NISTIR 4440

Summaries of

CENTER FOR FIRE RESEARCH

In-House Projects and Grants - 1990

Sonya M. Cherry, Editor
U.S. DEPARTMENT OF COMMERCE
National Institute of Standards and Technology
National Engineering Laboratory
Center for Fire Research
Gaithersburg, Maryland

United States Department of Commerce
National Institute of Standards and Technology

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SUMMARIES OF CENTER FOR FIRE RESEARCH IN-HOUSE PROJECTS AND GRANTS - 1990

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October 1990

U.S. DEPARTMENT OF COMMERCE, Robert A. Mosbacher, Secretary
National Institute of Standards and Technology, John W. Lyons, Director

PREFACE

This report describes the research projects performed in the Center for Fire Research (CFR) and under its grants program during FY 1990.

The Center is nationally recognized as the focal point for fire with an extremely competent multi-disciplinary technical staff that is supported by an excellent fire library and extensive laboratory facilities.

The Center was created by the Federal Fire Prevention and Control Act of 1974 which authorized the Secretary of Commerce, through the Center, to conduct a fire research program directly or through contracts or grants. Therefore, in addition to its in-house program, the Center maintains a fire research grants program that supplements most of the in-house programs and supports most of the academic fire research in the country. The Center, as a component of the National Institute of Standards and Technology (formerly the National Bureau of Standards), responds to the needs of other Federal agencies and private sector organizations. This report covers work performed with funds appropriated to the Center and work performed under contract to other agencies.

The goal of the Center's program is to provide the technical basis for the reduction of losses and costs of fire. The program is designed to meet the fire safety needs of the public, the fire services, and the manufacturing industry by upgrading the knowledge of fire and of the measurement and prediction of the performance of products in fires. The program is comprised of three elements:

- Basic research leading to the development of tools for "engineered fire safety; i.e., fire protection technologies and fire prediction methods as demonstrated in CFR fire models as: FIREFORM AND HAZARD.

- Timely response to current fire problems; for example, smoke toxicity, hazards of upholstered furniture, burning oil spills, and investigations support.

- Serves as a focal point for fire research in the nation by incorporating in its program academic and foreign Guest Researchers, collaborating and cooperating with work in fire research, working with academia on the development of fire related training programs, participating in standards and codes, operating a fire research information service and a Computer Bulletin Board, as well as organizing the National Fire Research Strategy Conference and other meetings.

The majority of our in-house priority projects and grants work fits into the first category, basic research and tools for engineered fire safety, and is
presented in Part I of this report. Our work for other agencies fits in the second, timely response to current fire problems, and is presented in Part II. Activities under the third element are diverse and are not included in this report.

Part I is organized to reflect the way in which the grants augment and support the in-house program. Many of the grants relate to different parts of the in-house programs, so each grant report is

presented immediately following its related in-house priority project. The projects are arranged in 12 groups:

Turbulent Combustion
Soot Formation
CO Prediction
Polymer Gasification
Flame Spread
Toxic Potency
Furniture Flammability
Building Fire Modeling and Smoke Transport
Fire Hazard Assessment
Engineering Analysis System and Fire Reconstruction
Suppression
Cone Calorimeter Development

The projects for other agencies, presented in Part II, although usually related to internally funded projects, are primarily designed to meet the missions of those agencies and organizations. The distribution of subjects prevents them from being classified in the same way as those in Part I so they have been organized into two groups:

Fire/Materials Interaction
Fire Protection Technology

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

TABLE OF CONTENTS

PART I. Basic Research and Tools for "Engineered" Fire Safety
(in-house projects and associated grants funded at NIST)

A. TURBULENT COMBUSTION

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

TURBULENT COMBUSTION SIMULATION

Staff

Howard R. Baum, NIST Fellow, Project Leader
Ronald G. Rehm, NIST Fellow
Daniel M. Corley, Physicist
James S. Sims, Physicist
Hai C. Tang, Computer Specialist

Project Objectives

Develop a fundamental understanding of the mechanisms which control gas phase combustion processes in fires and predictive capability which will allow the evolution of these processes to be calculated from basic principles.

Scope

A theoretical and computational approach to the study of the transport, mixing, diffusion, and reaction processes in an enclosure fire context. Each process is considered in detail at the appropriate level of description. Since these phenomena occur at widely different length and time scales, a large part of this effort is devoted to providing a set of overlapping analyses in frames of reference which permit the phenomena to be coupled together.

