or intercom communications systems; location of staging areas; ventilation systems and lighting; the need for coordination with the fire department; maintenance considerations; and the more intangible aspects of the problem such as promoting the creditability of the system to ensure acceptance of staging areas by occupants with disabilities.

An appendix of the report is directed primarily at anyone who is responsible for developing the emergency plan and for training occupant emergency organization members in the use of staging areas. This appendix provides detailed guidelines for selecting appropriate life safety strategies for protecting building occupants; and guidelines for developing, writing, and implementing fire emergency plans appropriate to the life safety strategies selected. Although the guidelines are tailored to buildings which contain staging areas, many of the suggestions have wider applicability and are useful for fire emergency planning in general.

Some of the Problem Areas and Recommendations.

Fire Emergency Plan and Training: A "Designated Official" is responsible for developing the occupant emergency plan, and for selecting and training occupant emergency organization members. More assistance should be given to Designated Officials for them to be able to perform these tasks adequately.

Existing Occupant Emergency Plans based on guidance from the GSA document "Occupant Emergency Program Guide" were good from the standpoint of establishing an organizational structure for emergency situations. However they were not designed to provide useful information to the typical building occupant. A document should be distributed to each employee that describes the fire emergency plan in simple language. Information regarding staging areas needs to be added to the Occupant Emergency Plan or a separate document regarding staging areas needs to be created.

Employees (called floor monitors, area monitors, etc.) who are assigned responsibilities in emergency situations need more assistance to perform their duties; e.g., formal training, group discussions, and feedback discussion sessions immediately after drills. Employees with disabilities need to be kept current as to who is assigned to assist them.

Employees with mobility impairments need to be instructed on the operation of the safety features of the staging areas and told how they provide safety. During our visits we did not find any such training underway or planned.

Potential users of the staging areas must have confidence in the safety of the staging areas. To build confidence, employees should be given information on the staging areas features as, for example, the existence of a special ventilation system to supply the staging area with clean outside air. Care must be taken not to destroy confidence in the system by, for example, having uncovered signs visible during the construction period and before the system is fully operational.

Coordination with the Fire Department: Building management must inform the fire department of the existence and design of staging areas. The fire department should be alerted during the design stage to give it the opportunity to make suggestions for improving the design and assuring that the design is consistent with their operating procedures. Staging areas should be included in the pre-fire plan and familiarization visits of the fire department.
Nature of the Staging Area: Some of the staging areas were too small to be comfortable or prevent employees from feeling "trapped." Some small staging areas may serve other functions, in addition to being a lobby or passageway, if those functions are carefully selected and the staging area is properly designed. Occupants with mobility impairments expressed the view that they would like to have a window in the staging area. It is anticipated that this will often not be practical. During our in-depth visits, none of the small staging areas had chairs or other furniture that would permit seating. Seating is needed for ambulatory occupants who have physical impairments that would make it difficult to stand for any period of time or to sit on the floor. Monitors accompanying employees with disabilities should also be able to sit.

Building Features:

1. Doors -- Many doors in fire barriers that had self-closers were kept open with wedges, etc. Self-closing devices should be replaced with automatic closers that will close the doors when the alarm sounds or power in the building is lost. Even some doors with automatic closers were kept open if frequent electric surges or interruptions closed the doors.

There were problems with the automatic folding doors as installed in the small staging areas in five of the six buildings. They did not have a viewing panel to provide the visibility outside the staging area which could decrease the anxiety of occupants awaiting rescue. The doors have a safety feature to stop the closing of the door when the door encounters an obstruction such as a slow moving person. This feature was not operating properly. (The manufacturer has informed us that this and other safety related problems were corrected.) The alarms associated with these doors should be properly deactivated (so as not to interrupt other associated safety features) or made much less intrusive. Their loudness would cause severe communication difficulties.

2. Communications -- For buildings with large staging areas, procedures must be developed to provide occupants with disabilities with the information as to which of the large staging areas they should go. (One may contain the fire.)

A phone or intercom system within the staging area, while not needed for the physical safety of those seeking refuge, would greatly add to their psychological comfort, and the information given the fire department by the occupants of staging areas could affect the priorities of actions by the fire department. The use of the phones or intercom is sufficiently complicated that informational signs and training of occupants for the setup particular to their building is needed.

If the communications systems are to function effectively, both the staging areas and the receiving office must be sufficiently quiet for the communicating persons to hear each other. More noise can be tolerated if phones rather than intercoms are used. Sounding alarms can make the systems useless.

3. Signs -- Signs should be included as part of the installation provided by GSA or, at least, guidelines for installing signs should be provided by GSA. If GSA provides the signs, the Designated Official should have the authority to add to or modify the signs. Signs should not be visible until the staging area is fully operational.

4. Ventilation systems -- Ventilation systems for the staging areas should be designed so there is a very high probability they will continue to operate throughout the fire. A lack of fresh air and moving air would most likely disturb occupants of the staging areas.
5. Lighting -- Some staging areas are normally dark and the switch is in the darkened room. Lighting for the small staging areas could be improved by connecting the alarm to the lights so that when the alarm sounds some light is automatically provided. This could be the regular lights with emergency backup. The emergency lights would be a possible alternative in some situations.

Safety Systems. In designing safety systems it is important to keep the systems as simple as possible. As systems become more complicated, it becomes difficult to assure: 1. that all components will contribute as anticipated to the functioning of the fire safety system; 2. that the hardware will be properly designed, installed, and maintained; or 3. that the building occupants and the security staff will be properly trained. Whenever staging areas are planned for additional buildings, it is important to be sure that there is an organizational structure that can design, install, and operate a system of this complexity.

Even if the system is relatively simple, it is vital to have one central point of responsibility and authority for ensuring that the system is designed, constructed and used as a coordinated system and that the human behavior aspects are integrated into the system design and implementation. As systems become more complicated, the need for this centralized authority increases. Even after the staging areas are designed and built, it is not too late to establish this central authority. There may still be a need for design changes and there is a need for continued oversight of the fire safety plan, its updating, and the associated training. We do not anticipate that the human behavior aspects of the system will be properly considered and handled without such a central authority.

Reports:


Professional Personnel

Richard W. Bukowski, P.E., Project Leader
Harold E. Nelson (Retired)
Scot Deal, Research Engineer
Charles Arnold, Computer Programmer

Project Objective

1. The development of separated and assembled fire protection analytical (computerized) tools and the transfer of these tools to practicing professionals.

2. The use of these tools and other resources to recreate and otherwise analyze one or more significant fires. To initiate verification of the results, to evaluate the tools, and to assist decision makers in actions to prevent recurrence.

Scope

1. Assemble useful data, formulas, and simple models. Program these into a common format with an accessible point of entry (menu, etc.) Develop this into a generalized engineering approach suitable for compartmented buildings. (This portion of the project is closely allied with aspects of the GSA sponsored project on Corridor Flows.)

2. Demonstrate procedures for fire reconstruction investigations. Conduct a reconstruction investigation of one or more fires of significance. Analyze the fire, determine and initiate research or testing needs required for a satisfactory reconstruction, prepare the appropriate report.

Technical Accomplishments

1. Engineering Analysis System

FPEtool, a computerized package of simple, easy to use, engineering equations and models has been upgraded and distributed broadly. New procedures to estimate the progress of a wave front propagating down a long corridor and then flowing into a target room (refuge area) has been incorporated.

2. Fire Reconstruction

Fires in Colorado Springs (CO) and Detroit (MI) were undertaken and reports were prepared. A prior, extensive analysis of the Happyland Social Club fire (Bronx, NY) was published after criminal proceedings against the accused arsonist were concluded. A prospectus for a modern, two-week training course in fire science for fire investigators was developed and proposed to the National Fire Academy (NFA) and the Bureau of Alcohol, Tobacco, and Firearms (BATF). The course, to be put on by BFRL in collaboration with NFA is awaiting developmental funding consideration by NFA and BATF.
Publications


Related Grants

"Fire Safety in Board and Care Homes", Carl M. Harris, George Mason University.
Institution: California Institute of Technology
Grant No.: 60NANB9D0958
Grant Title: Experimental Study of Heat Transfer and the Environment in a Room Fire
Principal Investigator: E. E. Zukoski
Jet Propulsion Center, 301-46
California Institute of Technology
Pasadena, CA 91125
Other Professional Personnel: T. Kubota, Professor Emeritus
R. Chan, Doctoral Student
S. Palm, Master’s Student
D. Revolinski, Doctoral Student
NIST Scientific Officer: Dr. Leonard Y. Cooper

TECHNICAL ABSTRACT

INTRODUCTION  The transient characteristics of large diffusion flames burning in a vitiated atmosphere, buoyancy driven flows in shafts, and the flow of gravity currents in hallways are under investigation in experimental programs.

The composition of the gas surrounding a large diffusion flame has a strong effect on the chemical species formed during the combustion processes and, in particular, on the production of carbon monoxide, a toxicant. We are studying the production of carbon monoxide and other species in large diffusion when the flame penetrates far above the interface between a cool lower layer of fresh air and a strongly vitiated upper layer. The emphasis in this study is to measure the products formed during the transient development of the upper layer.

The second area of interest concerns the transfer of heat and species in a vertical shaft. These processes are poorly treated now in most fire codes because the heat transfer and some of the mass transfer processes are not well understood. Mass and energy transfer between the inside and outside of the shaft can be driven by buoyancy forces which result from temperature differences between the shaft and ambient gas. This is the “stack effect.” A second mechanism is related to the Rayleigh-Taylor effect which occurs when a heavy gas lies above a lighter gas in a gravitational field. This process is slow and is important when the openings in the sides of the shaft are so small that the stack effect is unimportant. An accidental fire situation in which the Rayleigh-Taylor mixing is important would occur when a sealed shaft such as an elevator shaft is open at the bottom to a space which is involved in a fire. The influence of heat transfer to the walls of the shaft on both the stack and Rayleigh-Taylor mixing process are being investigated in an experimental program.
The third area of interest concerns an investigation of the influence of viscosity on the flow in a gravity current such as that which would develop in a long hall during an accidental fire. Because mixing between the gravity currents and the ambient atmosphere are very weak, these currents can transfer toxic species over long distances with almost no dilution. The influence of heat transfer to the walls and viscous effects on the propagation of these currents are being investigated in an experimental program.

**SPECIES PRODUCED DURING THE DEVELOPMENT OF A CEILING LAYER**

The chemical species produced in a hood during a transient experiment are being studied experimentally for configurations in which the steady state fuel-air ratio of the gas entering the hood is greater than stoichiometric. A numerical model for the process is also being developed.

The experiments are being carried out in a hood which is a 1.22 m high by 1.83 m on a side. A 19 cm diameter natural-gas burner is located 10 cm below the bottom of the hood and species formed within the hood are studied by analyzing gas samples withdrawn from the hood with either a gas chromatograph, which can be used to obtain a complete set of concentration data at a few times during a test, or on-line instruments which are used to obtain a continuous measure of the mole fractions of oxygen, carbon monoxide and carbon dioxide. Gas and wall temperatures are also measured. A complete set of data is taken every 20 ms.

A typical set of data is shown in Figures 1 to 4 for concentrations of oxygen, carbon monoxide, carbon dioxide, and gas temperatures for a 67.8 kW natural gas flame with the surface of the burner placed 10 cm below the bottom edge of the hood. Fuel flow is a step function starting at time zero and terminating at about 1800 s. The $Q^*$ value for this fire is 3.8, the flame height above the burner surface is about 1.1 m and the steady state equivalence ratio for the gases entering the hood is 2.2. Data obtained from six identical experiments, in which the sampling probe was located at different elevations, is shown in these figures.

The sudden initial changes in all parameters shown in these figures results from the initial filling of the hood with products of combustion. This occurs within the first 125 seconds, a time which is slightly shorter than rough estimates made of the filling time based on entrainment models.

At the end of this filling period, the composition of the gas within the chamber is still far from its steady state value, e.g., oxygen mole fraction about 10% and that for carbon monoxide below 0.15%, and subsequent changes occur as the species within the hood either react, in the flame or within the hood, or are displaced by the flow which enters the hood in the fire plume. The approach to a steady state is a relatively slow process requiring a total time of roughly 1000 s.

For the hood-flame parameters of this experiment, gas temperatures are low and do not rise above 500 K. Gas and wall temperatures rise with an almost constant difference and 80 to 90% of the heat release within the hood is transferred out of the gas.

We were interested to find that after the fire is extinguished, rapid mixing with the ambient atmosphere occurs. During the process, the oxygen concentration in the middle of the hood reaches levels of 10% within 300 seconds after the fuel flow is stopped. The transport of air into the hood is not caused by leaks in the hood and appears to be the result of mixing caused by natural convection currents. These currents are generated on the relatively cool side walls of the hood and mixing occurs when they reach the bottom of the hood and impinge on the ambient atmosphere.

For this test condition, species concentrations were measured at six elevations within the hood. Because a single probe was used to obtain this data six experiments were performed. As expected, stratification was observed during the filling period; however, once the interface reached the bottom of the hood, the species concentrations obtained from probes located at heights between six
cm above the bottom of the hood and 16 cm below the top were found to agree to within experimental accuracy. Thus, after the initial filling transient, the gas in the hood is well mixed for this hood-flame configuration. However, the gas temperature was not constant and increased monotonically with height due to heat transfer to the walls and ceiling. These results agree with steady state results obtained earlier.

A data set of this type is being collected for several fire-hood configurations so that the processes involved in the transient production of carbon monoxide and other species in the two layer configuration can be better understood. The data will also be useful in validating models for the combustion process in the two layered configuration.

A model of this transient process is also being developed with the aim of elucidating the chemical reactions which may occur in the bulk of the hood gas or as the hood gas recirculates through the flame.

**MIXING IN A VERTICAL SHAFT** The basic problem under investigation involves the transfer of heat and species into the shaft from a hot reservoir beneath the shaft when the sides and top of the shaft are sealed. At the beginning of an experiment, the shaft walls and the gas are cool and the experiment starts when the bottom is suddenly opened to a region full of hot, lower density gas. For this situation, the stack effect is not important and mixing occurs because of the Rayleigh-Taylor instability. The effect of openings from the shaft to the ambient atmosphere on this process will also be investigated.

The experimental apparatus constructed for this investigation will allow studies of flow in a 25 cm square shaft which is 250 cm high. The walls of the shaft and gas in the shaft will be initially at room temperature and the open bottom of the shaft will be suddenly exposed to gas at temperatures of 400 to 500 K at the beginning of the experiment. The subsequent motion of the hot gas front into the shaft and heat transfer to the shaft walls will be studied with fast response temperature and heat transfer instrumentation. The shaft and hot gas reservoir have been constructed and preliminary tests have been carried out.

**GRAVITY CURRENTS** The study of gravity currents has made use of the salt-water/water modeling of these currents in order to separate the influences of heat transfer and viscosity on the development of the currents in long halls.

A report on our gravity current experiments and a computational model for the current have been completed, and a description of the results are now available in a PhD thesis by R. Chan.

**REFERENCES**


Figure 1. Oxygen Concentration History

Figure 2. Carbon Monoxide Concentration History

Figure 3. Carbon Dioxide Concentration History

Figure 4. Gas Temperature History
FIRE AND THERMAL CHARACTERISTICS OF NAVY FIRE FIGHTER TRAINERS

Funding agency: Naval Training Systems Center, Orlando, Florida

Professional staff: Robert S. Levine

Project objective:
Support the development and implementation of prototype fire fighter trainers.

Technical accomplishments:
Measurements have been made of air and wall temperatures, atmospheric composition, radiant fluxes, vent flows, and other pertinent characteristics of prototype trainers to evaluate realism and to delineate possible training safety hazards. Prototype trainers are located at Mayport Naval Station, Florida; Groton, Conn., submarine station; Great Lakes Naval Station (recruit trainer); Treasure Island (San Francisco); San Diego; and Norfolk. Measurements are made with the BFRL instrument van and/or portable equipment, and the results are reported to the sponsors. Gas species analyses are performed and meetings to discuss them are arranged to obtain site permits from local Environmental Protection Agencies.

On occasion, special analyses are carried out by BFRL and other NIST personnel to obtain information of importance to solve developmental problems. These have included, for instance, metallurgical analysis of slag from a failed smoke generator, electron microscope examination of ceramic insulation to determine the cause of failure, and field equation modeling of a wind barrier solution to problems caused by wind affecting the flames on a carrier deck fire trainer.

Most of the necessary data from the complete stable of prototype trainers have been obtained and analyzed. But the production trainers will use somewhat different burners designed by a different Navy contractor. So measurements will be made to determine whether there are different effects. Also, the concerns of environmental authorities have not all been answered. These will require additional exhaust gas species measurements.

The project leader participates in design reviews, fleet project team meetings, and similar program activities when requested by the sponsor.

Reports and Publications:


NISTIR 4318, Levine, R.S., and Greenaugh, K., "Exhaust Gas Analysis for Harmful Species: 19F1A Fire Fighting Trainer at Mayport, Florida."
Institution: George Mason University
Grant No.: 60NANB9D0974
Grant Title: Fire Safety in Board and Care Homes
Principal Investigator: Prof. Carl M. Harris
Chairman, Dept. of Operations Research & Applied Statistics
George Mason University
4400 University Drive
Fairfax, VA 22030-4444

Other Professional Personnel: Dr. Bernard M. Levin
Dr. Norman E. Groner
Roseanne Paulsen

NIST Scientific Officers: Harold E. Nelson, Richard W. Bukowski

Technical Abstract:

Project Objectives

The goal of this project is to collect, analyze, and disseminate technical information that will help lead to a high degree of fire safety in board and care homes without incurring unnecessary expense or interfering with program goals. This information will be related, in large part, to the use of the Board and Care Chapter of the 1985 and 1988 editions of the Life Safety Code.

This grant involves several independent tasks, each contributing to the goal of the project.

Progress and Problems in Adoption of the Board and Care Chapter of the Life Safety Code

A major emphasis of this project is to determine the extent to which the Board and Care Chapter of the National Fire Protection Association's Life Safety Code has been adopted, and to uncover problems with its use and interpretation. Such knowledge can be helpful in developing recommendations for refinements of the Code and in promoting its use.

During the previous two years of the project, information and opinions were sought from various interested groups: state officials (mostly from social service agencies), persons from advocacy organizations, inspectors from the Veterans Administration, and "board and care" home providers. This year state fire marshal office representatives were queried. Responses were entered into a computer database using Paradox software. Analyses of the data, including essay type responses, were completed.
Interim Report

An interim report was completed and has been published by the National Institute of Standards and Technology as Report Number NIST-GCR-92-611 "Affordable Fire Safety in Board and Care Homes, A Regulatory Challenge--Interim Report" by B.M. Levin, N.E. Groner and R. Paulsen. It is not expected that subsequent work and investigation will result in any major changes in the format of the report or its conclusions. The final report should contain more documentation and substantiation. It should also contain some updated information.

The Life Safety Technical Committee on Board and Care Facilities met on July 23 and 24, 1992. The preparation of the interim report was timed so that it was available to the Committee for their information prior to the July Meeting.

Provider's Manual

A draft of a manual has been completed that could be used by those providers that are not knowledgeable about fire safety codes and regulations. Such providers must eventually rely on the advice of experts. However, they need a manual that will give them a simple explanation of the requirements in the Board and Care Chapter and advice on how they should proceed in preparing their facilities to meet the requirements in the Chapter. The manual should help them understand the type of professional assistance they will need. A draft of the manual has been completed and is being reviewed for clarity and accuracy.

Fatal Fire in Detroit Board and Care Home

Dr. Levin investigated the fatal fire of June 2, 1992 in Detroit, Michigan. A total of ten residents died on the day of the fire.

The facility occupied both sides of a three story (plus basement) duplex on a street with several homes providing personal care services. The state had considered it a board and care home (Adult Foster Care) until 15 years ago when the state withdrew its support and attempted to shut down the home. Since then it apparently has been considered by the city as a boarding and lodging house except it continued to provide personal care services to some of the same residents.

This fire supports a conclusion in the Interim Report that people with disabilities who cannot afford to live in code complying board and care homes may be housed in buildings that do not meet the state or local fire requirements for board and care homes. This problem was also highlighted in the local newspapers after the fire.

Highlights from the Interim Report

- The regulatory system for Board and Care Homes is complex. A Home may be subject to some combination of local, state, and federal regulations. It may need to meet separate sets of regulations in order to obtain a license, to obtain an occupancy permit, for funding, and/or for referrals from government agencies. The picture is somewhat simplified by the fact that more than one jurisdiction may adopt the same set of regulations (model code), and by the fact that one set
of regulations may be sufficiently more rigorous than another so that one can essentially ignore the less rigorous.