Support

Item 2 below was supported in part by the Department of Interior and item 3 was partially supported by the Air Force Office of Scientific Research.

Technical Accomplishments

1. Enclosure Fire Flows

The large eddy enclosure fire flow simulation capability has been extended in several directions. The existing three dimensional inviscid flow model now permits the direction of gravity to be oriented arbitrarily, permitting fire driven flows in inclined rooms and corridors to be studied. In addition, a new two dimensional high resolution Navier Stokes code with the same capability has been developed. The new code, used in conjunction with the Convex C120 mini-supercomputer, permits simulations with virtually all hydrodynamically relevant length scales resolved for floors at Reynolds numbers approach 10^5. Boundary conditions permitted include no slip or free slip for the velocity field, and cold or thermally insulated boundaries.

These codes have been applied to study the effects of this inclination on gravity currents in corridors generated by fires. This "trench effect" was a central issue in the disastrous Kings Cross underground fire in London in

1987. Figures (1) and (2) show individual frames from three dimensional and two dimensional simulations respectively. The figure captions give some idea of the resolution achievable with present computational fluid mechanics techniques.

2. Large Fire Studies

A vortex dynamics simulation of the wind blown smoke plume has been developed in collaboration with Professor A. Ghoniem of MIT. In its current state, it describes the descent of a cool particulate plume and its dispersal over a ground plane. Future work will include the systematic addition of the interaction of positive thermal and negative smoke buoyancy, stratification, combustion, and wind shear. Density contours thru the cross-section of the descending particle plume at several down-wind stations are shown in figure 3.

3. Eddy Scale Combustion

The concept of the Pseudo-Mixture fraction, an entity developed as part of the study of small scale combustion processes in fires, has been rederived in a very general context in collaboration with Professor J. Gore of the University of Maryland. In its new, more general form, it can be used in the two-dimensional Navier-Stokes simulation model after suitable modifications to that code.

Reports and Publications

Evans, D. D., Mulholland, G. W., Gross, D., Baum, H. R., and Walton, D., "Burning, Smoke Production and Smoke Dispersion from Oil Spill Combustion", NISTIR 89-4091, (Oct. 1989).

Rehm, R. G., Baum, H. R., Lozier, D. W., and Aaronson, J. J., "Diffusion-Controlled Reaction in a Vortex Field", Combustion Science and Technology, 66, p.293, (1989).

Evans, D., Walton, W., Baum, H. R., Lawson, R., Rehm, R., Harris, R., and Ghoniem, A., "Measurement of Large Scale Oil Spill Burns" Proceedings of the Thirteenth Arctic and Marine Oil Spill Technical Seminar, Canada, Cat. No. En 40-11/5-1990, p.1, (1990).

Related Grants

1. "Radiation Modeling of Laminar Diffusion Flames", J. de Ris, Factory Mutual Research Corporation.

2. "Radiation from Turbulent-Luminous Fires", G.M. Faeth, U. of Michigan.

3. "Structure and Radiation Properties of Pool Fires", J. Gore, U. of Maryland.

4. "Fire Propagation in Concurrent Flows", A.C. Fernandez-Pello, University of California at Berkeley.

5. "Fire Modeling", P. Pagni, University of California at Berkeley.

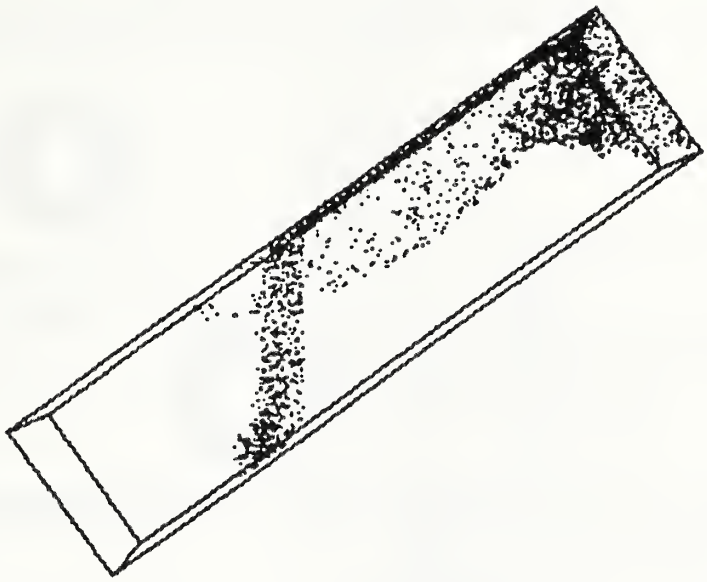

Figure 1 A three-dimensional flow computation in a 35-degree inclined corridor four times as long as high and wide using a grid $144 \times 36 \times 36$. Heat source is centered in the corridor one dimensionless unit from the end along the floor. The dimensionless time shown is 4.25 units. The model is based on the Euler equations.

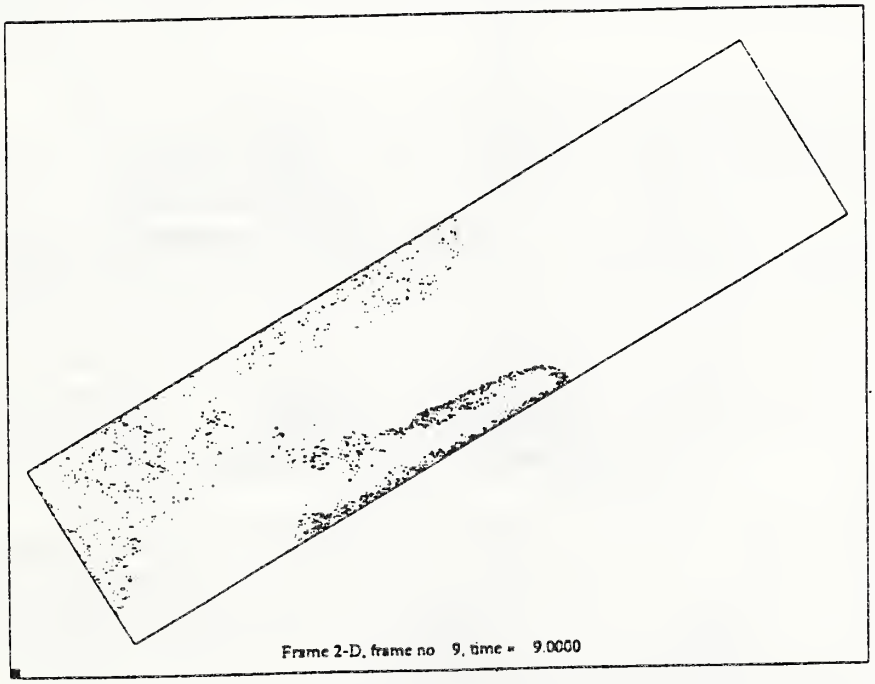

Figure 2 A two-dimensional flow computation in a 35-degree inclined corridor four times as long as high, using a high-resolution grid of 1024×256. The heat source is one dimensionless unit from the lower end wall, and the dimensionless time is 9. The computation is performed for a Reynolds number of $5x10^4$.