- There are very significant differences in the quality of life situation for the various disability groups and within each grouping. The entire gamut of possibilities is run. While some disabled persons are in high quality Homes with high levels of fire safety; others are in marginal or unregulated Homes of poor quality. Still others are homeless.

- The economic effect of requiring added fire safety can impact Homes very differently. The cost of fire safety improvements tends to be a much greater problem for a small family operation than for a well-financed corporation. There is controversy over the adequacy of care provided by these small operations. Some argue that these economically marginal homes do not provide an adequate level of care and safety, while others argue that the care is in fact better in these homes. The cost of fire safety requirements does affect decisions regarding establishing such Homes and increases in fire safety requirements do affect decisions regarding whether to continue in business.

- Placement of disabled persons outside institutional settings may result in additional risk to these persons in exchange for a better quality of life. It is reasonable to permit those disabled persons who fully understand the meaning and possible consequences of their choices to accept the risks most people accept for themselves and their families. A reasonable goal for small Board and Care Homes would be the fire safety record of private homes that meet current codes and whose residents follow good fire safety practices.

- State officials interviewed by staff were generally satisfied with current state fire regulations for Board and Care Homes, whether they were using the Life Safety Code or other sets of requirements. They did express some concern in two areas: cost of fire safety improvements and, where the Life Safety Code is being used, the need to classify the evacuation capability of the Home.

- The residents of Board and Care Homes on the whole may becoming more disabled. There is the trend to permit "aging in place." Instead of moving an elderly person with increasing disabilities from a Board and Care Home to a nursing home, the resident may be permitted to remain in the Board and Care with additional services being provided. Also, a disabled person who in the past would have been placed in a nursing home may now be placed in a Board and Care setting instead due to Federal Preadmission Screening and Resident Review (PASARR) programs. These programs are designed to prevent inappropriate nursing home placement for persons with disabilities. Whether or not these programs are resulting in Board and Care Homes having elderly persons who are on the whole more disabled than in the past needs to be studied.

- The 1991 Edition of the Life Safety Code requires that all new Board and Care Homes (including new facilities being established in existing buildings) have automatic sprinkler systems. There is considerable controversy about requiring the installation of sprinklers in private residences being converted to Board and Care Homes. Some experts believe that this requirement will discourage the development of new small Board and Care Homes for high functioning disabled people because of the added cost. Others claim that there often will not be any added cost, or only a minor added cost, because of the possible cost savings on other fire safety features when sprinklers are used.

- Some jurisdictions have adopted the Life Safety Code requirements but with significant restrictions. (To some extent these restrictions circumvent the intent of the developers of the Board and Care requirements which was to provide a set of flexible provisions covering a broad variety of
situations.) For example, an authority might not permit any classifications of "Prompt" (with its less stringent requirements). Regulators are concerned about the possibility of rapid deterioration of elderly persons' capabilities and possible frequent transfers of residents from one facility to another.

- Learning the Life Safety Code provisions is in itself not an easy task. Further, there are references to other standards and documents with which to deal. Inspectors need considerable training and frequent experience to perform inspections well and consistently. We received complaints from providers about alleged errors made by inspectors which have resulted in considerable expense to these providers.

- Proper labelling or classification of facilities is important to ensure that both an appropriate and adequate set of regulations is applied.

Classifying a small Home with low functioning residents as a Health Care Facility rather than as an "Impractical to Evacuate" Board and Care Home means that fire safety requirements designed for a large building are being applied to a small building. This forces the building to have an institutional (e.g., 6 foot wide corridors) rather than a homelike ambience.

Classifying a home with > 4 residents as a foster care home rather than a Board and Care Home could lead to a set of regulations being applied which are not strict enough.

- Using the Life Safety Code, Homes are classified as to their evacuation capability and given a rating of Prompt, Slow, or Impractical to Evacuate. The Code provides several alternative procedures to determine the appropriate rating. The two most commonly used are determination of an "E-score" for the facility and timed fire drills. However, both methods have their own possible shortcomings in predicting what would happen in an actual fire. Some officials make use of both procedures, one providing a check on the other.

- The Life Safety Code assumes that in Prompt or Slow facilities the residents can either self-evacuate or be assisted to evacuate with available staff. It follows that residents in such facilities should participate in fire drills, and this is clearly required by the Code. Some providers with nursing home backgrounds are unaware of the difference in fire drill requirements between nursing homes and Board and Care Homes. Improper drilling may have contributed to some of the fatalities in a Board and Care fire. We have recommended to the National Fire Protection Association that they add information about the need for resident participaton in fire exit drills in the Appendix of the Code -- which contains advice and guidance -- to heighten awareness of the problem. We are also preparing a relevant brochure.

- Some Homes having nonrelated disabled persons may be too small to come under Board and Care regulations (< 4 for the Life Safety Code, < 6 for the Building Codes). We did not find a lot of concern about a lack of a specific set of regulations for these situations. If an authority does have jurisdiction, it could apply the regulations for One- and Two-Family Dwellings or Apartments. If, in addition, the residents are trained in fire safety, we can expect the residences to be safer in general than the average home.

Introduction: Buoyancy induced flows in enclosures, with respect to the transport induced by fires in rooms and other compartments, have received a considerable amount of attention in the literature. However, not much work has been done on the flow through openings or vents such as those between connecting rooms in buildings and between quarters in ships. The work done on the flow through horizontal vents, such as the one shown in Fig. 1, is very limited. The flow rate can be estimated, as done for vertical vents, by using Bernoulli’s equation (Emmons, 1988 and Hinkley, 1986). However, this model breaks down, over certain ranges of the pressure and density differences, for problems where both density and pressure differences exist across the vent (Cooper, 1989).

Some experimental work has been done on the buoyancy driven flow through horizontal vents, particularly for the special circumstance of pressure difference across the vent $\Delta p=0$ (Epstein, 1988). Mercer and Thompson (1975) studied the flow between two fluid regions connected by an inclined circular pipe. Conditions for purging of the density induced flow were investigated. A total purging or flooding implies a unidirectional flow through the vent from one region to the other.

The standard vent-flow model, based on Bernoulli’s equation, assumes unidirectional flow and breaks down if a bi-directional flow exchange occurs under the combined effects of buoyancy and pressure. This model predicts zero flow when $\Delta p=0$. The volume flow rate $Q_u$ at the vent into the upper region from the lower region is taken as uniform and given by the model as $Q_u = C_D A_V \sqrt{2\Delta p/\rho_l}$, where $C_D$ is the flow discharge coefficient, $A_V$ is the vent area of cross-section and $\rho_l$ is the density of the fluid in the lower region (Heskestad and Spaulding, 1989). Similarly, if the pressure difference is reversed, the flow $Q_D$ is obtained. However, there is a flow across the vent due to the density difference $\Delta \rho$, even if the pressure difference $\Delta p$ is zero, due to the fluid in the upper region being heavier than that in the lower region. Cooper (1989) has developed an analytical model, employing an exchange-flow component and has determined the steady-state rate-of-burning in a ceiling-vented room, such as the one sketched in Fig. 1.
Experimental Arrangement: This work is directed at the flow through horizontal vents for nonzero pressure and density differences across the opening. An experimental system based on a fresh-water/salt-water flow arrangement is initially employed. The density difference ratio $\Delta \rho / \bar{\rho}$ is varied from 0.0 to about 0.2, in order to cover the range encountered in typical vented-compartment fires. The salinity is measured by means of a hydrometer. The pressure difference $\Delta p$ across the vent of diameter $D$ is obtained by keeping the upper region open to the atmosphere and pressurizing the bottom region, see Fig. 2. The volume flow rate across the vent is obtained by measuring the dilution of the brine solution contained in the upper region and the net flow rate $Q_o$, as discussed by Tan and Jaluria (1992).

Over the last year, the experimental effort has been expanded to consider air as the fluid. The density difference is obtained by heat input to raise the temperature level in an enclosure with a horizontal vent. Different experimental systems have been developed and fabricated, as sketched in Fig. 3. The heat input is provided by an electric heater. The first arrangement does not have an externally imposed pressure difference, but a pressure difference arises due to the heating up of air in the enclosure and the constriction imposed by the vent. The enclosure in Fig. 3(a) has a side vertical vent through which entrainment of ambient fluid occurs. The side vent may also be closed to obtain the circumstance of Fig. 1. Figure 3(b) is similar to the water/brine system employed earlier and sketched in Fig. 2. This portion of the study is undertaken to provide a better quantitative understanding of the flow mechanisms associated with fires in vented rooms and also to compare the results obtained with air as the fluid with those from water/brine simulation in order to check the validity of the latter for fire modeling.

Experimental Results: Several interesting and important results have been obtained from the water/brine system. Using a shadowgraph for flow visualization, a bidirectional flow was found to arise across the vent at $\Delta p=0$, with denser fluid descending in the central portion of the opening and lighter fluid rising in the outer portion. As the opposing pressure difference $\Delta p$ was increased, this downward flow was found to decrease, ultimately giving rise to a unidirectional upward flow. This purging, or flooding, pressure difference $\Delta P_c$ is of order $(g\Delta \rho L)$ for a vent of height $L$, $g$ being the gravitational acceleration. Some typical results on the flooding pressure difference $\Delta P_c$ are shown in Fig. 4. The measured values are in the range that may be derived on the basis of scale analysis. The results were found to be repeatable, within a few percent, of the measured values. However, the transition from bidirectional to unidirectional flow was found to be fairly gradual, indicating the downflow $Q_D$ to gradually reduce to zero as the pressure difference $\Delta p$ is increased. With increasing values of $(g\Delta \rho D)$, at a given $L/D$, the purging pressure difference $\Delta P_c$ was found to increase, as expected.

The net upward flow rate $Q_o$ was also measured and the other flow rates $Q_u$ and $Q_D$ determined from the measurements of density and overflowing fluid in the upper region. Figure 5 shows some of the characteristic results obtained. At zero $\Delta p$, the upward and downward flow rates are equal, yielding a zero net upward flow. As the pressure difference increases, the flow rate $Q_o$ increases, with the effect of the density difference $\Delta \rho$ diminishing as $\Delta p$ becomes large. Also, at very low pressure differences, the density difference effects dominate the flow across the vent. Thus, clearly the basic trends indicated by Cooper (1989) are obtained.

The results may also be given in terms of a flow discharge coefficient $C_D$, as defined earlier. This discharge coefficient is around 0.61 for an orifice (Emmons, 1988), if buoyancy effects are neglected. However, as seen in this work, the flow rates decrease if the opposing buoyancy effects are increased. Therefore, the discharge coefficient may be correlated in terms of the buoyancy parameter $B$ and $L/D$, where $B = (g\Delta \rho D)/\Delta p$. A correlation obtained from the data over the parametric ranges considered is of the form:

$$C_D = 0.61 + 0.07974B^a(L/D)^b$$

where the constants $a$ and $b$ were obtained as $-0.2246$ and $0.0278$, respectively. As $B$ approaches zero, the value of $C_D$ approaches 0.61. Also, the flow rate decreases as $B$ increases. This result applies as long as the buoyancy effect is not predominant, or the pressure difference is not close to zero, i.e., $B \to \infty$. For that case, the earlier results at $\Delta p=0$ may be employed.
The work done on the experimental systems using air as the fluid and temperature difference for the buoyancy effect has revealed very similar trends. The flows are much more disturbed than those in water and the transient effects are more significant. However the basic characteristics of the flow are well represented by the water/brine arrangement which is a much easier system to work with. The density differences are of the same order of magnitude as those encountered in typical fire situations. The determination of the flow rates is based on the density measurements in the water case and on velocity data in the air circumstance. The work is presently continuing and it is expected that quantitative comparisons on the flow rates will be made between the two arrangements, based on water and air respectively, in the near future. This work will indicate how accurately the flow through the vent is predicted by an equation such as the one given above in terms of $C_D$ or if any modifications are needed in the correlating equations obtained from the water flow simulation.

Acknowledgments: The authors acknowledge the several discussions with Dr. Leonard Y. Cooper on this problem. The help of Mr. R. Chiruvella in preparation of this manuscript and in obtaining some of the correlating equations is also acknowledged.

References:


Reports and Papers:


Fig. 1. Sketch of fire in a room with ceiling vent.

Fig. 2. Experimental system using water/brine as the working fluid.

Fig. 3. Experimental arrangements based on air as the fluid in the vented enclosure.

Fig. 4. Measured purging pressure difference $\Delta P_c$ as a function of the buoyancy effect.

Fig. 5. Measured volume flow rates for varying $\Delta \rho$ at $L/D=0.25$ and 1.0.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT -- FY92

INADVERTENT OPERATION OF FIRE PROTECTION SYSTEMS IN NUCLEAR POWER PLANTS

Funding agency: Nuclear Regulatory Commission

Professional staff: Robert S. Levine
   Other BFRL staff as required

Project objective: Collect data on the effects of fire suppressants on equipment important to safety in nuclear power plants. This is in support of SNL/INEL work on NRC Generic issue 57.

Technical accomplishments: Nuclear power plants have many installed fire protection systems. When inadvertent operation occurs, the suppressant (water or CO₂ or Halon are used) may damage operating equipment and/or interfere with safety circuits or create spurious signals. This project used Navy Safety Center data on a large variety of operating system incidents on ships and shore facilities to gain insight into effects that might occur and to enrich the limited statistical data from nuclear power plant experience.

This phase of the project is completed. It was found that the population of inadvertent events in shore facilities paralleled Nuclear Power Plant experience, yielding about 100 cases per year for the 10 years analyzed. Halon systems and carbon dioxide systems caused no trouble. This data allowed the Sandia analyst to derive a calculated unreliability about one-fifth that calculated from Nuclear Power Plant experience alone.

It was also found that on ships, when sea water was not used, the incidence of damaging effects was much less than the shore facility experience. The fresh water used on ships comes from a closely controlled pure potable water main. So it is postulated that the reason for many of the deleterious effects in Nuclear Power Plants is impure (high electrical conductivity) water. This may be largely due to rust buildup in water residing in sprinkler systems. Incidentally, when sea water is used to extinguish fires, there is a very large probability that electrical equipment exposed to it will be damaged.

A survey found that very little work has been done on the purity of water in fire protection systems. Bell labs has analyzed water that comes in contact with central station equipment and finds that potassium is a significant contaminant.

Future work may look at ways to solve that problem, either by making inadvertent operation of the suppression system less likely, less damaging, or require redundant initiation.

Reports and publications:

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - FY92

LIVE FIRE TESTING

Funding agency: Office of Live Fire Testing, OSD, Pentagon

Professional staff: Robert S. Levine
Other BFRL staff as required.


Technical accomplishments: The Office of Live Fire Testing is mandated by congress to review and analyze independently, military agency Live Fire Test Plans and Analysis. The BFRL is a consultant to this office on fire related phenomena and effects, such as personnel burns, fire damage to equipment and structures, and toxic gases caused by fire.

This program is still in the study phase, and is closely related to activities of persons at the Institute for Defense Analyses. Several memos on effects to be considered have been written to IDA and the Live Fire Test Office. Most emphasis to date is on a new submarine design that will be "all up" tested about 1995.

BFRL fire models are being enriched so that they can calculate bulkhead and other surface hot spot temperatures. This is being tested by comparison with HULVUL" surface ship tests performed by the Royal Navy in 1990. Additionally they will be tested against data developed by the US Navy at China Lake when the report on that work is available. Once validated, the programs will be used to predict fire spread by ignition of the next "fuel package" in ships and submarines.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - FY92

LARGE SCALE SMOKE MOVEMENT

Professional Staff: John H. Kloe, Project Leader
Leonard Y. Cooper
Glenn P. Forney
William D. Davis
Daniel M. Alvord
Takayuki Matsushita

Project Objective:

Over the next six years develop and verify algorithms for modeling large scale smoke movement in buildings. The building configurations of interest are corridors, atria, open shafts, and stair shafts.

Technical Accomplishments:

Takayuki Matsushita, Guest Worker, from BRI developed a hybrid model of corridor smoke flow with consultation from Howard Baum, Walter Jones and Glenn Forney. This model considers properties in the corridor as constant across the corridor width, two zones vertically, and varying over the corridor length. Partial differential equations for the model were derived from the conservation equations, and a computer model using a packaged PDE solver was written for adiabatic flow. Results of the model were in good agreement with experiments, considering the lack of heat transfer in the model.

Work started on a joint NIST/FRI plan for studying atrium smoke movement. Cooper went to Japan where a scale model atrium facility was built with an adjustable top vent and pressurization capabilities. Many of the experiments for this project have been conducted. In some cases, the flow through the vent is about 30% of what would be calculated by a simple orifice equation model. This flow difference has significant implications for atrium smoke control technology, and work has started on a generalized model for this atrium vent flow.

The field model, Harwell FLOW3D, has been used to gain an understanding of smoke transport in corridors and large spaces. In addition, the field model has been applied to other fire problems including simulation of flow and combustion in a fully involved compartment fire and the interaction of a fire plume and wind in a simulation of a Navy Fire Fighter Trainer.

Reports and Publications:


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.
STAGING AREAS FOR THE HANDICAPPED

Funding Agency: General Services Administration (GSA)

Professional Staff: John H. Klotz, Project Leader
Harold E. Nelson
Scot Deal
Daniel M. Alvord

Project Objective:
Develop the capability to evaluate the fire safety of staging areas for the handicapped. Staging areas are intended as spaces in which people with disabilities can safely wait during a fire.

Technical Accomplishments:
The GSA has installed staging areas in six existing buildings. Spaces that were turned into staging areas included passenger elevator lobbies, service elevator lobbies, sections of corridor, and rooms. The BFRL project consisted of field tests, human behavior studies, and threat analysis. Pressurization tests were conducted to evaluate to leakage area between the staging areas and other parts of the building. The threat analysis evaluated tenability in route to staging areas and within staging areas due to transport of smoke from post flashover fires, sprinklered fires, and smoldering fires. The sprinklered fires were based on a model of post-sprinkler heat release recently developed by Madrzykowski of BFRL. It was concluded that staging areas can be either a haven of safety or a hazard. The difference is highly dependent on details of design, the type of fire exposure, outside wind and temperature conditions, and the capability and reliability of the smoke control pressurization system. Without pressurization all staging areas studied are subject to lethal failure. In many cases the persons most needing the staging area protection may be unable to reach that area before their pathway (corridor or aisle ways) become lethal. Further, it was concluded that the operation of a properly designed sprinkler system eliminates the life threat to all occupants regardless of their individual abilities and can provide superior protection for people with disabilities as compared to staging areas.

Reports and Publications:

Related Grants:
Effectiveness of Staging Areas in Office Buildings, George Mason University.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - FY92

FIRE EVACUATION BY ELEVATORS

Funding Agency: General Services Administration

Professional Staff: John H. Klotz, Project Leader
Scot Deal
Daniel M. Alvord

Project Objective:

This project is a study of the feasibility of using elevators for general fire evacuation.

Technical Accomplishments:

Throughout most of the world, warning signs next to elevators indicate they should not be used in fire situations. However, the idea of using elevators to speed up evacuation and to evacuated people with disabilities has gained considerable attention. A method of calculating the time required to evacuate people by use of elevators was developed, and an interactive computer program for elevator evacuation (ELVAC) was written. The engineering considerations of doors opening onto fire, activation, elevator doors jamming, fire resistance, water damage, reliability of electrical power, fire in the elevator system, and smoke in the elevator system were studied. Human considerations about system acceptance and functionality were addressed based on experience with other systems.

The feasibility of adapting four existing buildings for combined elevator and stair evacuation was studied. The buildings consisted of a wide range of heights (7, 13, 18 and 35 stories) and consisted of single and multiple rise arrangements. For all of these buildings, combined stair and elevator evacuation would have the advantages of (a) reduction of estimated building evacuation time, (b) people with disabilities can use elevators to evacuate the building in the same way that they entered, (c) the fire service can use the elevators to rescue occupants, and (d) the fire service can use the elevators to move men and equipment for fire fighting. The reduction in evacuation time ranged from 10 to 50% of the time needed for stair only evacuation. The study concluded that elevator evacuation of buildings is feasible, but it involves significant organizational and engineering challenges.

Reports and Publications:


Related Grants:

Use of Elevators During Fire Evacuations - Human Factors Considerations, George Mason University.
RISK ANALYSIS FOR THE FIRE SAFETY OF AIRLINE PASSENGERS

Funding Agency: Federal Aviation Administration

Professional Staff: Dr. Richard L. Smith

Objective:

To develop the generic methodology and an intelligent computer program that will compute the fire risk for passengers of airlines assuming the implementation of various fire safety regulations.