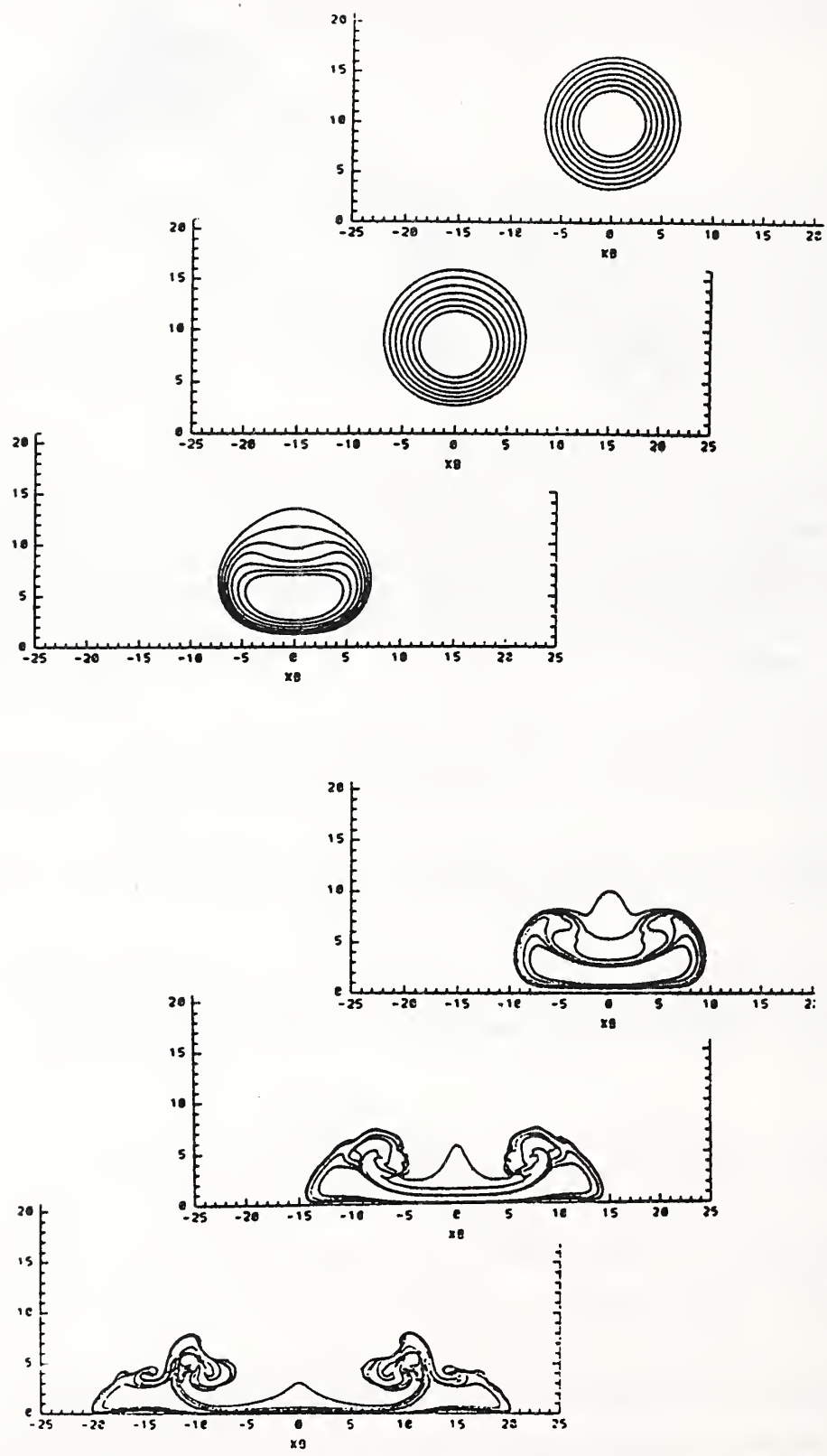

Figure 3. Density Contours Through Cross-Section of Vortex Simulation of Descending Particle Plume

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: The University of Michigan

Grant No.: 60NANB8D0833

Grant Title: Radiation from Turbulent Luminous Flames

Principal Investigator: Professor G.M. Faeth
Department of Aerospace Engineering
218 Aerospace Engineering Building
The University of Michigan
Ann Arbor, MI 48109-2140

Other Professional Personnel: M.A. Kounalakis, Doctoral Student
O.V. Koylu, Doctor Student
Y.R. Sivathanu, Doctoral Student

NIST Scientific Officer: Dr. Howard R. Baum

Technical Abstract:

Introduction. This investigation is considering two aspects of unwanted fires: (1) the relationship between CO and soot emissions, and (2) the effects of turbulence/radiation interactions. The findings have application to modeling fires in structures, developing materials test codes, and developing fire detectors. Progress on both phases is briefly discussed in the following; additional details can be found in the reports and papers listed at the end of this report.

CO and Soot Emissions. Carbon monoxide and soot represent major hazards of fire environments: inhalation of carbon monoxide is a significant cause of fatalities in fires while the presence of soot obscures fire fighting efforts and increases flame spread and combustion rates by increasing flame radiation. Additionally, CO and soot oxidation processes have similarities that suggest a relationship between the two emissions — yielding a synergism of fire hazards that has important implications concerning materials properties for improved fire safety as well as a better understanding of the phenomena responsible for these emissions. Thus, the objective of the present investigation is to study the emission of carbon monoxide from overventilated buoyant turbulent diffusion flames, and to examine whether there is a relationship between CO and soot emissions. This involved experiments with hydrocarbon/air flames whose soot properties had been studied earlier, to allow comparison with present CO emission measurements.