Introduction:

Airline fire safety is important for the airline passengers and for the potential flying public that needs to be assured of the safety of flying. The public has demonstrated a willingness to pay for flight safety when it is cost effective. Therefore, it is critical that FAA’s fire safety regulations provide demonstrable safety improvement at an acceptable cost.

Injuries or death due to airplane fire are a rare event. Therefore, there is not a large body of relevant statistical data that can be used to determine the impact of various fire safety strategies. In this respect, airplane fire safety is similar to the safety problem faced by the Nuclear Regulatory Commission for the safety of nuclear power plants or NASA for its space shuttle program.

Approach:

In the last decade considerable progress have been made in developing and/or improving risk analysis. The major motivators were the Three Mile Island disaster and the Challenger space shuttle disaster. Similarly, there have been major advances in Artificial Intelligence in dealing with reasoning with uncertainty or vague knowledge. Some advances have used such approaches as Bayesian Probability Theory, Dempster-Shafer’s rule for combining evidence, and expert systems. Also, probability theory has been impacted significantly by developments in Bayesian Probability Theory and new applications of the Maximum Entropy theory.

This project will apply the advances in these three fields to the risk analysis for the fire safety of airline passengers. The project’s objective will be to develop the generic methodology and a computer program that will enable one to calculate the risk due to fire for airline passengers. The program will be capable of utilizing the state-of-the-art safety analysis technology, the historical data on fire losses in airplanes, the results of experiments and tests, the predictions of physical science models, and experts’ opinions. However, the user will control exactly what knowledge is used and what assumptions are made. The program will be capable of recording an individual analysis so that it can be reviewed by others.
Funding Agency: National Forest Products Association

Professional Staff: Vytenis Babrauskas
Kenneth D. Steckler

Project Objective:

Under this project, NIST lent technical support to the implementation of U.S./Japanese negotiations on wood imports. The implementation measures provided for changes in the Japanese Building Law. The revised provisions of this law were to be derived from a research program conducted by the Building Research Institute of Japan. NIST cooperated with BRI in this research program and assisted in analyzing and developing U.S. positions on this issue.

Technical Accomplishments:

NIST staff worked directly with BRI staff involved in reviewing the test plans for the full-scale earthquake + fire testing. NIST staff cooperatively worked with BRI staff to make leakage measurements in conjunction with the full-scale earthquake testing; they also observed the earthquake and the fire tests and conducted laboratory and computer analyses. The materials for the test house were analyzed according to heat-release-rate based principles of non-combustibility. These data were found to be very similar to those from corresponding U.S. materials. NIST staff also participated in the analyses of various draft regulation provisions and in developing a U.S. position on the acceptability of these provisions.

Reports and Publications:

None.
Technical Abstract:

Objectives. For twenty years the American public has been trained to avoid the use of elevators during fire emergencies. Warning signs at elevators tell people not to use the elevators during fire evacuations. The dangers of using elevators during fire emergencies are well known and accepted by both laymen and experts. Nevertheless, it is likely that the technology now can be developed to provide a safe fire evacuation using elevators in tall buildings.

In this study, we are attempting to identify the human behavioral issues associated with evacuating occupants from office buildings using elevators. It is part of a larger project at the National Institute of Standards and Technology that is considering all aspects of the possible use of elevators for evacuating building occupants during a fire emergency. Our approach is to use a system perspective to identify relevant human factors issues. However, we are limited by the lack of empirical evidence directly applicable to the problem and the impracticality of collecting such empirical data.

Because there are no data from building evacuations using elevators, the findings of this study will be necessarily speculative and general. They will be based on the authors' combined experience and on one study of installations (staging areas) that are similar in some respects. Some of our conclusions are expected to be tentative.

Final Report. The final report of the entire NIST project is Report # NISTIR 4870 "Feasibility and Design Considerations of Emergency Evacuation by Elevators by J.H. Klote, D.M. Alvord, B.M. Levin, and N.E. Groner. The project staff assisted in the preparation of this NIST report.
The final report to NIST contained the following conclusions:

Summary of Conclusions. There should be no problem getting those occupants who cannot descend stairs to use elevators. They basically have no choice. However, the evacuation system cannot be deemed a success if occupants with mobility limitations, who must rely on the elevators, have serious doubts about their own safety in fire emergencies. It is important to teach them about the fire safety features in the elevator system so that they will support the fire safety plan and use the elevators with confidence.

There are several obstacles to getting mobile building occupants to use elevators in fire emergencies. First, there has been a twenty year campaign to teach people not to use elevators in fires. Secondly, occupants in many buildings may not have sufficient confidence in the building management to entrust their safety to a mechanical device that is designed and maintained by current building management. Also, people have strong needs to exert control over their own fate and relying on elevators in fire emergency evacuations decreases such control.

On the other hand, the use of elevators should be appealing for several reasons. People tend to leave buildings by the same route they used for entering; those who used elevators to arrive at their desired destination will tend to return by the same means. If the occupants are on an upper floor, the physical effort required to leave the building by stairs might encourage elevator use. The congestion on the stairs of office buildings, especially if the evacuation is not phased by floor, might be very unpleasant. (Most people are probably not aware of this potential congestion. However, even if the elevators were not used by the general building population in fire emergencies and fire drills, there would be a need to inform the occupants of tall buildings of this congestion, especially if the occupants are to accept a phased evacuation by stairs.)

In a well run and well maintained building, a good training program should be able to overcome obstacles to occupant acceptance of elevator use for fire evacuations. This training program should include:

- An explanation and discussion regarding why most buildings prohibit the use of elevators in fire emergencies and how their building has been designed to permit fire safe elevator evacuations in fire emergencies. This will help overcome the previous training which encouraged people not to use elevators in fire situations.

- An explanation of how the use of elevators decreases the time to evacuate the building (or portion of the building). This item is based on the assumption that some occupants will use the stairs and others will use elevators.

- A discussion of potential congestion problems on the stairs.

- An explanation of how the system works including who gets priority use of the elevators (or stairs if there is a phased evacuation), how the communication system works, how the system assures that no one is left behind in an elevator lobby, etc.

- Fire drills where the occupants can practice their evacuation assignments and obtain a more concrete understanding of how the system works.

It is clear that fully mobile occupants from the fire floor should always be assigned to use stairs rather than elevators: this should satisfy some of the concerns regarding controlling one’s own fate,
and help make the system appear reasonable. Alerting occupants to the availability of stairs as a backup that can be used before a floor becomes dangerous—and informing occupants that they would be alerted well before conditions become dangerous—should satisfy some of the other concerns regarding controlling one’s own fate.

Occupants will have more confidence that the fire safety features were properly designed and installed and are being properly maintained if the building, in general, is well run and well maintained. This confidence is important in getting occupant acceptance for the Building Emergency Plan and for the use of elevators.

It is generally accepted that there should be a written Building Emergency Plan. This written plan can serve at least three purposes. It can be a management tool, assuring management that the emergency evacuation system has been well designed and implemented. It can also serve to provide information to the emergency team (including the monitors and wardens) regarding their assignments and responsibilities. Finally, it can inform the occupants about the plan, that is, it can supplement the formal training or even be used as a textbook for the training. The written plan, which can be printed as several documents, should meet all these functions. It should be revised frequently, as appropriate, to assure the occupants that the system is not falling into disrepair.

Some of the occupants will be required to wait for a considerable time in or near the elevator lobby before the first elevator arrives, perhaps in a few cases more than the approximate 10 minutes in buildings recently studied by Klote et al. Even with a good training program, people are unlikely to wait that long before deciding to use the stairs unless information is provided to them about the progress of the fire and the progress of the elevator evacuation. A good two-way communications system, including both a control center and the elevator lobbies, is vital. (Fire drills can be conducted where only part of the building is evacuated so that the maximum wait at the elevator would be shorter.)

It may appear obvious to some, but it cannot be emphasized too strongly, that all the tasks assigned to the emergency team (and the associated equipment and computer programs) be carefully designed from a human factors engineering standpoint. The emergency team should be thoroughly trained, including drills where they can practice their assignments.

Each building will need to have a command center or control room where the priorities for assigning elevators to floors are made and controlled, and from where information is sent to the elevator lobbies. The design of this center, and the training of the security staff manning it, is of special importance.

Reports:


A5. Fire Hazard Assessment
Institution: University of Maryland
Grant No.: 60NANB1D1164
Grant Title: Development of the Fire Data Management System
Principle Investigator: Dr. Frederick W. Mowrer
Department of Fire Protection Engineering
University of Maryland
College Park, MD 20742
Other Personnel: Amy Cheng, Graduate Student
Jeffrey Collins, Undergraduate Student
Jay Torner, Undergraduate Student
NIST Scientific Officer: Dr. Vytenis Babrauskas

Technical Abstract:

Introduction. The Fire Data Management System (FDMS) is a database of fire test data being developed with international cooperation among numerous fire research and testing laboratories worldwide. Such data are essential for the application of quantitative fire hazard analysis techniques, such as computer-based fire modeling, and for evaluating the expected performance of a product under actual fire conditions. In the past the retrieval, exchange and use of fire test data has been difficult because a standard format did not exist for storing or exchanging the data or for entering the data into fire models. The FDMS provides a standard format for data storage and exchange. The development of the FDMS should permit substantive advances in the application of quantitative analysis methods to fire protection engineering problems.

Research Plan. The work being conducted under this grant has three components:

- Incorporation of existing data from NIST into FDMS format. A large body of fire test data exists in various formats at NIST. This data is being converted to FDMS format for incorporation into the FDMS.

- Generation of additional critical data. Much of the existing data at NIST has been acquired for specific research programs. Consequently, gaps exist within the current database. These gaps should be filled to make the FDMS more useful for practical fire protection engineering purposes.

- Development of engineering guidelines for use of the FDMS database. This task includes the development of a morphological chart for grouping test data and the development of simplified engineering relationships to aid in the screening of tested materials for particular applications.
Progress to Date. With respect to the three tasks identified above, the following progress can be reported:

- We have been transferring Cone Calorimeter data in chronological sequence from the original formats of the various data acquisition systems to the FDMS. We have adopted this approach due to concern that data stored on older systems may not be transferrable much longer due to failure of the systems or the data diskettes. To date, data from approximately 1500 Cone Calorimeter tests have been transferred to MSDOS diskettes. We are in the process of transferring this data to the FDMS. We have obtained a copy of the DCS data conversion software from SINTEF in Norway, which can be used to convert data from some of the formats used at NIST to the FDMS format. For other formats used at NIST, we are writing data conversion algorithms to accomplish this task.

- We have not generated any additional critical data yet. This task is planned for the second year of this project.

- We have begun the development of engineering guidelines for use of the FDMS. Development of the morphological chart has been initiated to categorize Cone Calorimeter test data. For example, the broadest distinction can be made between furnishings, finishes and structural elements. For finishes, the next level of distinction would be between floor, wall and ceiling coverings. Further distinctions could be made between mounting methods, substrates, etc. With such distinctions, a user should be able to find more readily data appropriate for a particular application. Such distinctions should also permit gaps in the existing database to be identified. A literature review is also being conducted to survey existing simplified methods for using Cone Calorimeter data for engineering applications.

Acknowledgements: We would like to acknowledge Emil Braun for his assistance in finding and recovering much of the Cone Calorimeter test data acquired at NIST over the past decade. We also wish to acknowledge Kristen Opstad of SINTEF in Norway for sending us a copy of the DCS data conversion program developed in his laboratory.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT – FY 92

FIRE HAZARD ASSESSMENT METHODOLOGY

Professional Personnel

Richard D. Peacock, Project Leader
Walter W. Jones, Group Leader, Fire Hazard Analysis Group
Glenn P. Forney, Computer Scientist
Rebecca W. Portier, Mathematician
Paul A. Reneke, Computer Scientist

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. While initially limited to residential-style occupancies, the software design is aimed at an across the board use of 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 which state-of-the-art 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. This latter includes new phenomenon and features to continue providing a state-of-the-art tool for hazard analysis for use by fire protection professionals. One of the new features is mechanical ventilation. We have also improved the documentation by providing a step-by-step learning guide and integrating the example cases in the technical reference.

Simultaneously, work is continuing on improving the modeling capability for version 1.2. New physical routines which have been added: flow through holes in ceilings and floors; another zone for each compartment that contains a fire. This is the ceiling jet and makes the estimate of heat loss from 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 significant portion of the priority project on the hazard methodology this year involved improving the internal structure of the CFAST model. The project has two basic goals: 1. Improve the numerics of CFAST so that it will run more correctly and faster, and 2. Improve program and data structures so that
future improvements to CFAST can be more easily accomplished. To achieve these goals, we have taken a “divide and conquer” approach to systematize the data flow between the physical phenomena and the model’s implementation of the differential equation set (the “physical interface routines” referenced below). This was done in two steps:

1. Implement a new “state-of-the-art” differential equation solver, DASSL, that can handle algebraic equations. The incorporation of conduction and the HVAC system directly into the set of equations solved by CFAST could then be implemented.

2. Reorganize the single physical interface routine in CFAST (DSOURC) by creating multiple physical interface routines (one interface routine per phenomenon) and a single control routine to replace DSOURC. Each interface routine provides communication between the physical phenomena and CFAST, using data structures natural to the phenomenon it implements (i.e., order vent properties by vent number, room properties by room number, fire properties by fire number). Each interface routine will calculate flow and/or flux terms and return. The control routine uses these terms to formulate the differential equations. The flux terms are also used as boundary conditions for the wall heat conduction calculation.

The calling sequence for a suite of procedures defines their relationship to the calling program and to order in which they are called. A summary of the subroutine structure of CFAST is illustrated in Figure 1. The program modules on the bottom row of the figure are the physical interface routines which interface the CFAST model with the actual physics of each phenomenon. Additional routines, not shown on this summary figure, implement the physics.

Each physical interface routine calculates flow and/or flux terms as appropriate for all rooms and/or surfaces of the simulation being modeled. These flow and flux terms are the effect of the phenomenon on each of the layers and/or surfaces and includes flows due to mass, enthalpy and products of combustion. Rather than using multiple variables for each room, these are organized into a single array for each phenomenon. This structure is shown in Figure 2. To illustrate the organization of the physical interface routines, the following outlines the steps in calculating one of the phenomena — the fires.

The physical interface routine, FIRES, calculates the rates of addition of mass, enthalpy, and species into all layers in all rooms from all fires in a simulation. For each fire, the following scheme is employed:

1. Initialize the fire data structure, FLWF, to zero.

2. For each specified fire, the routine PYROLS (for the main fire) or OBJINT (for object fires) calculates time dependent quantities for the time of interest by interpolating between the time
points specified by the user. The routine DOFIRE calculates the plume entrainment rate.

3. For a type 1 (unconstrained) fire, the routine DOFIRE sets the burning rate to the pyrolysis rate. The heat release rate is found by multiplying the burning rate by the heat of combustion.

4. For a type 2 (constrained) fire, the prescribed chemistry scheme, discussed above, is used to constrain the burning rate based on both the fuel and oxygen available. This chemistry scheme is implemented in the routine CHEMIE. This calculation is done for both the lower layer (from the mass entrained by the plume) and for burning in the upper layer (with oxygen and fuel available in the layer).

5. Sum the contributions from all fires into the fire data structure for return to the control routine. The following code fragment is typical of those in all of the physical interface routines:

```latex
XTL = ZZTEMP(LFBO,LOWER)
FLWF(LFBO,M,UPPER) = FLWF(LFBO,M,UPPER) + EMS(LFBO)
FLWF(LFBO,M,LOWER) = FLWF(LFBO,M,LOWER) - EMS(LFBO)
GEME = CP*EME(LFBO)*XTL
GEMP = CP*EMP(LFBO)*TE
FLWF(LFBO,Q,UPPER) = FLWF(LFBO,Q,UPPER) + QF(LFBO) + GEME + GEMP
FLWF(LFBO,Q,LOWER) = FLWF(LFBO,Q,LOWER) - GEME
QLPQUF(LFBO) = QLPQUF(LFBO) + QF(LFBO) + GEMP
DO 40 LSP = 1, NS
   FLWF(LFBO,LSP+2,UPPER) = FLWF(LFBO,LSP+2,UPPER) + XNTMS(UPPER,LSP)
   + FLWF(LFBO,LSP+2,LOWER) = FLWF(LFBO,LSP+2,LOWER) + XNTMS(LOWER,LSP)
40 CONTINUE
```

We have not, by any means, done a comprehensive comparison of the two versions of the model for all possible test cases. However, for the ones we have completed, the comparison is quite good. The following simple example (a fire in a single closed room) is illustrative of the comparative execution speed of this same test case with the two versions of the model (in hours:minutes:seconds): Original CFAST (damped) - 0:0:34, original CFAST (full solution) - 0:0:34, new CFAST (full solution) - 0:0:13. For a more complicated test case (a three room case with multiple vents), the comparison is even more dramatic: Original CFAST (damped) - 0:1:15, original CFAST (full solution) - 14:34:00, new CFAST (full solution) - 0:1:36.

More time was spent this year completing a paper on validation of the model, that is comparing the output from the model with full scale experiments as well as fires in actual buildings. An example is shown in Figure 3. We chose five examples which push the limits of the modeling capability. This was intended to show the abilities and limitations of the model, and to provide guidance on what areas need
to be addressed to improve its capability in a significant manner. This work is discussed in one of the papers cited below. It shows reasonable agreement between the two, with difficulties where we expected.

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.

Reports and Publications


Associated Grants


FPETOOL UPGRADE

Funding Agency: General Services Administration

Professional Personnel

Harold E. Nelson, (retired)
Scot Deal, Research Engineer
Charles Arnold, Computer Programmer

Project Objective

Add two modules to FPETool. The two new modules extend the users' ability to analyze fire effects from the room of origin by predicting conditions in the adjoining corridor and rooms off of the corridor.

Technical Accomplishments

FPETool, a computer program containing quick and easy-to-use fire safety engineering equations, has extended the capabilities of its room FIRE SIMULATOR model. Postflashover smoke from the room of fire origin is tracked, in terms of temperature, layer depth and speed, as these products advance down a corridor in a wave. Results from this CORRIDOR module are compared with several experimental data sets.

Smoke conditions from the corridor are then used to predict smoke leakage rates into areas of refuge. Temperature, gas concentrations and time to lethality are determined in the refuge room. Smoke infiltration rates are based on theory and await experimental comparison. The smoke toxicity model developed by Bukowski et al.¹ and based upon experimental analogs was implemented to evaluate conditions within the refuge areas.

Engineering calculations used by CORRIDOR and the smoke leakage model made significant contributions to a recent study for the GSA. In this study, times to lethality were predicted when the source of the smoke was located at remote distances.

Publications and Related Grants


"The Effect of Open Windows on Smoke Movement in a High-Rise Building," Technical Note (to be released), NIST, Gaithersburg, MD, 1992.

Institution: Clemson University
Grant No.: 60NANB0D1023
Grant Title: Mathematical Modeling of Human Egress from Fires in Residential Buildings
Principal Investigator: Michael M. Kostreva, Professor
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Other Professional Personnel: Malgorzata Wiecek, Assistant Professor
Teodros Getachew, Doctoral Student

NIST Scientific Officer: Richard Peacock

Technical Abstract: In this research the movements of human occupants of a building who are reacting to the presence of a fire in the building are considered. Such movement is generally known as egress and thus the present study is concerned with fire egress analysis. Our work seems to be the first to apply multi-objective programming models to this problem. The motivation to introduce more than one objective function to be minimized is quite natural in the fire environment. A building fire contains multiple hazards to be avoided, by simultaneously minimizing travel time, distance of travel, amount of smoke inhaled, amounts of toxins encountered, etc. It is the goal of fire egress analysis to find all nondominated paths for each such occupant and then to make further study of the paths and their corresponding cost vectors. By obtaining such a detailed solution one obtains a deeper understanding of the building structure, the occupants and how occupants might best manage the risk of a fire.

A building fire and the reaction of the occupants to the fire form an inherently dynamic phenomenon. As such, the data to be considered in decision making is comprised of functions of time which may be derived either from actual fire measurements or from the output of mathematical models of fire and smoke dynamics. At the Building and Fire Research
Laboratory, research on the physics of fire and the mathematical modeling of fires in buildings is well established. Recently the Fire Hazards Analysis group has published a computer package called HAZARD I. It contains a model in which a network is superimposed on the floor plan and the occupants behavior is simulated by a set of heuristic decision rules. The occupants move around in the network until they find an egress path by which they leave the building. The research of this paper is designed to provide additional insight into the people-fire interaction within a building. Theoretical foundation for this research work is given by advanced vector dynamic programming. Kostreva, Wiecek, and Getachew (1991) applied several network models to fire egress analysis for residential buildings. A pair of algorithms is introduced in Kostreva and Wiecek (1993) which seems to be the first paper to study a network with vector time dependent costs. In a continuation of the research effort reported above, a new approach will be applied to performing multicriteria decision making in fire egress analysis.

In the dynamic programming literature two problem formulations are considered: find all nondominated paths 1) from each node to the destination node or 2) from the origin node to every other node. The former formulation is based on the backward approach to DP while the latter uses the forward approach. An algorithm based on the forward technique will be described here and its applicability to fire egress analysis will be demonstrated.

Consider a general network, not assumed to be acyclic, that consists of N nodes \{1, 2, ..., N\} and a set of links (i, j) connecting the nodes. Associated with each link is a vector cost \([c_{ij}(t)]\), where the cost functions \((c_{ij}: \mathbb{R}^+ \rightarrow \mathbb{R}^{m+})\) are assumed to be positive vector valued functions of time. Let \([c_{ij}(t)]_1\) be the time to travel from node i to node j, given that travel starts at time t. The cost to traverse a path p between two nodes of the network is defined as \([c(p)] = \sum_{(i,j) \in p} [c_{ij}(t)]\). It is assumed that the cost of traveling along a link is a function only of the arrival time at the starting node at the link. This assumption, referred to as the frozen link model, allows for fixing a link cost not at the time of leaving the origin node, but later, at the time of arriving at the starting node of the link and, thus, for updating the link cost according to very recent data about the fire.

Let time \(t\) be a continuous variable, that is \(t \geq 0\), and let the functions \([c_{ij}(t)]_1\) take any positive value. Let node 1 be the origin node. Assume that the departure time from the origin node is \(t = 0\). Finally an assumption is introduced which allows the formulation of the principle of
optimality for dynamic multiple objective networks. The assumption seems to be very realistic for any fire egress scenario: part a) states that evacuees may not pass each other during evacuation, and part b) refers to deterioration of evacuation conditions over time.

Assumption. For any link (i, j) in the network and all $t_1, t_2 \geq 0$, if $t_1 \leq t_2$, then

a) $t_1 + [c_{ij}(t_1)]_1 \leq t_2 + [c_{ij}(t_2)]_1$, and

b) $[c_{ij}(t_1)]_r \leq [c_{ij}(t_2)]_r$ for all $r \in \{2, ..., m\}$.

Theorem: Principle of Optimality for Dynamic Multiple Objective Networks

Under Assumption a) and b), a nondominated path $p$, that leaves the origin node at time $t = 0$ and arrives at node $j$ at time $t_j$, has the property that for each node $i$ lying on this path, a subpath $p_1$, that leaves the origin node at time $t = 0$ and arrives at node $i$ at time $t_i$, for $t_i \leq t_j$, is nondominated.

Applications made to date have been to sample problems of moderate size. Constructing an example from available data in The Greenville News, a model representing the recent food processing plant fire in Hamlet, N.C. in which 25 people lost their lives was solved. It demonstrated that from certain locations within the plant there were multiple nondominated egress paths. For details see Kostreva and Wiecek, (1992). Many different studies on houses have been conducted, using real floor plans and plans from the literature. An analysis has been performed using a sequence of starting times for exit for the occupants of a building, see Getachew and Kostreva (1992). By such analysis one may learn the characteristics of certain rooms or sets of rooms, for occupants who respond with varying amounts of delay to the existence of a fire. Finally, in a first step toward solution of very large scale models, an approximation method has been developed in Kostreva and Wiecek (1992). Such a method is simpler than the mathematically provable algorithms of Kostreva and Wiecek (1993), but it suffers two defects: it does not always get the whole solution set and sometimes it produces paths which are not solutions. Some additional research into approximation methods is needed in order to solve very large models representing hotels or other high-rise buildings.

Reports and Papers:


Introduction. This grant supported the modifications to the furniture fire model (FFM) for eventual inclusion in the HAZARD system. By the beginning of the current fiscal year, our simpler version of FFM had become the Flame Spread Model (FSM). Further development of FSM required demonstrating the code, creating a stand-alone version, and merging the code with CFAST. Other task activities involved developing algorithms to simulate "strip" fire spread, to modify flame spreading due to air vitiation, and to more easily determine model constants with the preproccessing PC based routines.

Implementing FSM on the PC with CFAST. Before converting FAST/FSM to CFAST, the code was used to demonstrate simulation of different fire scenarios in a room. The flame spread model has been applied to simulate a burning panel of HO/FRPU (heavy Olefin foam material/fire retarded polyurethane) in a single compartment where the fire has been specified as one of the constrained fires. The simulated panels have different orientations (horizontal panel and vertical walls), different geometries with different thicknesses, and different fire positions in the room of fire origin (center of the room and along a wall of the room) with different ignition locations on the panels. In these applications, the effect of door open (width and height of the door of the room of fire origin) on the flame spread rate developed on the panel, the pyrolysis rate, and the upper hot gas layer depth has been demonstrated and analyzed.

In order to begin conversion of FSM to CFAST from FAST, a stand-alone version of FSM was also developed. This code (now called FSMSAV) was shown to be very efficient and it still retained the basic fire growth features as that for FFM, except that only a single panel was used. The predicted fire growth was shown to be equivalent to that predicted with the FAST/FSM code. Since there is a renewed interest in modeling furniture fires, we developed a stand-alone FFM so that it too will be incorporated into CFAST.
However, the main activity of Task 1 consisted of incorporating FSM into CFAST, which meant developing CFAST/FSM version before the FFMSAV version. CFAST has been designated for the second version of HAZARD. The software implementation of CFAST and its differences with the FAST-18 was recently published by the National Institute of Standards and Technology (NIST) in two documents: "Refinement of a Model for Fire Growth and Smoke Transport" and "A Programmer’s Reference Manual for CFAST, the Unified Model of Fire Growth and Smoke Transport". Since these documents show how to modify or incorporate new subroutines into CFAST, they were examined in detail for incorporating FSM and FFM. The grantee, Dr. Mark Dietenberger, has interacted closely with the developers of CFAST to develop software for interfacing FSM and FFM to CFAST. This software development was collaborated on-site at the Building and Fire Research Laboratories (BFRL) with Dr. Walter Jones and Dr. Gamal Ahmed.

Additional activities of Task 1 were to improve CONEPROC and LIFTFIT for easier calibration of the FSM model constants. The code for LIFTFIT was delivered to NIST and a mini-User Guide was provided as well.

**Developing the Strip Fire Algorithms** The objective of Task 2 was to develop algorithms to simulate "strip" fires and to permit indentation of the flame spread regions. The wall fire originating at a point source first spreads rapidly upwards; then spreads rapidly in the lateral direction as the upper surface regions are heated by the upper gas layer. The flame spread region takes on a "T"-shape that should be accomodated by the flame spreading logic. In addition, the flame shape algorithm will need modifications to simulate the strip flames for this wall fire scenario. In some fire scenarios, the burn-out region can develop to such an extent that the flame structure and the burn history needs to be calculated with a new subroutine. In the algorithm for such a "strip fire", the use of very small surface elements should be avoided to maintain computational efficiency. This would enhance the flame spread model to simulate burning on thin or fire-retardant combustible materials. By permitting indentation of the flame spread region the flame spreading process can gradually transition from a circular ignition region to a strip fire proceeding along the wall.

**Study of Air Vitiation on Flame Spread** Task 3 objective was to study effects of oxygen concentration (and other environmental conditions) on the fire spread. A practical analytical model was developed to calculate the flame spread rate in opposed flow as a function of ambient environments such as oxygen concentration, temperature, pressure, relative gravity, and thermal radiation. The model constants were calibrated for PMMA and paper materials using some of the routines in the LIFTFIT program. The mathematical modeling for the structure and emissions of the fire plumes as a function of the vitiated air environment is needed to calculate the surface heat flux distribution that determines the flame spread rate in assisting flow. An interim combustion model was suggested for this task. In many realistic fire scenarios, there may be sufficient fuel loading in a room that the hot and vitiated air will affect the fire-growth processes. In particular, the lateral, downward, and horizontal flame spreadings are particularly sensitive to the oxygen concentration, gas temperature, and external irradiances. Thus, the vitiated air can actually retard the fire-growth process, perhaps allowing a significantly longer containment of the fire in the compartment. Since this is an important process, it would be worthwhile to simulate the containment of fire, if only imperfectly. Thus, validated models of flame spread in opposed flow and combusting plume for vitiated air should be incorporated. Since the codes for these two models already exist and are compact enough to fit in FSM and FFM, minimal programming will be required.

These developments should find applications in fire scenarios relating to compartmentation, structural fire resistance, ignitibility of a secondary combustible item, and room flashover.
References.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - FY92

SUPPORT OF THE NAVY FIRE MODELING PROGRAM

Funding Agency: Naval Research Laboratory

Professional Staff: Walter W. Jones, Project Leader
Paul A. Reneke

Project Objective:

Develop specific algorithms to incorporate phenomena into the BFRL fire models which address problems unique 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 mechanical ventilation and vertical flow through hatches and other openings in decks. In addition, CFAST was restructured this year to increase its speed for real time applications of damage assessment, and to allow more easily other Navy Commands to incorporate their own changes and additions.

Reports and Publications:


A6. Large Fires
CHARACTERIZATION OF LARGE FIRES

Professional Staff: David D. Evans, Project Leader
Kathy A. Notarianni, Fire Protection Engineer
Daniel Madrzykowski, Mechanical Engineer
Robert Vettori, Fire Protection Engineer
Howard Baum, NIST Fellow

Project Objective:

Develop understanding of the burning characteristics and environmental effects of large wind blown fires.

Scope:

This project is directed at measurement and prediction of large wind blown fires that occur as the result of industrial accidents and natural disasters. Research effort is directed at the development of non-intrusive means to assess major burning characteristics of large fires including geometry, motion, heat release rate, and emissions. The fate of wind blown combustion products in the near fire region that in meteorological terms may extend downwind 100 km are included in this study of fire effects.

Technical Accomplishment:

In May 1991, measurements were made to characterize the fires and smoke in the Al Ahmadi Oil Field, 30 km south of Kuwait City. Heat release rate is the single best indicator of fire characteristics. A rapid assessment of the heat release rate from the high pressure gas and oil spray flames could be made from measurements of the flame length. Although data from high pressure flames with heat release rates (HRR) order one gigawatt is not available, other studies of heat release rate vs. flame height for buoyancy dominated flames is available. One available correlation from McCaffrey¹ is:

\[ Q = (Z/0.2)^{5/2} \]

\[ Q = \text{Total HRR (kW)} \]

\[ Z = \text{Flame Height (m)} \]

Even though the crude oil flares in the Kuwait oil fields were high pressure releases, equation (1) provides an estimate of the rate of heat release. Using this correlation with ground level and aerial measurements of flame height for 12 flare fires, it was determined that the average heat release rate of

measurements of flame height for 12 flare fires, it was determined that the average heat release rate of fires in the Al Ahmadi oil field was 760 MW. In addition, radiative heat flux measurements were made around one of the larger fires, estimated to be 1.7 gigawatts in total heat release rate. At 183 m from the fire, the radiative flux per unit area was 1.8 kW/m². Using a radiative fraction of 0.43 and an assumption of uniform emission, the total heat release rate of this fire agrees with that obtained using equation (1). The effort to quantify the characteristics of the Kuwait fires without knowing the fuel flow rate presented a challenge beyond that usually taken in ordinary scientific studies. This technical work would have benefitted from measurement methods and increased knowledge about the behavior of large fires.

To pursue the understanding of wind blown fires and the predictions of the wind blown plume trajectory, a first step is to provide a facility to make measurements. Towards this end, the feasibility of modifying part of the Fire Research Building traditionally used for room and corridor fire tests to function as a fire wind tunnel facility is being examined. The addition of a blower to the facility, provides a maximum of 2 m/s wind speed in a 2.4 m square cross-section and 12 m long test section. Experiments have shown that this configuration is sufficient to measure the plume from a 0.3 m diameter pool fire for approximately 30 fire diameters downwind. This facility, or its successor, will be the experimental vehicle to experiment with traditional and non-intrusive measurement technology that may be capable of characterizing larger fires in the field. Data from the facility will be used to validate simulations of the near field smoke plume flow like those being performed in the Simulation of Turbulent Combustion and Transport in Fires priority project and OA funded In-Situ Burning of Oil Spills.

**Publications:**


**Related Grants:**

"Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes," Ahmed F. Ghoniem, Massachusetts Institute of Technology.

"A Study of Simulated Oil Well Blowout Fires," Jay Gore, Purdue University.
IN-SITU BURNING OF OIL SPILLS

Funding Agency: Minerals Management Service, DoI
U.S. Coast Guard, DoT
American Petroleum Institute

Professional Staff: David D. Evans, Project Leader
William D. Walton, Fire Protection Engineer
Howard R. Baum, NIST Fellow
Kathy A. Notarianni, Fire Protection Engineer
James R. Lawson, General Physical Scientist
Daniel Madrzykowski, Mechanical Engineer
Kurt Keydel, Mechanical Engineer

Project Objective:
To develop and implement the instrumentation and data use methodology for quantifying the combustion of crude oil on water during field experiments of current oil spill burn technology.

Technical Accomplishment:
Data from the 1991 mesoscale crude oil burns were analyzed. Results for burning rate and smoke yield from the pool fires up to 15 m square were as expected from previous testing. The oil surface regression rate, a measure of burning rate, was found to be 0.055 mm/s. Smoke yield, the fraction of the fuel converted to particulate, was 13 percent. In cooperative research between NIST and the Massachusetts Institute of Technology (MIT), a method has been developed to simulate smoke dispersion and settling from crude oil pool fires burning in a uniform wind. Calculation of the smoke plume trajectory and smoke particulate deposition from a 114 m² (110 MW) mesoscale crude oil burn have shown that with 6 m/s wind speed, particulate deposition would cover a downwind distance of 258 km.

Publications:

Related Grants:
"Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes," Ahmed F. Ghoniem, Massachusetts Institute of Technology.

"A Study of Boilover Mechanism on Crude Oil Combustion," Kozo Saito, University of Kentucky.
Institution: Purdue University
Grant No: 60NANB1D1172
Grant Title: A Study of Simulated Oil Well Blowout Fires and Flares
Principal Investigator: Professor J. P. Gore
                  School of Mechanical Engineering
                  Purdue University
                  West Lafayette, IN 47907
Other Personnel: Mr. C. Q. Jian, Doctoral Student
                 Mr. P. Dutta, Doctoral Student
                 Dr. Y. Sivathanu, Research Associate
NIST Scientific Officer: Dr. David D. Evans

Technical Abstract:

Introduction: The overall objective of this project is to develop capabilities for predicting radiative heat loads from oil well blowout fires, diverter fires and boom-flares to surrounding objects. Three aspects of the overall project were addressed during the past year: (1) evaluation of total radiative output of a jet flame based on a single point radiance measurement; (2) measurements and predictions of temperature and velocity distributions in buoyant, turbulent, horizontal flames representative of diverter fires; and (3) development of a two-fuel spray atomizer/burner with very low (5% to 20%) gas to liquid mass ratios.

(1) Total Radiative Output from Single Point Radiance Data: The total radiative output per unit combustion energy release (defined as radiative heat loss fraction XR) of a fire is used as a parameter in many engineering sub-models. This parameter influences the peak reaction temperatures, radiation hazard to surrounding objects and personnel, and emission of smoke, CO, NO and NOx from the fires. Past measurements have shown that for highly buoyant flames, XR tends to be constant for a given fuel. For forced jet flames, XR decreases with increasing Reynolds number (Re) beyond a critical Re. Values of XR for laboratory flames have been obtained by traversing a wide-angle total radiation heat flux gauge to measure the distribution of the radiation heat flux on the surface of a semi-infinite cylinder. These data are then integrated to obtain the total radiant output of the flame.

In order to utilize a single measurement of the radiative heat flux to infer the total radiant output of the flame, a scaling relationship between these quantities must be established. Calculations of radiative heat flux to various locations using the multi-ray method in conjunction with a calibrated turbulence model showed that X/Lf and R/Lf where X is the vertical distance from the injector exit, R is the radial distance from the axis of the flame and Lf is the axial distance of the point at which the mean local mixture fraction is stoichiometric. The results of the calculations showed that for identical values of the above two parameters the ratio of the total radiant output of
the flame and the chemical energy release collapsed for a range of flame sizes. Since measurements of the $L_f$ defined in the above manner can not be obtained in practical fires such as those in Kuwait, the $L_f$ was defined as the visible flame length for the sake of comparison.

Figure 1 shows the predictions of radiant output normalized by the chemical energy release and the radiation fraction plotted as a function of $X/L_f$ for $R/L_f$ = 0.5 and 1.0. The experimental data for a wide range of flames (heat release rates between 10 and 100 kW) and three different fuels are also plotted in Fig. 1. The scatter in the data result from the uncertainty in the determination of the visible flame heights of flames burning fuels of different sooting tendencies.

(2) Horizontal Turbulent Buoyant Diffusion Flames: Oil and gas well diverter fires form this type of flame. Pipe leaks may also cause horizontal fires. Predictions of the trajectory and radiation heat loadings of these fires are important in the assessment and design of structures around diverters and minimum safe distances from possible pipe leaks. In previous work, a 2-dimensional boundary layer analysis for predicting the centerline trajectory of horizontal flames was developed. The results of this analysis showed good agreement with the experimentally observed trajectories over a range of Reynolds numbers (Re= 4000 to Re= 12000). Measurements of flame shapes and temperature and velocity distributions showed that the flames are unsymmetric around the curvilinear axis due to the plume-like flow that develops along the upper interface. It was therefore necessary to extend the analysis to a 3-dimensional boundary layer method.

During the past year, a three dimensional boundary layer method was developed for the treatment of the unsymmetric flow. The centerline trajectory predicted by the 2-dimensional calculations was used to economize on the computational domain by attaching a curvilinear coordinate to the centerline of the visible flame. Calculations in two directions orthogonal to the curvilinear axis made the procedure 3-dimensional. Diffusion in the axial direction was neglected since the flow is predominantly axial and the difficulty of specifying the downstream boundary conditions is avoided.

Figure 2 shows the measurements and predictions of axial velocity distributions along a direction normal to the curvilinear axis in the vertical plane. The predictions capture the unsymmetric plume flow qualitatively. However, the magnitude of the velocity is under-predicted. Measurements of temperature in this region have shown relatively low values. Therefore, this level of agreement is sufficient for calculating radiation properties. However, the reasons for the low values of predicted velocity are being studied.

(3) Two-Fuel Spray Atomizer Burner: Jet flames resulting from oil well accidents contain approximately 5 to 20% gaseous fuel. Past laboratory studies have been limited because the atomization quality with such low gas to liquid mass ratio is not sufficient for flame stabilization. A new type of atomizer/burner has been developed and tested during the past year. Figure 3 shows the measurements of drop size using a Malvern instrument for a representative location in the spray generated by the atomizer. The drop sizes seen in Fig. 3 are between 5 and 300 microns and the mean drop size is 36 microns. With this size distribution, two-fuel spray flames can be stabilized with a gas/liquid mass ratio of 0.05. Combustion tests with this burner are currently in progress.

Acknowledgement: The oil well blowout and diverter fires program at NIST is supported by the Mineral Management Service of the U. S. Department of Interior with Mr. Ed Tennyson, Mr. Charles Smith and Mr. John Gregory serving as program monitors.
Reports and Papers:


Figure 1: Measurements and Predictions of Radiative Heat Flux Surrounding Turbulent Jet Diffusion Flames.

Figure 3: Malvern Measurements of Probability Density Function of Drop Sizes Produced by the Effervescent Atomizer/Burner.
Figure 2: Measurements and 3-D Boundary Layer Predictions of Velocity Distributions in Turbulent, Buoyant, Horizontal Jet Diffusion Flames
Introduction: Burning rates of objects on fire determine safe egress times, heating rate of surrounding objects and flame spread rates. Radiative heat flux from fires to surrounding objects determines the possibility of ignition, flame spread and flashover. Improved understanding of phenomena that determine the burning rates and radiation loading of pool fires when incorporated into design and emergency management procedures can reduce fire losses.

The overall objective of the current grant is to study the effect of fire size, fuel type and turbulent fluctuations on the radiative heat feedback and radiative output to the surroundings from liquid fueled pool fires. During the three year study fires burning methanol, ethanol, hexanol, heptane, MMA, toluene and styrene in 4.6, 7.1, 30, 60 and 100 cm pools were studied. Table 1 shows various properties of these flames. The heat release rates varied between 0.6 and 2480 kW and the flame heights varied between 16 and 340 cm. Up to 30 cm pool size, the methanol fires shown in Table 1 have total heat feedback rates comparable to those of the heptane fires. This is due to the shape of the methanol fires in the region near the fuel surface that leads to very high convective heat fluxes. For larger fires, the radiative component for heptane increases significantly leading to almost a factor of 2 difference between the feedback rate of the two fuels.

The heat feedback rates of the toluene fires are much larger than those for the heptane fires for smaller pools. However, for the 100 cm pools, the heat feedback for the two fuels are comparable. The radiant fraction for the two fuels shows little variation with fire size except for the 100 cm toluene fire which shows lower $X_R$ (24% for 100 cm fire compared to 36% for the 60 cm fire) possibly due to the effects of blockage by dark cold soot on the outer surface. The reduced heat feedback rate (34 kW/m² instead of 40 kW/m²) is also probably due to the presence of cold soot in the region near the surface.

The directional radiative heat flux incident on the fuel surface was measured for the 30 cm methanol, heptane and toluene fires using a N₂-purged radiation flux gauge. The
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<th>( \dot{m}^\infty ) (kg/s)</th>
<th>( Q^\infty ) (KW/m^2)</th>
<th>( Q_{chem} ) (KW)</th>
<th>( H_f ) (cm)</th>
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Table 1: Properties of Pool Fires Over a Range of Fuel Types and Fire Diameters.
hemispherical radiative heat flux incident on the surface was obtained from the directional data using area-weighted integration.

The local distribution of soot volume fractions and temperatures are important in determining the radiation heat fluxes to the surroundings and to the fuel surface in luminous fires. During the present investigation, a five wavelength emission/absorption probe was used to the measure in 7.1 cm diameter toluene (Klassen et al., 1992a), 30 cm toluene (Klassen et al., 1992b) and 30 cm heptane fires (Klassen, 1992).

Measurements of soot volume fractions and temperatures in the 30 cm toluene fires were used to calculate the radiative heat flux incident on the fuel surface under the following approximations: (1) radiation from gaseous molecules is negligible compared to that from soot particles; (2) fuel vapor and all other intermediate species except soot particles are transparent; and (3) the integral length scale for radiation fluctuations could be estimated by trial and error. The first two assumptions were tested by measuring spectral absorption and emission properties in toluene fires. The effects of these on the calculated incident heat flux are estimated to be less than 10%. Two point measurements in toluene fires are planned to obtain a more rational method for the treatment of length scales.

The multi-ray procedure used in the calculations is illustrated in Fig. 1. The details of the procedure are given by Klassen (1992) and Klassen et al. (1992b). Figure 2 shows the comparison between measurements and predictions of radiative heat flux incident on the surface. In view of the approximations, the agreement between measurements and calculations is encouraging.

Since the time series from the experimental data are available, a filtering technique was applied to find the frequencies of scalar property fluctuations that have a significant impact on the radiation intensity leaving the fires. Klassen and Gore (1992) found that for spectral radiation intensities leaving a diametric path in a 7.1 cm toluene fire, at least the characteristic pulsation frequency (approximately 10 Hz) must be resolved to obtain reasonable estimates. Data filtered at frequencies lower than 10 Hz yield substantial under-prediction.

The multi-ray calculations show that due to the different optical thicknesses, bulk of the energy incident on the liquid surface originates within 0.5 diameters of the surface for toluene and within 3.5 diameters of the surface for heptane fires. The work in progress on the current grant involves: (1) measurements of CO2 concentrations to develop a methodology for the treatment of radiation from gaseous species in nonluminous fires; (2) two point measurements to examine if the assumed integral length scales for radiation fluctuations are rational; and (3) interpretation of the radiative heat feedback for different fuels in terms of an energy balance at the surface. It is recognized that surface reflection (which can be 100% for directional heat fluxes beyond a certain angle from the normal) can play a role in determining the fraction of the incident energy that is absorbed by the liquid.

Acknowledgement: The contributions made by Dr. Hamins of N. I. S. T. are gratefully acknowledged.

Reports and Papers:


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**Figure 1:** Narrow Angle Directional Radiative Heat Flux Measurements and Calculations for Pool Fires.

**Figure 2:** Measurements and Calculations of Total Radiative Heat Flux to the Fuel Surface.
B. Fire Safety of Products and Materials

B1. Materials Combustion
Professional Personnel

T. Kashiwagi, Group Leader
J. Brown, Chemist
A. Hamins, Mechanical Engineer
K. Steckler, Physicist
J.C. Yang, Post-Doctoral Associate

Principal Objectives

(1) To improve our understanding of the physical and chemical gasification processes of various polymers and to develop theoretical models to predict the gasification rates of polymers exposed to fire conditions.

(2) To improve our understanding of energy feedback mechanisms of pool fires and to develop theoretical models to predict energy feedback rates from a pool flame to the fuel surface.

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 heat transfer 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. A simple global energy feedback model is developed which takes into account fuel effects and the influence of pool diameter on the energy feedback rate.

Technical Accomplishments

I. Polymer Gasification

1. Experiments

An experimental apparatus for studying transient gasification of materials exposed to radiant heating in a nitrogen atmosphere is being 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. Measurements will include temperature profiles within the sample, depth of the bubble layer in the sample, and mass of the sample as a function of time.
2. Gasification Rate Model

Work continued on the numerical model developed last year for the one-dimensional gasification of a non-charring thermoplastic material. Sub-surface, in-depth degradation of an opaque solid via a one-step Arrhenius reaction was considered. The model accounts for temperature-dependent thermal properties and time-dependent external radiant flux. It assumes that degraded material is instantaneously removed from the solid. Gasification rates calculated with this model, however, were much larger than experimental results for PMMA.

The model was modified to account for in-depth absorption of external radiation in semi-transparent materials such as PMMA. Again, the calculated results were much larger than the experimental data. It is suspected that lack of an in-depth re-emission heat transfer mechanism is the major source of this discrepancy. The next step is to provide for the re-emission of absorbed external radiation.

II. Pool Burning

1. Experiments

The energy flux at the surface of a pool fire was characterized. A narrow view angle, nitrogen purged, water cooled radiometer was used to measure the radiative portion of the heat feedback to the surface of 30 and 60 cm pool fires. The intensity was measured at several angles above the fuel surface. The effect of gauge heat up was measured with the fire burning by placing a water cooled cap over the radiometer (nitrogen purge maintained). The radiometer was calibrated using a standard flux gauge. The fuels tested were methanol, heptane and toluene. The intensity, I(θ), profiles were integrated to give the hemispherical total emissive power at various locations: flux = \int \int I(θ)(1-R(θ))\cos(θ)\sin(θ)dθdϕ, where R(θ) represents the incident energy reflected by the fuel surface.

The measured radiative flux incident varied as a function of location. Figure 1 shows the results for the three fuels tested in the 30 cm diameter pool. The largest radiative heat flux was in the toluene fire, followed by heptane and methanol.

Total feedback to the fuel surface was calculated from fuel burning rates measured in a pool fire apparatus consisting of four concentric rings with the burning rate in each ring independently monitored. In addition, heat losses to the cooling water and increases in sensible heat of the fuel were determined to be small. Thermocouple measurements indicated that heat conduction from the flame to the fuel surface via the burner rim was negligible. A comparison of the local radiative and local total heat feedback for 30 cm pool fires showed that radiation is the primary heat transfer mechanism for all fuels. The difference between radiative and total heat feedback was attributed to convective heat transfer which was significant in the methanol fire only.

Characterization of the soot field by laser extinction for pool fires burning a range of diameters is being conducted. Figure 2 shows the maximum soot volume fraction at 0.5 and 1.0 diameter above the fuel surface for fires burning acetone and heptane in 5.0, 7.5 and 10 cm pools. Additional radiance measurements are being planned for large pool fires (1 m).

2. Burning Rate Model

A simple global model was developed which predicts the mass burning flux for pool fires consuming liquid fuels in a quiescent environment. The model assumed constant bulk properties such as flame
temperature, soot volume fraction, and species concentrations. The computational procedure required knowledge of the fuel smoke point height and fuel properties such as the heat of vaporization, heat capacity, and boiling point. A cylindrical flame shape was assumed and the flame height was calculated using Heskestad's correlation. A mean beam length approach for radiative heat transfer was utilized and emission from both gas species and soot particles was considered. The global flame temperature was taken as the average of the maximum flame temperature and the fuel boiling point. The maximum temperature was based on the adiabatic flame temperature less the energy lost through radiation and combustion inefficiency. The predicted mass flux was within a factor of two of measured burning rates for pool diameters greater than 0.2 m and within a factor of three for smaller diameters.

Recent Publications


Related Grants


"The Structure and Radiation Properties of Pool Fires", J.P. Gore, Purdue University.
Fig. 1 Radiative heat feedback to the surface of 30 cm pool fires burning methanol, heptane and toluene.

Fig. 2 Maximum soot volume fraction at 0.5 and 1.0 diameter above the surface as a function of pool diameter for acetone and heptane pools.
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. If the solid phase consists of an organic macromolecular material, the complexity is compounded by the need to account for a host of pyrolytic phenomena in addition to the gas phase processes. This is unfortunately the situation in study of fire phenomena. 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 when small scale laboratory pyrolysis data can be reliably used to model fire situations.

The role of a char layer in complicating the analysis of the combustion process has been recognized by many workers in the field. The char has a high emissivity and may thus participate in mechanisms of extinguishment by heat loss from the surface. If not screened by the outward flux of volatiles, the char may itself react with oxygen, and become a local heat source, as in glowing combustion. The char may also be highly catalytic in promoting cracking reactions of volatiles, changing the composition of the volatiles from that which exists in the active pyrolysis zone. The cracking may also result in additional carbon deposition in the char layer. If the volatiles contain carbon dioxide or water vapor and the char temperature is high enough, some gasification reactions may occur, resulting in release of hydrogen and/or carbon monoxide from the char. Such possibilities have been often recognized, but generally not studied in a systematic manner. A significant difficulty in performing such studies in a controlled environment is that the mass transfer in the char layer is imperfectly understood. For example, in real fire situations, wood forms a char layer with a partially crazed (alligatored) surface, and that suggests the possibility of cracks carrying volatiles out from below the char layer. This means that the residence time of the volatiles in the char layer (or extent of contacting between the two) is unknown, and thus difficult to quantitatively model.

Experimental Approach. The 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

Institution: Brown University
Grant Number: 60NANB0D1042
Grant Title: The Behavior of Charring Materials in Simulated Fire Environments
Principal Investigator: Prof. Eric M. Suuberg
Division of Engineering
Brown University
Providence, R.I. 02912
(401) 863-1420
Other Professional Personnel: Mr. William Lilly, Senior Research Engineer
Mr. Ivan Milosavljevic, Graduate Student
Mr. Jack Liang, Undergraduate Student

Technical Abstract:

Building and Fire Research Laboratory
Fire Research Program
National Institute of Standards and Technology
Grantee Project - FY92
Brown University, and it 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 environment can then simulate either a diffusion flame environment, in which little or no oxygen reaches the surface of the sample, or a pre-ignition environment, in which pyrolysis begins in the presence of oxygen and a radiative flux from a fire elsewhere in the environment. The sample surface is heated by radiant quartz heaters which can provide a flux of up to about 100kW/m², which should cover the range of relevance in fire situations (somewhere around 40kW/m² is a "standard" condition).

The sample itself is instrumented within its interior with thermocouples, to provide a temperature profile, and the surface temperature can also be measured optically. We can determine the emissivity of the char in-house, using diffuse reflectance techniques on a FTIR spectrometer. 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 or MS provides information only on the gaseous species, and the tars must be separately collected by condensation, or determined by difference.

In a few cases, the samples were pyrolyzed in an ordinary thermogravimetric analyzer (TGA) equipped for gas product analysis by FTIR.

Results Obtained Work thus far completed has involved examining in detail the pyrolysis behavior of high density cellulosic samples. These samples have densities approaching those in wood (ranging from about 0.4 to 1 g/cc), but have the advantage of uniform, known composition and low impurity levels. The samples are pressed in house from cellulose pulp. The tests performed under nitrogen (with a surface radiative flux of 40 kW/m²) in the simulated fire apparatus displayed the expected behavior, involving progressive penetration of a thermal wave into the sample. The results are shown in Fig.1. These results are for different initial sample thicknesses, as noted, and show that the penetration of a thermal wave into the samples controls the rate of the pyrolysis process, and that the process is thus conduction limited. It is apparent that the usual diffusion-limited behavior is, however, not observed (wherein the process slows as the thermal wave penetrates more deeply). This is the case because there is a prescribed incident surface flux that drives a continual increase in surface temperature. For example, in the case of a 12.25 mm thick sample, the surface temperature rises more or less linearly with time, for the first 750 seconds. It should be noted that in the case of the data of Fig. 1, the heat lamps are only switched on at 270 seconds.

Generally speaking, the mass loss rate from pyrolyzing cellulose samples varies proportionally with sample density. This is noted in Fig. 2. There is no such variation noted in small particle samples pyrolyzed in a thermogravimetric analyzer (TGA).

The linear variation of mass loss rate with density in the large-scale tests reflects the fact that the thermal conductivity of the char layer formed during pyrolysis varies with the initial density of the samples. The density of the char layer is, in fact, proportional to the initial sample density.

The yield of char has been observed to be only a weak function of sample density, in experiments conducted in a TGA. This is in contrast to "char yields" from samples in the simulated fire apparatus, in which heat losses from the back of the sample effectively prevented the process of pyrolysis from going to completion. Thus density itself is not a key factor in determining char yields. It has a role only insofar as it affects the heat transfer (and possibly mass transfer) within the system.

It appears as though mass transfer limitations play a measurable, but not very large role in determining char yields. It is observed that much of the tar that is evolved emerges from around the sides of the sample, rather than through the front face of the sample, indicating a movement lateral to the band structure induced during pressing, and analogous to the preferential movement of volatiles in an along-the-grain direction as opposed to cross grain. Tests with thin samples indicate that this can result in differences in char yield of only a few percent.

It was also noted in this work that the alligatoring behavior commonly seen in wood could
induced, and could be suppressed or enhanced, depending upon sample configuration. Alligatoring involves the macroscopic cracking of the sample, due to shrinkage during pyrolysis. Allowing small samples to shrink inward during pyrolysis largely prevents alligatoring, whereas confining the edges of a sample to prevent inward shrinkage, causes cracking failure in the middle of the sample. Such alligatoring cracks potentially serve as important conduits of volatiles, and an assumption of uniform surface flux of volatiles may be rather poor in some situations.

Sample density affects the ability of volatiles to escape the pyrolyzing material. The higher the density of the starting material, the higher the density of the char layer left behind, and the lower the rate of mass transfer out of the sample. We have observed the effect of sample density variations on the gas products of pyrolysis, in experiments with identical 3 mm cubes of sample. The results are shown below in Table 1.

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</table>

It is obvious that there is a slight trend towards higher yields of gaseous cracking products with increasing density. This is accompanied by an increase in final char yield from about 4% to 5.5% in going from the lowest to the highest density. Thus with small particles, the effect of density on the process of cracking of heavy, tarry volatiles is small, but measurable. It is not believed that the effect will be much more substantial in larger samples, insofar as sample cracking dictates in large measure the ability of the volatiles to escape. Examination of this point continues.

It is then concluded that the primary factor determining char yields in the large scale apparatus tests of the present study is differences in the heat transfer environments. It has however also been concluded that the kinetics of cellulose pyrolysis as determined from fine particle TGA-type studies is inadequate for predicting the course of pyrolysis in large samples, even if heat transfer limitations are properly accounted for. The process of pyrolysis deep within the sample is considerably slower than would be predicted from fine-particle kinetics. The material involved is also obviously quite different from virgin cellulose; it is quite brown, and of obviously different composition. The implication is that at slow heating rates, as experienced within the bulk of the sample, the pyrolysis involves more than a single controlling step, and the competitive nature of different pyrolysis pathways becomes apparent. This can be missed in fine particle work involving the same surface heating rates, because in those cases, the bulk heats as quickly as the surface. This aspect of the problem is currently being further examined.

**Reports and Papers**


Figure 1. Mass as a function of time for 1 g/cc samples. The initial values of sample mass have been shifted to a common value so as to make comparison easier.

Figure 2. Mass loss rate as a function of sample density, from the simulated fire apparatus and the TGA device. Parallel and perpendicular refer to the orientation of sample band structure relative to the direction of the incident radiative flux.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1992

CIGARETTE IGNITION METROLOGY

Funding Agency: U.S. Consumer Product Safety Commission

Professional Staff: Richard G. Gann, Project Leader
Emil Braun
Richard H. Harris, Jr.
Henri Mitler
Magdalena Navarro
Thomas J. Ohlemiller
Kay M. Villa
George N. Walton

Project Objective:

Fulfill NIST responsibilities under P.L. 101-352, the Fire-Safe Cigarette Act of 1990, by August 9, 1993. The Act directs NIST to perform three tasks for the CPSC: develop a standard test method to determine cigarette ignition propensity, compile performance data for current cigarettes using the method, and conduct laboratory studies on and computer modeling of ignition physics to develop a predictive capability.

Technical Accomplishments:

BFRL has developed both a primary (direct measurement of ignition) and secondary (measurement of another property related to ignition propensity) test method. The former uses flat furnishing mockups consisting of commercially available fabric/foam combinations. The latter replaces these substrates with multiple layers of filer paper, determining the number of layers for which the test cigarette continues to burn. An interlaboratory evaluation of the methods will occur early in FY1993. A computer model of a substrate degrading in the presence of a moving heat source has been developed, eventually to run in conjunction with one of a cigarette burning on a non-reactive substrate. The former solves the time-dependent heat diffusion equation and includes an asymmetric, variable size, moving computational grid; two pyrolyzing layers with an air gap in between; and temperature-varying thermophysical properties.

Reports and Publications:


FUNDING AGENCY
FEDERAL AVIATION ADMINISTRATION

PROFESSIONAL PERSONNEL:
Marc R. Nyden, Research Chemist
James E. Brown, Research Chemist
Barry Bauer, Research Chemist (MSEL)
Charles Dick, Research Physicist (Physics)

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:
Synthetic polymers comprise a significant fraction of the fire load borne by commercial aircraft. The flammability and combustion toxicity of these materials impact the passenger survivability of in-flight and post-crash fires. Research conducted in BFRL has focused on finding ways to increase the tendency of plastics to char when they are burned. We have used computer modeling to identify factors which promote the formation of char during the thermal degradation of polymers. Computer movies based on molecular dynamic simulations of degrading polymers indicate that cross-linked polymers tend to undergo further cross-linking when burned and eventually form high molecular weight, thermally stable chars. This prediction has been confirmed in Cone Calorimeter flammability measurements made on both \( \gamma \) and \( \beta \) - irradiated polyethylene and on chemically cross-linked poly(methyl methacrylate). The behavior of the \( \beta \) - irradiated polyethylene was particularly striking. The more highly cross-linked layer on the top of the sample, charred and formed a large bubble in the process of retaining the gases generated in the degradation of the interior. Eventually, the gases broke through and ignited, leaving behind a thin skin of carbonaceous material. These experiments suggest the possibility of using ionizing radiation to graft fire resistant shells on to processed plastics. In this way, it may be possible to achieve a significant reduction in flammability without altering the bulk material. New experiments, which involve grafting poly(vinylidene chloride) to the surface of polystyrene sheets, are underway.

REPORTS AND PUBLICATIONS:
FLAME RETARDANT STUDY

Funding Agency: General Electric Co.

Professional Staff: Takashi Kashiwagi, Project Leader
Thomas G. Clearly

Project Objective: To understand the effects of polymer structure and certain flame retardant treatments on flammability properties of engineering thermoplastics.

Technical Accomplishment:

Various flammability properties, ignition, flame spread rate, heat release rate, CO and soot yields, and smoke extinction, are measured for various GE's polycarbonates, polyimides and polyphenyleneoxides with and without flame retardant treatments. The effects of external radiant flux on the flammability properties of these sample were determined using Cone Calorimeter and LIFT devices. Since all of these samples intumesce during burning, two sample mounting configurations are used. One of them is with a metal frame and a course grid to retain the sample surface at the original location. The other is without any frame or a grid and the sample intumesces without any restriction. The former tends to generate lower heat release rate and the latter higher heat release rate. Since the sample size used in the Cone Calorimeter is relatively small (about 10 cm x 10 cm), the amount of intumescent might be affected by the size. In order to study this effect samples with the size of 38 cm x 38 cm will be tested to measure the amount of intumescent and also heat release rate.

Gasification rate, temperature distribution in the sample, and evolved gaseous products of selected combinations of polymer samples will be measured using the new radiative gasification device. The gasification experiment will be conducted in nitrogen atmosphere to make certain that there are no gas phase reactions. The sample will be exposed to external flux up to 75 KW/m². Samples with and without the treatments will be studied to determine the effects of the treatments on the gasification process and hopefully to understand the mechanism of the flame retardant treatment.

Reports and Publication:

"Effects of Sample Mounting on Flammability Properties of Intumescent Polymers", Kashiwagi, T. and Cleary, T.G., accepted in Fire Safety J.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - FY92

HEAT FLUX MEASUREMENTS IN NBS SMOKE BOX

Funding Agency: Federal Aviation Administration

Professional Staff: Dr. Richard L. Smith

Project Objective:
To provide a faster and more accurate method of setting the heat flux in the NBS smoke density chamber for use by the FAA.

Technical Approach:
A series of heaters will be selected or designed and then their profiles will be measured using a 0.635 cm Gardon gauge. A profile measurement technique will be developed for the new heater and this Gardon gauge.

Technical Accomplishments:
Reliable measurements of the rate of heat release and the generation of smoke are needed for the evaluation of aircraft cabin interior materials. FAA has chosen to use the ASTM E 662-83, "Standard Test Method for Specific Optical Density of Smoke Generated By Solid Materials." In this method as implemented by FAA, they believe there is a significant variation of the incident heat flux over the surface of the specimen. In addition FAA is not satisfied with the heat flux gauge prescribed in this test method and they want one that can make a measurement faster and is easier to calibrate.

A prototype heater has been developed that provides a more uniform radiation field on the target specimen. Application of a gauge similar to the one used in the OSU calorimeter for use in the smoke box for measuring the heat flux has been demonstrated. Using this heater and gauge, a method that allows one to measure the radiation field at the center of the specimen to infer the average radiation field over the specimen has been developed. Smoke chamber tests on FAA samples have been run to compare the operation before and after the modifications to the heater. A final report describing how to incorporate these three items into the FAA test procedure has been prepared.

Reports and Publications:
Funding Agency: US Navy, David Taylor Research Center

Professional Staff: James E. Brown, Research Chemist
Thomas J. Ohlemiller, Research Engineer
Thomas G. Cleary, Chemical Engineer

Project Objective:
To develop bench scale and intermediate scale test methodology to evaluate the fire performance properties of fiber-reinforced composites in order to assist the U.S. Navy in selecting these materials for ship and submarine use.

Technical Accomplishments:

1. Effect of Edge Clamping on Measured Small Scale Flammability Behavior of Composites

Composite materials comprised of several layers of woven glass and an organic binder tend to delaminate when heated. This has the effect of allowing pyrolysis gases to escape out the edges of the sample. This can produce behavior from small scale samples which is not typical of the same materials at full scale. This issue has been pursued in the context of heat release rate of composites as measured in the Cone Calorimeter. Heat release rate is one of the inputs in predicting the upward spread of flames on a material.

The normal sample holder used in the Cone Calorimeter allows the escape of gases from the sample edges. A modified holder, which clamps the sample edges, prevents this escape but produces two pronounced changes in heat release behavior: first, the sample may exhibit multiple heat release peaks whereas before it produced one; second, the average heat release rate is lowered and extended in time. The first effect appears to be inherent in the layered structure of the composite. By testing various combinations of samples in the regular holder and in the clamped holder, with the samples in some cases having a pattern of small holes to assist gas escape, it has been shown that the second effect above is an artifact produced by heat losses to the edge clamp. An empirical means for correcting the data to eliminate this effect has been devised but it requires several tests on the same sample (at any heat flux of interest). Because of the considerable inconvenience this involves, we have proceeded to look at larger scale flame spread behavior on these materials to see if it really is sensitive.
to the details of the heat release behavior. If not, these corrections may be irrelevant.

2. Medium-Scale Upward Flame Spread on Composite Materials

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 is now being adapted to the measurement of flame spread on the same composite materials as were tested above with the Cone Calorimeter. No definitive results are available as yet.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - FY92

RADIATIVE IGNITION AND SUBSEQUENT FLAME SPREADING
IN MICROGRAVITY ENVIRONMENT

Funding Agency: NASA Microgravity Science Program

Professional Staff: Takashi Kashiwagi, Co-Project Leader
Howard R. Baum, Co-Project Leader
Kazuyoshi Nakabe, Guest Researcher

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.

Technical Accomplishment:
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. Preliminary 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 will be studied. It appears that transition from spontaneous ignition to flame spread tends to be difficult without the slow flows. 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, CO₂, H₂O and O₂. The development of an apparatus to measure global gas phase oxidation reaction rates for the degradation products from the cellulosic sheet will begin shortly.

Reports and Publication:


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.

Technical Approach

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 γ 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. Our preliminary experiments have indicated PE does char when burned in the presence of small amounts of MnCl₂.

Technical Accomplishments

We have demonstrated that molecular dynamics modeling is useful in providing concepts for the development and design of fire resistant materials. In particular, we have established that the flammability of certain polymers can be reduced by using ionizing radiation and/or copolymerization with multivalent monomers to introduce cross-links.
Reports and Publications


SHORT-DURATION AUTOIGNITION TEMPERATURE APPARATUS

Funding Agency: United States Air Force Engineering & Services Laboratory

Professional Staff: Nelson Bryner, Project Leader
                 Erik L. Johnsson, Mechanical Engineer
                 Kermit C. Smyth, Research Chemist

Project Objective:
To provide US Air Force Engineering & Services Laboratory (ESL) with apparatus necessary to collect short-duration autoignition data for hydrocarbon fuels.

Technical Accomplishments:
This project is designed to transfer short-duration autoignition technology developed at NIST [1] to USAF ESL. This apparatus allows short-duration autoignition temperature measurements of hydrocarbon fuels under conditions where the fuel/air stoichiometry, the nature of the hot metal surface, and the contact time are well controlled. This approach provides a much more reliable database to establish the importance of fuel structure effects than the current ASTM E659 procedure [2]. This transfer of technology will provide ESL with the capability to collect short-duration autoignition data for hydrocarbon fuels.

An improved version of the NIST autoignition apparatus was designed, ordered, and assembled during FY92. After preliminary testing, apparatus will be delivered to USAF ESL in September of 1992.

Publications and References
B2. Furniture Flammability
Professional Personnel

Andrew Fowell, Division Chief
Vytenis Babrauskas, Fire Prevention Engineer
Thomas Ohlemiller, Research Engineer
King-Mon-Tu, Mechanical Engineer
Thomas Cleary, Chemical Engineer
Kay Villa, Textile Technologist

Projective Objective

Develop by 1994 a method by which furniture manufacturers can predict the rate of heat release of residential furniture.

Technical Approach

Analyze and report the results of studies on the effect of mode and location of ignition of residential upholstered furniture. Acquire full scale burn data in the required range from testing laboratories and manufacturers. Perform small scale tests on samples of the fabric, foam and combinations of them used in the full scale test pieces. Develop a correlation between component and fabric-foam combination performance, and an understanding of the mechanisms involved. Test the Dietenberger model's ability to predict furniture burning rate. Develop simpler alternatives to that model for predicting maximum rate of heat release. It is hoped the prediction process will involve no more than charts, but if this cannot be attained, a simple PC based program will be developed.

Technical Accomplishments

A set of upholstered chairs constructed from five different fabric/foam combinations was subjected to a variety of ignition sources suggested by fire statistics. The sources included a cigarette, a small match-like flame, an incandescent lamp, a space heater, and a large flame source (CTB 133 equivalent gas burner). For any chair type, the time to the peak heat release rate depended on the ignition sequence, but the magnitude of the peak did not, within the scatter of the data for any given chair. HAZARD I, the fire hazard assessment method developed at NIST, was used to quantify the hazard posed by the different ignition scenarios. It is recommended that the hazards of upholstered furniture for residential use be assessed on the basis of resistance to small flame and cigarette ignition combined with peak heat release rate and time to peak subsequent to ignition by a strong source such as the CTB 133 equivalent gas burner.

Full scale fire experiments were conducted on three fabric-foam combinations using four ignition locations, center of the seat cushion, lower center back, front and side of the chair. These ignition locations had negligible effect on the peak heat release rate or total heat released, but did have a significant effect on time to reach peak heat release. The results of full scale burn tests performed by California Bureau of Home Furnishings and Omega Point Laboratories have been examined and
discussed with the testing lab staff, but there is insufficient detail to develop ignition and fire spread models from this data. We were unable to run bench scale tests on the materials used to construct the furniture tested in full scale by the above laboratories because there was insufficient extra material available. Bench scale tests will instead be performed on material used to construct the furniture used in the ignition mode studies.

The Deitenberger model for fire growth on upholstered furniture has been recoded into Fortran. Preliminary ideas for a material classification system have been developed.

Publications:

B3. Wall Fires
Institution: Factory Mutual Research Corporation
Grant No: 60NANB1D1177
Grant Title: Prediction of Fire Dynamics
Principal Investigators: Ronald L. Alpert and John de Ris
Other Professional Personnel: H.W. Emmons, G.H. Markstein, L. Orloff

NIST Scientific Officer: Dr. Henri Mitler

Technical Abstract:

This work is divided into four tasks, each of which is designed to provide essential inputs for comprehensive models of burning and fire growth.

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

The ceiling jet from a fire is described by field model analysis with what appears to be high precision (and high cost). The actual precision has never been experimentally checked. The attempt last year to develop an adequate simpler analysis, as is so successful for river flow, fails when there are significant density changes in the ceiling jet by heat loss to the environment. The cooling of the ceiling jet with resultant density increase causes the depth and Richardson number to increase without limit. This was explained in some detail by a report presented in the 3rd IAFSS Symposium (1).

Since vertical motions are required for a ceiling jet to meet source and end boundary conditions and vertical accelerations influence the pressure distribution, the vertical momentum effects have been introduced into the horizontal momentum equation. This raises the differential equation from a first order to a third order, thus making it possible to meet the additional conditions. The resultant steady flows show large standing waves not reported from experiment. Some field model calculations show some waves for a short distance in back of the front. Perhaps the present model correctly has these waves, but without damping, they persist from the front all the way back to the source. Future work will attempt to add some suitable damping.

The nonsteady terms have been added to the simple theory and are being applied to the ceiling jet flows without heat transfer. Since what happens under these conditions is well known from liquid flows, these results will serve as a test of the present transient theory.

The above work is directed toward development of a simple, engineering accuracy description of all ceiling jet phenomena, which are as important in some fires. However, fire predictions do not require as high an accuracy as many other more mature engineering fields (at least at the present time). Thus some of the ceiling jet phenomena may not be of much importance to fire modeling. However, we have to
consider ceiling jet sources of various kinds. The plume striking the ceiling has not yet been adequately modeled and hence its range of parameters, depth, velocity, Richardson number is not yet considered. The source flow of hot gas out of a fire room door into a corridor must be better understood. Similarly the end conditions are important. The end may be open, as a corridor ending in an atrium or the edge of a balcony over a fire. The end may be a door so that the ceiling jet is at first doubled back as a hydraulic jump, or partially doubled back and partially flowing through the door. Important transient effects occur not only as a ceiling jet first advances along a ceiling, but also include the later development of the ceiling jet as the mass flow changes with fire intensity. All these effects are being considered, although not yet quantitatively.

Reference

Task 2. Models for Turbulent Flame Chemistry and Radiation (J. de Ris, L. Orloff)

Radiation from turbulent diffusion flames controls the burning rates of moderate and large-scale fires (1) and is, therefore, of central importance to the flammability problem. Recently, we have developed a global flame radiation model (2) which predicts the radiant fraction from buoyant turbulent (fuel-jet) diffusion flames in terms of the fuel's laminar flame smoke-point value. The model considers the separate roles of soot and gaseous radiation. The effective flame radiation temperature is predicted by the model in terms of the: 1) incompleteness of combustion, 2) radiant heat loss and 3) turbulent mixing, resulting in good agreement with experiment (3).

It is argued that the soot absorption coefficient (or soot volume fraction) is: 1) proportional to the turbulent macro-scale flow time in the soot formation region of the flames, and 2) inversely proportional to the chemical time for soot formation. The chemical time for soot formation is shown to be approximately proportional to the smoke-point heat release rate on the basis of the laminar flame smoke-point models of Kent (4) and Gulder (5). Markstein's general correlations (6,7) of smoke-points in terms of the stoichiometric oxidant to fuel mass ration, S, and adiabatic stoichiometric flame temperature, T_{ad} for nitrogen diluted fuel and oxidant mixtures show that: 1) the soot formation is quite sensitive to S which controls the local velocity of the gas flowing through the diffusion flame toward the fuel side, while 2) the soot formation is relatively insensitive to T_{ad}. The latter result allows us to generalize the turbulent flame radiation model to include nitrogen diluted fuel mixtures and nitrogen diluted/oxygen enriched oxidants.

The predicted radiant fractions are in excellent agreement with experiment for different oxidant and fuel mixtures covering a wide range of flame sootiness. The model is tested against both axisymmetric (8) and planar (9) free-jet buoyant turbulent diffusion flames over a range of heat release rates. We are currently applying the model to wall fire flames which have smaller radiant fractions due to: 1) convective heat loss to the surface, 2) significant dilution of the supplied fuel gases by products of combustion diffusing back toward the fuel source, and possibly 3) reduced macro-scale mixing times due to wall shear stress.

The model requires knowledge of the fuel smoke point which effectively characterizes the fuel's chemical structure. Methods are now available for evaluating the required smoke point of gaseous, liquid, and solid (charring and non-charring) fuels of interest.

By developing algebraic curve-fit formulas for the soot and gaseous emissivities, the model is self-contained and can be readily implemented using spread-sheet software.
References
2. de Ris, J. and Orloff, L.: submitted to Combustion and Flame.

Task 3. Turbulent Flame Heat Transfer to Surfaces (G.H. Markstein)

The scientific understanding of wall-fire combustion and in particular the development of pertinent theoretical models (1-4) require experimental data on flame radiation so that these models can be applied to fires of hazardous scale where radiative energy transfer plays a controlling role. The purpose of the present work is to extend the range of such data beyond the upper limits of fuel sooting tendency and flame height attained in previous investigations (2,5-8). In the approach used here, wall fires of solid fuels are simulated by burning gaseous hydrocarbon fuels under steady-state conditions. The four fuels, methane, ethane, ethylene and propylene, are used to cover a sufficiently wide range of sooting tendency.

Initially, the study concentrated on the simulated overfire region by releasing the entire fuel flow from a horizontal slot burner placed adjacent to a vertical water-cooled metal plate (9,10) while more recent work (11) is concerned primarily with the pyrolysis region, simulated by supplying gaseous fuels from a water-cooled vertical sintered-porous-metal surface. The burner developed for this study consists of ten 132-mm-high and 380-mm-wide vertical porous-metal panels topped by a 660 mm high water-cooled solid-metal heat transfer plate divided into five similar segments. To approach two-dimensional flow conditions as closely as possible, water-cooled side walls of 150 mm depth are attached to the burner over the entire height of 1980 mm.

The water-cooling passages embedded in the porous metal and the heat transfer plate are instrumented with differential thermocouples for measurement of the total heat transferred to each panel and segment by the flame. Other instrumentation includes a wide-view-angle radiometer measuring total radiant emission and a slit scanning radiometer to determine the vertical distribution of radiant emission by horizontal slices across the wall fire.

In the slot-burner work (9,10) it was found that the radiative fraction of total heat release rate was reduced significantly by placing the burner adjacent to a water-cooled wall, compared to values obtained with free-
burning slot-burner or jet flames. This work also yielded dimensionless correlations of radiant emission as a function of height independent of heat release rate, by introducing a radiation flame-length parameter. The latter vary with the 1/2 power of heat-release rate, suggesting that flame heights are controlled primarily by radiant cooling rather than turbulent mixing, and implying a mean volumetric heat-release rate independent of fire size and fuel type.

Work with the porous-metal burner (11) showed that for any fixed fuel mass flux, the radiance \( N_o \) increases linearly with height, \( z \), after an initial jump at the flame base. At fixed \( z \), linear relationships between reciprocal radiance \( N_o^{-1} \) and reciprocal mass flux \( \text{m}^{-1} \) were obtained. For methane and ethane these relationships held over the entire range of mass flux, while, for ethylene and propylene, an abrupt transition separating two regimes occurred at critical mass fluxes. The ordinate intercept \( N_o^{-1} \), representing an asymptotic radiance, and the slope \( s \) of the linear relationship, are functions of height \( z \). \( N_o^{-1} \) and \( s^{-1} \) increase with fuel sooting tendency at fixed \( z \).

Heat fluxes to the porous-metal panels decreased with increasing mass flux near the flame base, but were nearly independent of mass flux near the top portion of the porous-metal burner. These heat fluxes increased with fuel sooting tendency except for a reversed trend between methane and ethane. At sufficiently high mass flux, a jump of heat flux occurred at the junction between the porous-metal burner and the solid-metal heat transfer plate, and the heat flux increased further with height in this over-fire region. In this zone, the data were separated into a lower overlapping set for alkane fuels, methane and ethane, and a higher overlapping set for the alkenes, ethylene and propylene.

Additional results beyond those included in Ref. 11 will be presented. In particular, separation of total heat flux to the wall into its radiative and convective components is an essential requirement for the development of a predictive theoretical model. Instrumentation for performing pertinent measurements is currently being developed. However, preliminary estimates of the separation can be obtained from the current data and will be reported.

References


Task 4. Measurement of Charring Fuel Smoke Points (J. de Ris, Xiaofang Cheng)

The objective of this task is to measure the smoke points of several charring solid materials by moving horizontal samples under a controlled CO\textsubscript{2} laser heat source, and to compare results with smoke points obtained by the existing vial technique, and correlate both results against measurements of incompleteness of combustion.

It is now well established that the smoke point of a material provides a direct measure of a material’s flame sootiness and it is anticipated that the smoke point may also provide various other non-thermal damage\textsuperscript{1} characteristics of a material. The smoke point also correlates the radiant fraction of the total heat release rate and the incompleteness of combustion of turbulent diffusion flames typical of fires. Clearly, the smoke point is a very important material flammability property which needs to be measured for practical fuels. It can readily be measured for gaseous, liquid and non-charring solid fuels which can be made to support a controlled steady laminar "candle-like" diffusion flame. The smoke point is defined as the maximum flame height which just does not emit smoke from the flame tip. A typical 10 cm high smoke-point flame requires a fuel supply rate of only 4x10\textsuperscript{-4} g/s. The small amount of material required for such measurements should make the smoke-point measurement particularly attractive to chemical industry researchers involved in developing new materials.

The major problem with using the smoke point as a material flammability property is the difficulty in measuring it for charring fuels. The pyrolysis rates of charring fuels are usually transient. The char produced during transient pyrolysis may chemically react with the pyrolysis gases causing them to change chemically and alter their smoke-point value. There is also the possibility that the pyrolysis vapors may change chemically when coming into contact with a heated surface before entering the laminar candle-like flame. These issues need to be resolved as part of the development of a practical smoke-point test method.

Previously, as part of this grant, M.A. Delichatsios established that it is possible to measure the smoke-point of a charring fuel. He placed samples of PMMA, wood and neoprene in a small quartz vial and exposed the vial to a controlled quartz-halogen radiant heat source in our flammability research laboratory. By manually increasing and decreasing the radiant exposure, he obtained a preliminary smoke-point measurement for all three fuels. The PMMA value agreed with previous results obtained by Tewarson.

\textsuperscript{1}Damage due to CO, soot particles and corrosive chemical compounds.
We have recently assembled an apparatus for measuring the smoke point of a charring material by slowly moving a horizontal slab under a focused beam from a CO$_2$ laser. By adjusting either the horizontal feed rate or CO$_2$ laser power we can control the height of the steady laminar flame. The flame height is measured by video camera while the smoke release is measured by its extinction of an electrically chopped IRLED optical beam passing across an exhaust chimney above the flame. A threshold circuit powers a light bulb seen by the video camera when the smoke release exceeds some specified small value.

Initial measurements of the smoke point for PMMA and two types of particle board show that the smoke-point flame height is independent of the horizontal feed rate. Greater feed rates require more laser power. A laser power of less than 50 W should be sufficient for all materials of interest.

The laser technique has the particular advantage of allowing the fuel gases to immediately enter the attached laminar flame without coming into contact with any neighboring hot surface, such as the mouth of a heated vial or other fuel holder. The flame remains well anchored to the fuel surface because of the intense flame to solid heat transfer characteristic of creeping flames.

The goal of the current task will be to compare results from the two rather different techniques (vial and laser heat source) for measuring the smoke point of practical charring materials. These results will also be compared with measurements of smoke yield and incompleteness of combustion for larger (10 cm diameter) samples which generally correlate with the smoke point. We expect this task to be complete by the end of the grant period (1992).
Institution: The University of Kentucky

Grant No.: 60NANB1D1142

Grant Title: A Study of Fire Induced Flow along the Vertical Corner Wall: Part II

Principal Investigator: Kozo Saito
Associate Professor
Dept. of Mechanical Engineering

Other Professional Personnel: Cheng Qian, Doctoral Student
Wen Lin, Master Student
Hiroki Ishida, Visiting Scientist
Ted Oizumi, Visiting Scientist

NIST Scientific Officer: Dr. Henry Mitler

TECHNICAL ABSTRACT:
Upward flame spread is a severe phenomenon due to its rapid growth rate and radiation emission from the flame [1–3]. The modeling of upward flame spread along the vertical corner wall must deal with the transient three dimensional nature of the flow pattern which causes complex convective and radiative heat transfer to the wall, and the generating two dimensional spread pattern.

To supply needed experimental data to develop prediction models on room corner fires, a project — experimental studies on fire spread along the vertical corner wall, was initiated at the Combustion and Fire Research Laboratory at the University of Kentucky. In the first phase of the project, a one-half scale room corner model, a square fool burner whose exit surface area is 15 x 15 x 8 cm, and a flow visualization system were designed and built in the Combustion and Fire Research Laboratory at the University of Kentucky.

Flow Visualization Experiments
Fire induced flow along the vertical corner wall was visualized as a function of six different burner heat flux (4.5, 9.0, 13.5, 18, 22.5, and 27 kW) and six different burner stand—off distances (0, 2.5, 5, 10, 15 and 20 cm). Results obtained through these experiments are: (1) Under some conditions, a vortex tube appeared near the burner corner and propagated along the corner to the ceiling. If the vortex tube formation occurs during upward flame spread, it may enhance the flame spread rate significantly [1,2]. The effect of burner geometry on fire—induced flow and the vortex formation was also studied, and no significant effect was found [4–6].

Infrared Imaging Temperature Measurements
To predict flame spread rate on vertical corner walls, the detailed temperature profiles of the wall surface must be understood. The nature of the upward flame spread along the vertical corner wall is two dimensional, highly transient, and unstable.
Conventional thermocouple techniques, if applied, have limitations due to their complexity of implementation, and the uncertainty of pyrolysis temperature (particularly for charring materials), as can be seen in previous work [1,3]. Visual observation techniques which were previously applied for spread rate measurement can produce ambiguous results in the determination of the transient pyrolysis front location. To overcome the limitations associated with these conventional methods, infrared radiometry, which is useful for non-contact temperature measurement, was applied with automated image analysis to obtain transient temperature distributions. The infrared camera was located away from the fire source and it measured the temperature of the wall through the flame. The main difficulty faced was that the wall temperature was considerably lower than the flame temperature, therefore, the flame radiation caused interference — i.e., infrared system would detect some intermediate flame temperature instead of the wall. The infrared image obtained through a 10.6 μm ± 0.5 μm band width filter showed good agreement with the thermocouple data and the infrared image data obtained without flame interference [7]. Based on this, the infrared technique was applied to the measurement of upward flame spread.

**Measurements of Visible Flame Height, Temperature and Heat Flux Distributions at the Vertical Corner Wall**

The one-half scale room corner model was used for these measurements. A propane—air premixed flame was established on a square floor burner to heat up the Marinite—made corner walls. After a steady state temperature distribution was established on the wall surface, visible flame height (in time average), the temperature and heat flux distributions at a corner wall were measured [9].

Visible flame shape was recorded by a video camera, then visible flame height was obtained by averaging (in time) the flame tip location. The frequency of the flame fluctuation was estimated from the video film to be approximately a few Hz, therefore, the averaging was made over a three second period. The flame height measurements were performed changing the burner heat release rate between 4.5 and 31.5 kW and the burner stand—off distance between 0 and 25 cm. Figure 1 shows average flame height as a function of the burner stand—off distance for two different burner heat release rates.

Temperature was measured with 100 μm diameter Chromel—Alumel thermocouples as a function of burner heat release rate and burner stand—off distance. The thermocouple measurement was intentionally designed to compare with the previous infrared measurement results. The thermocouples were placed approximately 1 mm below the Marinite wall surface by drilling a small hole. The thermocouple beads were then covered with Marinite powder to prevent direct exposure of radiation from the flame and convective heat. The thermocouple readings were recorded in a computerized data acquisition system. These thermocouple readings confirmed that the wall temperature achieved a steady state temperature distribution within 30 minutes after the burner was on.

Total heat flux was measured using water cooled heat flux meters at the same eighteen locations as the temperature measurements. Temperature and heat flux distributions for the burner heat flux, \( Q = 13.5 \text{ kW} \) and the burner stand—off distance, \( \text{BSD} = 0 \) are shown in Fig. 2; and those for \( Q = 13.5 \text{ kW} \) and the \( \text{BSD} = 5 \text{ cm} \) (in which vortex formation was observed) are shown in Fig. 3. Interestingly, figure 3 shows both temperature and heat flux distributions have a "dip" near the corner, while figure 2 has no dip and both temperature and heat flux distributions have a monotonous increase with accessing the corner. The existence of the dip may contribute to flow instability near the corner. When this flow instability is coupled with the corner geometry, vortex may be generated. But only this dip may not be sufficient to generate the vortex [7].
References


Fig. 1 Visible average (in time) flame height as a function of burner stand-off distance.

![Graph showing the relationship between burner heat release rate and flame height as a function of burner stand-off distance.](image-url)
Fig. 2 Temperature (left) and heat flux (right) distributions at a vertical corner wall. Burner heat release rate is 13.5 kW and BSD is 0.

Fig. 3 Temperature (left) and heat flux (right) distributions at a vertical corner wall. Burner heat release rate is 13.5 kW and BSD is 5 cm.
Introduction: The overall objective of the present project is to understand the upward flame spread phenomenon under simulated surrounding fire conditions. This is achieved by conducting experiments on upward flame spread under external radiation, developing a mathematical model, measuring the relevant basic material properties needed, and checking the validity of the model by comparing predictions with data. Emphasis is placed on studying and predicting the behavior of practical wall materials used in building and vehicle interiors and textiles. A detailed description of the tasks described below can be found elsewhere in reports.

Technical Accomplishments: A comprehensive series of flame spread experiments on samples of several different materials at various external radiant heat flux levels, under preheat and no preheat conditions, and for a range of line-burner igniter strengths is in progress. In each test, measurements are made as a function of time for total heat feedback and surface temperature at five different heights, and the flame height is read from the video record. Wall samples are 0.3m wide by 1.2 m high (1' x 4') and are subjected to external radiation fluxes of up to 29 kW/m² using two large electrically heated panels. In addition to the flame spread experiments, other complementary tasks were carried out to support the overall investigation. Following is a summary of results and technical accomplishments for the past year.

Effect of External Radiation: Figure 1 shows the flame height as a function of time at six different heat fluxes for particle board samples. The samples were not preheated and the igniter was set at 18 kW/m in all tests. The external flux not only enhances the upward flame spread significantly, but also determines whether the upward flame spread will be sustained. At 5.4 kW/m² and above the flame spread was self-sustained; at heat flux levels tested below that threshold it did not.

Effect of Preheat: When the particle board sample was preheated to steady state and then ignited, the flame spread was substantially greater compared to the sample which was simultaneously
Tests

When the igniter failed, the PMMA board ignited up and produced a small flame that produced an average upward spread of 12 mm. Figure 3 shows a comparison of the flame spread for these materials tested under identical conditions with an average external radiation flux of 12.9 kW/m². Continuous and rapid flame spread was seen on the samples of PMMA and particle board. The flames on the untreated plywood spread to the top but then dropped back down. The fire retardant plywood showed only a slight increase in flame height for a short time. Additional tests are in progress.

Effect of Igniter Strength: The igniter strength determines the height of the flames from the line burner. A large ignition source can produce sufficient size of the initial pyrolysis zone to sustain the upward spread. Figure 3 shows interesting results of the effect of the igniter strength on particle board samples. The largest igniter flames clearly produced a sustainable fire, the smallest failed to do so, and the middle size initially created flames up to the top, however, the flames became intermittent and then dropped back to a much lower level.

Tests on Other Materials: Tests were conducted on samples of four different materials, 3.2 mm PMMA, 12.7 mm fire retardant plywood, 12.7 mm untreated plywood, and 15.9 mm particle board. Figure 4 shows a comparison of the flame spread for these materials tested under identical conditions with an average external radiation flux of 12.9 kW/m². Continuous and rapid flame spread was seen on the samples of PMMA and particle board. Flames on the untreated plywood spread to the top but then dropped back down. The fire retardant plywood showed only a slight increase in flame height for a short time. Additional tests are in progress.

Role of In-depth Radiation Absorption: When in-depth absorption is ignored, all the energy is assumed to be deposited on the surface. This results in a more rapid rise in surface temperature and consequently in a greater rate of predicted upward flame spread. The objective of this task is to study the effect of in-depth radiation absorption on the surface temperature of a semitransparent material, using PMMA as an example. In the mathematical model, the medium is modeled as a one-dimensional slab, insulated at one end and subjected to external radiation at the other. To examine the effect of in-depth radiation absorption, the material is then considered to be either semitransparent or opaque. A 14-band model is employed to simulate the spectral distribution of absorption coefficient and reflectivity, which were determined using a standard Fourier Transform infrared (FTIR) spectrometer.

Figure 5 shows data and the 14-band model for the absorption coefficient of PMMA. The net effect on energy absorption depends on both the spectral distribution of incident radiation and the spectral properties of the absorbing medium. Therefore, a carefully selected multiband radiation model is needed to accurately account for the in-depth absorption. The spectral radiation properties of absorptivity and reflectivity property data are then used as an input to the mathematical model.

To verify the model, a series of experiments were carried out to determine the rise of surface temperature on two sets of PMMA samples, those with clear surface and those with soot-layer covered surface, at different values of external heat flux. As an example, comparisons for blackened samples are shown in Fig. 6 at 6.8 kW/m². The difference between the opaque and semitransparent cases represents the effect of in-depth radiation absorption. It is clearly seen that it takes longer for a semitransparent sample to reach a fixed temperature than the opaque sample.

Surface Reflectivity Measurements: A unique type of heated cavity reflectometer has been designed and is being built to measure the spectral hemispherical reflectance of burning samples. Such data will be useful in enhancing our understanding and predictive capability of the behavior of materials in strongly radiative environments in general, and in vertical flame spread studies in particular. The reflectometer consists of a cavity which can be heated to approximately 1100 deg. C. The sample is mounted on a water-cooled sample holder which may be rotated to provide a variation in the polar angle. Air for combustion, butane pilot for ignition, and nitrogen for extinguishing are provided by a burner rod which is inserted through the bottom face. The
fabrication of various components is nearing completion. The reflectometer will be used in conjunction with the FTIR spectrometer to obtain reflectance measurements.

Acknowledgements: The authors would like to gratefully acknowledge the overall guidance of Dr. Henri Mitler of NIST, the help of Dr. King-Mon Tu and Ken Steckler of NIST in identifying and providing some of the sample materials, and the numerous technical discussions with Prof. Thynell of Penn State.

Reports and Papers

1. Periodic Reports on the project, "Upward Flame Spread on Vertical Walls under External Radiation," sponsored by NIST under Grant No. USDC60NANNB8DO849.

Fig. 1: Flame Spread Under Various External Heat Fluxes; Igniter = 18 kW/m; No preheat

Fig. 2: Effect of Preheat on Flame Spread; Heat Flux = 5.4 kW/m²; Igniter = 18 kW/m

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Fig. 3: Effect of Igniter Strength on Flame Spread; Heat Flux = 5.4 kW/m²; No preheat

Fig. 4: Flame Spread on Various Materials; Heat Flux = 12.9 kW/m²; Igniter = 18 kW/m; No preheat

Fig. 5: Absorption Coefficient and 14 Band Model

Fig. 6: Effect of In-Depth Absorption on Surface Temperature Rise of Blackened Samples
WALL FIRE SPREAD

Professional Personnel

H.E. Mitler, Project Leader
K.D. Steckler, Physicist
J.G. Quintiere, Mech. Engineer
M. McClain, Programmer

Project Objective

To develop a method for predicting the rate and extent of fire spread on interior surfaces in a room using the fire properties of the materials involved. A general model including char-forming materials and composites burning on flat walls, and including burnthrough, will be completed and experimentally verified by the end of FY 92. It will be designed so that it can be readily incorporated into CFAST.

Scope

This project addresses the problem of fire growth on walls in enclosures, the kind of fire which most rapidly leads to flashover. The upward growth rate (especially in a corner) may be thought of as characteristic of the flammability of the burning wall material. Several aspects of wall fire growth will be considered, including lateral and upward growth and burnout on flat walls. The burning materials will be arbitrary: from simple, uniform, isotropic, subliming solids to heterogenous, nonisotropic, charring, melting, laminated, and composite materials. Lateral (creeping) spread will also be covered, as well as spread under a variety of external conditions.

Technical Approach

1. Devise algorithm for calculating upward spread of fires on walls
2. Find generic expression for heat feedback fluxes from flames to wall
3. Calculate temperature profile in wall as a function of height and time
4. Devise mass-loss algorithm, to find pyrolysis rate at each point, as a function of time
5. Generalize pyrolysis submodel to use input data from Cone calorimeter
6. Validate numerical implementation, at each stage of development
7. Generalize program to use external fluxes
8. Include lateral spread in a two-zone environment
9. Incorporate burnout front
10. Validate model, experimentally
11. Make program compatible with CFAST
12. Document computer program (SPREAD)
Technical Accomplishments

Done so far this fiscal year:

The article "Heat Fluxes from Flames to Vertical Surfaces" by J.G. Quintiere and T. Cleary for delivery at the 1992 ASME Winter Annual Meeting has been approved by WERB.

H.E. Mitler and G. Gallina are finishing the report "A Sensitivity Analysis of the Wall-Fire Program SPREAD," to be a NISTIR.

The program (SPREAD) has been restructured for insertion into CFAST:
   a. The nomenclature is now consistent with the approved list.
   b. Modularization and simplification of the program has been carried through.
   c. The data structures have been made consistent with the approved form.

A new expression for wall flame heights has been derived. It is

\[ x_f = (x_{fo}^4 + x_p^4)^{1/4} \]

where \( x_{fo} \) is the wall-flame height calculated for a line burner against a wall, and \( x_p \) is the pyrolysis height. When this replaced the usual expression in the program \( x_{fo} \), difficulties which we had validating SPREAD against the Japanese experiments disappeared, and the results are satisfactory.

A new scheme was devised for determining and handling the location of the lower burnout front. Some more work has been done towards the completion of the vitiated-air test apparatus.

Done to date:

The computer program SPREAD calculates the burning rate and upward spread rate of fires on flat walls, by calculating the wall temperature at a number of heights, and noting that the pyrolysis front reaches a point when the temperature there reaches \( T_{ig} \). This is done numerically, rather than analytically. It also includes the simultaneous lateral spread of the burning zone. This is calculated using the expression

\[ v_s = \frac{\Phi}{k \rho c (T_{ig} - T_s)^2} \]

for the lateral spread rate, where \( T_s \) is the instantaneous wall temperature. In a two-zone room fire model, therefore, the spread rate in the upper region will generally be greater than in the lower region.

The model has been validated against full-scale experiments carried out by K. Steckler on PMMA and on wood; see Figs.1 and 2. It has also been validated against experiments carried out by Y. Hasemi, at the BRI (Japan). Those involve external irradiation of the wood samples; see Fig.3.

As part of the overall calculation, the pyrolysis rate of an arbitrary material subjected to an arbitrary heating-flux history is calculated. The method depends on measuring the heat of gasification as a function of time, in the Cone Calorimeter, then making an appropriate transformation.
Reports and Publications

Steckler, K.D., and Mitler, H.E., "Experimental Study of the Pyrolysis Rate of a PMMA Wall Panel in a Reduced-Scale Enclosure," Combustion Institute/Eastern States Section; Chemical and Physical Processes in Combustion; Technical Meeting, Clearwater Beach, Fla., 73/1-4 pp., Dec. 1988


Mitler, H.E. (1990) "Predicting the spread rates of fires on vertical surfaces," 23d (International) Symposium on Combustion; The Combustion Institute, Pittsburgh, PA, p.1715


Related Grants

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


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

UPWARD FLAMESPREAD
PMMA

Q_{ext}=0. kW
Q_{b'}=25.6 kW/m

Experimental
peak
average
calculated

TIME [s]
UPWARD FLAMESSPREAD

UC Particle Board

\[ Q_{\text{ext}} = 0 \text{ kW/m}^{2} \]
\[ Q_{b'} = 25.6 \text{ kW/m} \]

\[ X_f - 1/2 \text{ power} \]

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Figure 8 Summary of the Experiment No.17(Particleboard, \( q, 5 \text{ kW/m}^{2} \))
C. Advanced Sensing and Suppression

C1. Fire Detection
ADVANCED FIRE DETECTION SYSTEMS

Professional Personnel

William Grosshandler, Project Leader
Richard L. Smith
Marc Nyden
Richard Harris, Jr.
Margaret Jackson

Project Objective

To demonstrate principles for the response of detection systems to the stimuli of early fire events while discriminating against false signals

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.

The general approach in this research is to increase the amount of information upon which a decision is to be made, and to do this in the minimum amount of time. Advances in the sensing of temperature, species concentrations, particulate matter, and acoustic and electromagnetic radiation have been surveyed to determine their applicability to fire detection. Of particular interest are optical and solid-state sensors for CO, infrared sensing of hydrocarbons and acid gases, fiber-optic integrated sensors, micrometer-size sensors, and sub-acoustic and super-acoustic sensors. Software is to be developed to recognize unique acoustic and electromagnetic signatures of various fire events.

Technical Accomplishments

1. Assessment of Advanced Fire Detection Technologies - The majority of fires are sensed either by the heat or the smoke they produce at a set location in space, with an alarm signal being issued when a threshold temperature or particulate level is exceeded. Many of these sensors are inexpensive and perfectly suitable for certain applications, but issues such as false alarms and increased performance can necessitate alternative sensing techniques. Advances in sensor technology, in microelectronics, and in our understanding of ignition and flame spread provide an opportunity to greatly enhance the performance
of fire detection systems in traditional applications. Technological advances have also led to new situations with unique protection requirements at a time when environmental considerations have eliminated our most effective suppressants (halons), making the early detection of a fire even more critical. A review describing some of these developments has been completed (Grosshandler, 1992), suggesting possible applications and indicating limitations to the technologies which need to be overcome before exploitation is feasible.

Detection systems identified as having high potential for improved protection of residential, commercial or specialized high risk spaces, but in need or research, include the following:

- discriminating smoke/CO detectors, including point and integrated sensors
- remote FTIR fire detection, with research into detectability limits in mixtures of pyrolysis gases, spectrum analysis in non-isothermal environments with concentration gradients, and instrument development for field installation required
- wide-band optical and audio detection systems, including visible/IR fire signatures and acoustic signatures of fires
- laser and fiber optic detection systems, including thermal sensors, gas sensors, and laser-based particle sensors

2. Remote FTIR Fire Detection - The portable open-path FTIR (OP-FTIR) spectrometer is a recent innovation which offers distinct advantages over conventional fire and emission measurement techniques. Portability is an asset which will allow researchers to make on-site measurements of both industrial emissions and uncontrolled fires. Furthermore, in situ measurements of the atmosphere of interest can be made directly and in real time, circumventing problems of extractive sampling. The limits of detection decrease in direct proportion to the path length over which the spectrum is collected, with the result that extended path lengths using multiple passes can produce high sensitivity. The ability to operate the spectrometer in the passive and active modes can be exploited to measure both the infrared radiation emitted from a fire and the IR absorption in cooler atmospheres surrounding the fire.

A deficiency of many existing fire detectors is that they are based on point sampling, often from a location remote from the fire. Since an IR spectrum from 4 to 12 μm can be measured with 1 cm⁻¹ resolution in about 2 seconds, an OP-FTIR fire detector could locate a variety of combustion gases anywhere along its line of sight within seconds of their production, and could scan a large warehouse or outdoor storage facility in less than a minute. Research is required to analyze spectral features of these data and to interpret, unambiguously, those characteristic of an early fire event. The limits on sensitivity, spatial resolution, and smoke interference need to be determined so that the technique can be to early warning fire detection.

3. Acoustic Emission Detection System - An experimental study (Grosshandler and Jackson, 1992) has been initiated to assess the viability of using the acoustic signal emitted by a variety of structural materials exposed to nonuniform heating as an early indicator of a fire. Beams of aluminum, gypsum, plywood, poly-methylmethacrylate and poly-vinylchloride, simply supported across a 0.5 m span, were subjected to a 0.9 kW open flame. Piezoelectric sensors were mounted directly on the beams, 0.3 m from the center of the flame, to record high frequency acoustic emissions (AE). The samples varied between 3 and 18 mm in thickness and the heat flux was maintained approximately constant over a circular area about 50 mm in diameter. The time of exposure to the flame was adjusted between one and six minutes, depending on the temperature rise in the material, to prevent the AE sensors from overheating. For the gypsum board the maximum temperature increase above the ambient was 0.8 °C at the location of the AE sensors.
The measured signals varied in power and in number with the material and thickness of the specimen. The acoustic emission from a bulk material is associated with an abrupt change in stress following a microscopic dislocation. The stress relief generates an elastic wave which radiates throughout the material at the speed of sound. The thermal energy released by the flame impinging on the beam, plus the combustion of the material itself, creates a temperature gradient, and leads to thermal stresses in the material. The strength of the acoustic source depends upon the suddenness with which the stress is relieved and the number of AE events increases with the number of defects or discontinuities in the material; hence, a composite material is likely to be more active than a pure substance.

The number of AE events in a minute and the accumulated energy release during the heating cycle provide a good measure of the overheated state of some structural materials. The 12 mm thick plywood was particularly susceptible to acoustic emission, with about 43 events/minute being recorded in one test. The gypsum board produced 16 events/minute and the 12 mm aluminum just 0.5 events/minute. The thinnest aluminum plate did not respond above the background level (0.3 events/minute) even though it reached the highest temperature. The differences in cumulative energy associated with the AE event were equally striking, with one test of the plywood producing four times more energy than the gypsum board even though the heating period for the wood was half as long. One conclusion of the study is that the use of AE transducers as early sensors of hidden structural fires remains a viable concept. However, critical issues remain to be investigated if this technique is to be practical for fire detection; eg., false signal discrimination must be verified, the maximum practical area covered per sensor must be determined, and durability and reliability must be examined.

4. Low False Alarm Rate Residential Fire Detection - New approaches to low false alarm rate fire detection with specific application to residences are also being contemplated. The objective would be to provide the proof of concept for a detector system that will reduce the incidence of false alarms to no more than twice the incidence of a real fire. The targeted universe would be a three room suite as represented in the Bldg. 205 test facility. Ignition events which would be considered include a smoldering cigarette on a bed, a grease fire on the kitchen stove, and an electrical space heater malfunction. Discrimination between an unwanted ignition/fire and the interference caused by a person smoking a cigarette, steam generated during cooking, blowing dust, and frying food would be sought. Sensors would be chosen from commercially available smoke, CO, thermal and acoustic detectors. The system would consist of an array of detectors in the three rooms and a central processor to analyze the information and determine the appropriate response. Three levels of warning would be planned; eg., that there is a reasonable probability of a fire in the kitchen; that there is a high probability of a fire in the bedroom; or that there is definitely a fire in the family room: call the fire department!

Reports and Publications


C2. Fire Suppression
AGENT SCREENING FOR HALON 1301 AVIATION REPLACEMENT

Funding Agency: U.S. Air Force, Wright Laboratory

Professional Staff: William Grosshandler (Project Leader), Richard Gann, Anthony Hamins, Greg Linteris, Marc Nyden, William Pitts, John Yang, Michael Zachariah

Project Objective: Establish a comprehensive experimental program to screen eleven specified gaseous agents, sodium bicarbonate powder, and other promising chemicals as a means to identify (by 9/30/93) the best three candidates for a subsequent full-scale aircraft fire extinguishment evaluation program.

Technical Approach: A search is underway for chemicals to replace halon fire extinguishing agents which have both a low ozone depletion potential and a high fire suppression efficiency. The federal government uses halon 1301 in a multitude of aircraft applications, including engine nacelle and dry bay protection, with little understanding of phenomena which control extinguishment in these situations. The effectiveness of a fire suppression agent is related to its thermodynamic properties, its behavior during two-phase flow, its interaction with flame chemistry, the timing of its release and the nature of the fire. A series of carefully designed experiments is being conducted to examine each of these factors, singly and in combination. Theoretical models will be used to interpret the results, to increase our understanding of the suppression process, and to predict behavior over an expanded range of operating conditions. In particular, control of those phenomena which dominate the actual suppression process is sought, be they the chemical reactivity of the agent, the thermal quench or dilution provided by the agent, or the properties associated with the physical mixing of the agent into the fire.

There are five separate tasks to be accomplished:

- determination of the thermal properties and dynamics of the agents as they exit the containment vessel
- agent dispersion and fluid mechanics outside the vessel
- flame extinction measurements using a cup burner, an opposed flow diffusion flame burner, a turbulent jet diffusion flame, and a detonation tube
- understanding flame/agent chemistry
- identification of additional agents

A pressure vessel with a rupture disc will be used to discharge the agent (initially at 4 MPa) into the atmosphere. Nine pure fluorocarbons, two mono-chlorinated fluorocarbons, a fluorocarbon azeotrope, and sodium bicarbonate powder are to be tested mixed with nitrogen or CHF₃. The exiting spray will be illuminated by a laser sheet and recorded with high speed cinematography. Schlieren photography, Mie scattering from the droplets, and quantitative Rayleigh scattering in the gaseous plume will also be used to determine the penetration of the agent. Chemical kinetic modeling and the results of diffusion flame measurements will determine whether the dominant mechanism of suppression is chemical or physical.
BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
GRANTEE PROJECT - FY 92

Institution: Michigan State University
Grant Number: 60NANB8D0861
Title: Evaluation of Fire Suppression Effectiveness
Principal Investigators: Dr. Arvind Atreya
Department of Mechanical Engineering
Michigan State University, East Lansing, MI 48824
Other Professional Personnel: Todd Crompton (M. S. candidate) & Dr. Sanjay Agrawal
NIST Scientific Officer: Dr. David D. Evans

TECHNICAL ABSTRACT:

INTRODUCTION:
Literature on 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. The current knowledge of suppression mechanisms of halons is also insufficient to provide a clear understanding of the important chemical mechanisms. Most importantly, there does not exist a scientific basis for comparing the suppression effectiveness of physical and chemical suppression agents. This prevents development of new, perhaps more efficient, suppression agents and application strategies.

Thus, as a first step, it is necessary to develop an experimental and theoretical framework that will: (i) provide a quantitative understanding of the mechanisms (chemical and/or physical) responsible for extinguishment, (ii) enable determination of the suppression rate, time to extinguishment and agent application strategies, (iii) enable evaluation of suppression effectiveness which is needed for rational comparison of various suppression agents. The present work addresses this research problem through well-controlled small-scale laminar stagnation-point flow and counterflow diffusion flame experiments and modeling. This configuration is chosen because the results can be easily extrapolated to larger scale via mathematical models.

SUPPRESSION EXPERIMENTS:

For quantitative measurements, two unique experimental facilities have been constructed. These are: (i) Stagnation-point flow apparatus: which allows studying both the gas-phase and the condensed-phase suppression actions and enables transient chemical measurements in the exhaust gas. These
measurements are being used to study the suppression mechanisms and quantify the suppression effectiveness. (ii) **Counterflow diffusion flame apparatus**: which allows detailed flame structure measurements but is limited to gas-phase suppression agents. Initially, the work is being done using the stagnation-point flow apparatus with water as the extinguishing agent.

The stagnation-point flow apparatus and the associated equipment developed for suppression studies are schematically shown in Figure 1 and the details of the suppression apparatus are shown in Figure 2. This apparatus consists of a cylindrical 1200 °C furnace (approximately 15" tall) with a center ceramic tube for gas supply/exhaust. This ceramic tube supports a ceramic honeycomb heat exchanger and a ceramic honeycomb flow straightener (not shown in Figure 2). This furnace is used to supply external radiation on the sample surface and is supported by a specially designed ceramic flange which is supported by a stainless-steel cylinder that hangs from a 16" dia. water-cooled aluminum plate. A 10" diameter quartz tube that can slide over the stainless-steel casing is used as an observation window. This glass tube sits on a soft silicone foam rubber support to prevent gas leakage. A 1.5" dia. PMMA sample is fed into the flame by a motor-driven mechanism. It is surrounded by ceramic insulation to ensure one-dimensional heat conduction. The entire bottom sample assembly is also supported by a 12" dia. water-cooled aluminum plate. A water-cooled droplet injection tube that can swing in and out of the hot burn zone is used to release water droplets on the sample surface (this tube can be seen in Fig. 2).

In addition to suppression by water droplets (representative results described below), the stagnation-point flow and counterflow experiments are designed to be used for studying and consistently quantifying the suppression rate (defined by the attenuation in the energy release rate and measured by the exhaust gas composition) as a result of: (i) changes in the gas-phase composition due to addition of diluents (CO\textsubscript{2}, H\textsubscript{2}O or N\textsubscript{2}) or halons and their effect on the flame structure, and (ii) increase in the strain rate. Later, heterogeneous surface reactions such as glowing char combustion will also be studied in the same configuration. In the counterflow experiments, flame structure measurements across the diffusion flame in conjunction with an appropriate models will be used to determine the chemical heat release rate and species production and destruction rates.

**Experimental Results on Suppression by Water:**

Typical experimental results of the overall species composition measurements made in the exhaust duct of the stagnation-point flow apparatus during suppression by water are shown in Figures 3 & 4. These results reveal a very interesting effect of water application. Figure 3 shows the CO\textsubscript{2} production rate and the O\textsubscript{2} consumption rate. Clearly, an increase in the CO\textsubscript{2} production rate and the O\textsubscript{2} depletion rate correspond to an increase in the burning rate and vice versa. Figure 3 shows that when small amounts of water was applied (< .2ml), the burning rate was not significantly affected (or the small transient response could not be measured because a change in CO and total hydrocarbon concentrations was noted; see Fig. 4). As the amount of water applied is increased (see small arrows on the time-axis of Figures 3, 4), the burning rate first substantially increases and it then decreases. For droplets < .3ml, the subsequent decrease was negligible. The increase in the burning rate was substantial and unexpected because it implies that instead of suppressing the flame we have enhanced it by applying water droplets. This increase is also consistent with a decrease in CO and total hydrocarbon concentrations and visibly corresponds to the disappearance of soot. Thus, as a result of water evaporation CO, total hydrocarbons and soot are oxidized to CO\textsubscript{2}, depleting O\textsubscript{2} in the process. This chemical hypothesis is supported by the fact that a non-sooty flame containing little CO, soot & unburned hydrocarbons does not show a similar increase in the burning rate due to water application. It seems that there are two simultaneous effects as a result of water application: (i) **chemical enhancement** of the burning rate (which is important only when the flames are sooty; Note: most fires are sooty), and (ii) **physical cooling** of the solid via water evaporation. This work is continuing and more quantitative results will soon be available.
FIG. 3: CARBON DIOXIDE AND OXYGEN DEPLETION MEASUREMENTS DURING SUPPRESSION BY VARIOUS AMOUNTS OF WATER

Note: For small amounts of water the effect was not noticeable. As the quantity of H₂O increased, first the burning rate increased and then it decreased.

FIG. 4: TOTAL HYDROCARBONS AND CARBON MONOXIDE MEASUREMENTS DURING SUPPRESSION BY VARIOUS AMOUNTS OF WATER

Note that both CO and HC decrease upon water application.
EVALUATION OF THE EFFECT OF RECESSED SPRINKLER INSTALLATION ON SPRINKLER ACTIVATION TIME

Funding Agency: U.S. General Services Administration

Professional Staff: Daniel Madrzykowski, Project Leader

Project Objective:
To develop factors, which modify the RTI to account for the effect of recessed sprinkler installation, for input into sprinkler activation models.

Technical Accomplishments:
Sprinkler activation models are being used by engineers in their design/evaluation of fire protection systems. These models have evolved from direct application of single step engineering correlations to models considering the secondary effects of; heat loss to the ceiling, plume flow through two layers, and the standoff distance of the sprinkler link below the ceiling. All of these models assume the sprinkler link is fully exposed to the hot gas flow across the ceiling.

In an effort to make the ceilings in sprinklered buildings more aesthetically pleasing, sprinklers have been recessed into the ceiling or recessed and covered with decorative temperature activated plates. Currently, the models do not account for the effects of recessing or covering the sprinklers.

One of the critical input parameters to the sprinkler activation models is the response time index (RTI) of the sprinkler. The test used to measure the RTI does not consider the effects of the recessed installation on the RTI. Large scale fire experiments are being conducted by the Building and Fire Research Laboratory (BFRL) to evaluate the effect recessing the sprinkler has on the sprinkler activation time. Results from the large scale experiments will be compared to RTI values obtained in the BFRL plunge test apparatus with similar sprinklers. Factors will be developed as required to modify the measured RTI for the effects of recessed sprinkler installations. Modified RTI's will be used with the GSA Engineering Fire Assessment System to predict sprinkler activation times which will be compared with activation times measured in large scale experiments.

Reports and Publications:

New Project

Related Grants:

None
EVALUATION OF THE USE OF THE GSA ENGINEERING FIRE ASSESSMENT SYSTEM FOR PREDICTING THE RESPONSE OF SPRINKLERS AND DETECTORS IN LARGE SPACES

Funding Agency: U.S. General Services Administration

Professional Staff: Kathy A. Notarianni, Project Leader
Daniel Madrzykowski, Mechanical Engineer

Project Objective:

To verify and provide recommendations for the use of the GSA Engineering Fire Assessment System for predicting the response of sprinklers and detectors in large spaces.

Technical Accomplishments:

Fire sprinkler and thermal detector activation predictions are an integral and important aspect of the GSA Engineering Fire Assessment System. Large spaces represent some of the most difficult fire protection challenges. While there has been a substantial effort to verify the use of activation predictions in small and medium size rooms, virtually no verification experiments have been conducted for large spaces.

Conducting verification experiments for large spaces is difficult due to the availability of adequate facilities for live fire experiments. The largest fire test facility in the United States is limited to a ceiling height of 18.2 m. The Building and Fire Research Laboratory has completed measurements during live fire tests conducted in an aircraft hanger with a ceiling height of 30.4 m. Fire gas temperatures and disk temperatures were measured above the fire and along the ceiling in locations corresponding to the expected location of sprinklers or detectors.

The results of the fire experiments were compared to the predictions from the two computer models, FPETOOL and LAVENT, in order to determine the limits of applicability of the models and to develop recommendations for use in large spaces. Both computer fire models underpredicted the ceiling jet temperatures measured in these tests, and thus would be conservative in their activation predictions. For high ceiling heights, future versions of these models should include hot gas transport time and fire plume dynamics which were shown to be key for modeling of large spaces.

Reports and Publications:

New project

Related Grants:

None
Technical Abstract:

Introduction. The phenomena associated with extinguishment of a solid fuel fire are investigated experimentally. In particular, the evaporative cooling of a hot non metallic surface subjected to the impingement of a random array of droplets is quantified. The relevance of this study to the extinguishment process is two-fold: a) it describes the cooling of the surfaces exposed to fire and b) it quantifies the vapor generation in the fire environment.

Experimental Results. The experimental results reported here refer to a simplified situation with respect to the actual water-fire-solid interaction process to provide a controlled, repeatable and quantifiable set of data which will be used to validate the multi-droplet model which was obtained earlier [1,2,3].

The fire environment is simulated by three, radiant panels mounted above the surface of a macor square tile (0.1524 x 0.1524 x 0.0254 m). The panels are capable of temperatures in excess of 800 °C and can be approximate to black bodies. Two panels are conical in shape with an external diameter of about 0.2 meters. These two panels are positioned above the macor tile, on two opposite sides of the tile with their axis at 30° from vertical and facing the tile surface and each other. The third panel is conical in shape with an external diameter of 0.3 meters. This panel is mounted horizontally just above the tile. The three
panels are identical in electrical load and are fed by a three phase power supply which is controlled on a temperature feedback and are held at a constant temperature set point.

The tile is pasted onto a chilled plate which is kept at near ambient temperature by chilled water flow. The radiant boundary condition as well as the thermal condition at the lower surface of the tile are designed to obtain a linear temperature profile in the tile depth and to insure that the tile exposed surface is isothermal over the spray impingement region, prior to the initiation of the transient.

The droplet distribution used in the experiment is random. However, all droplets are identical (their volume is approximately 10 \( \mu l \)) and the spray impingement region has a constant diameter of 0.06 meters. The water mass flux is controlled by changing the droplet generation frequency. The droplet dispenser is constituted of a cavity which gradually tapers to a small opening at the bottom where a needle pointing downward is attached. The cavity is bounded at its top by a plastic disk which is pulsated downward by an electromagnetically activated plunger at the desired frequency. The dispenser is suspended from four parallel vertical wires and is moving above the deposition region under the action of three pulsating bumpers which are moving toward each other symmetrically. To insure continuous motion of the dispenser, a periodic displacement of one of the four suspending wires is provided by a rotating device. Figure 1 shows a typical droplet distribution as recorded by a camera looking at the dispenser from above. Typical droplet frequencies are of the order 0.1 to 0.8 Hertz. This range of values is adequate to induce surface flooding at high frequencies while achieving steady state conditions for low and intermediate values.

The water used in the experiment is de-ionized and de-gassed. In order to obtain a constant feed of water, a mineral oil sealed reservoir and head control tank has been used. This system allows control of the fluid head above the distributor within 0.01 m and at the same time it keeps any gasses from diffusing back into the water. Experiments with de-ionized water are also being conducted to assess the effect of gasses coming out of solution during the evaporative process. Additional consideration will be given to the effect of impact momentum on the droplet shape on the surface, which greatly affects the evaporation rate. To this effect, a modified version of the single droplet model is currently being derived. This code is based on the heat transfer unidimensionality in the liquid layer which was observed previously [6].

The macor tile transient surface temperature distribution is recorded with an infrared camera. The infrared image is correlated to a temperature distribution (see [4,5]). The 256 shades of gray are related to a temperature scale of about 120 °C. The scale is set by simultaneously measuring the temperature of a given surface point with a thermocouple probe and via the infrared camera reading. The spacial resolution is of about 0.0001 m/pixel and the temperature resolution is of 2 °C/gray-shade which yields an accuracy of about ± 1 °C. The transient temperature distribution is recorded on a VCR and selected frames during the transient are grabbed by a PC to be analyzed. The camera has a field of view of a circular area with a diameter of about 0.06 meters. This area is viewed through a black-painted chilled pipe which eliminates stray radiation from other sources than the macor surface in direct view. Figure 2 shows a typical snap-shot of the temperature
distribution of the sprayed surface. In order to condense the information available, the averaged transient temperature is calculated for selected frames (e.g. Fig. 2) during the evaporative transient. A detailed description of the components of the experimental set-up will be provided along with a sample data record of the phenomena to illustrate the data processing. The surface averaged transient temperature for various conditions is presented in Fig. 3. The oscillatory nature of the average surface temperature is due to the selection of a small portion of the surface sprayed. Depending upon the number of evaporating droplets present in this portion of the solid surface at any instant of time, the temperature fluctuates above or below the overall surface average. It is evident that for times greater than 800 seconds, a steady state conditions has been reached with an average surface temperature of 108 °C.

**Analytical Results.** Two major analytical tasks are under way. The first deals with the formulation of the model for the prediction of the thermal behavior of a single droplet evaporating under radiant heat input. This model has been completed and a manuscript, which describes the various findings, is currently in preparation. The second task is ongoing and concerns the simplification and generalization of the single droplet model to include the effects of impact momentum and of more complex droplet configurations on the solid surface (i.e. effect of dissolved gasses, boiling, etc.).

**Acknowledgement.** The authors are indebted to Dr. H. Baum (BFRL-NIST) for his guidance in the development of the single and multi-droplet codes.

**Reports and Papers.**


FIGURE 1 - Droplet distribution obtained over 180 seconds at a frequency of about one droplet per second over a circular surface with 0.05 meters of diameter.

FIGURE 2 - Typical instantaneous macor surface temperature distribution obtained after 60 seconds with a water mass flux of 0.0015 kg/m².s with an initial solid surface temperature of 140 °C and droplets of 11 μ-liters.

FIGURE 3 - Transient average solid surface temperature with an initial solid surface temperature of 151 °C, a mass flux of 0.0010 kg/m².s and droplet deposition frequency of 0.33 Hertz.
Part 2. Alphabetical Listing of BFRL Fire Research Grantees and Their Grants
## Alphabetical Listing of BFRL Fire Research Grantees and Their Grants

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This report describes the research projects performed in the Building and Fire Research Laboratory (BFR) Fire Research Program and under its grants program from October 1, 1991 through September 30, 1992.