The experiments involved three burners, having diameters of 5, 50 and 234 mm, operating over conditions ranging from buoyant jet flames to soot-like fires. The fuel-lean far-overfire region of the flames was sampled and analyzed, using NDIR to find CO concentrations and gas chromotography to find mixture fractions. The fuels were all gases — acetylene, propylene, ethylene, propane and methane — burning in still air.

It was found that variations in CO concentrations in the overfire region for any given flame were consistent with passive mixing and with CO concentrations and mixture fractions being relatively constant when chemical reactions are quenched near the flame sheet The last observation is surprising, since it is expected that regions of CO emission

near the base of the flame sheet would have shorter residence times, and thus different outcomes of finite rate CO chemistry, than regions near the tips of turbulent flames. Nevertheless, similar behavior was found for soot, so this behavior seems plausible due to the somewhat related oxidation processes of CO and soot. As a result, it was possible to find CO generation factors (the mass of CO emitted per unit mass of fuel carbon burned) that were relatively uniform for given flames, analagous to the behavior of soot generation factors found earlier.

Figure 1 is an illustration of CO generation factors plotted as a function of characteristic flame residence time normalized by the smoke point residence time. Data are only identified by fuel and burner size to reduce cluttering: a variety of burner Reynolds numbers and flame sampling positions were used. The behavior is similar to soot generation factors: CO generation factors vary at short residence times but approach asymptotic values for residence times an order of magnitude longer than smoke point residence times. This latter condition is most important for practical fires, providing a concise description of CO emissions from overventilated flames. A second feature of the results is that the asymptotic CO generation factor increases in the order of the sooting tendency of the fuel: propane, ethylene, propylene and acetylene. No smoke point has been found for methane so it is not plotted in Fig. 4, however, its asymptotic CO generation efficiency is less than half that of propane — consistent with its weak sooting tendencies.

The relationship between CO and soot emissions is illustrated quantitatively in Fig. 2. In this case, results for each burner and fuel are averaged to reduce cluttering. The correlation between CO and soot emissions is striking — extending nearly two orders of magnitude, with H/C ratios in the range 1-2.67, a wide variety of flame residence times, and various maximum temperatures within the flames. Consideration of earlier findings during study of the laminar flamelet concept suggest that emitted CO leaves the flame sheet with the soot layer so that the two have similar chemical environments. Then in circumstances where soot oxidation is not completed, it is not surprising that CO oxidation is incomplete as well.

Extensive measurements at Factory Mutual suggest that this correspondence between CO and soot emissions persists for other fuels, including liquids and solids. Thus, current work is turning to the CO and soot emission properties of liquid hydrocarbons in overventilated flames, to see whether generation factors are constant for given flames, whether they approach asymptotic values for long residence times in comparison to the smoke point residence time, and whether the correspondence between CO and soot emissions seen in Fig. 2 for gaseous fuels is preserved for a wider range of liquid fuels.

Turbulence/Radiation Interactions. Past work has shown that turbulence/radiation interactions cause mean radiation levels to be biased upward from estimates based on mean scalar properties (often by factors of 2-3). This is problematical for fire models while radiation fluctuations provide a basis of discriminating fires from background sources during early fire detection. Motivated by these applications, this phase of the investigation is studying turbulence/radiation interactions for both nonluminous and luminous flames. Earlier work had made some progress in treating turbulence/radiation interactions with somewhat ad hoc stochastic and turbulence models, in conjunction with the laminar flamelet concept. The objective of the present work was to test the robustness of the laminar flamelet concept for radiation fluctuation predictions using rigorous stochastic methods and direct measurements of the required statistical properties of the flames.

Experiments for nonluminous flames involved direct measurements of mixture fraction and radiation statistics for horizontal radiation paths through carbon monoxide/air flames. Predictions were based on extension of statistical-time-series methods to simulate mixture fraction distributions along the radiation paths (satisfying probability density functions and spatial and temporal correlations of mixture fractions), the laminar flamelet concept to relate all scalar properties to mixture fraction, and a narrow band radiation model. The resulting radiation statistics — mean and fluctuating values, probability density functions and the temporal spectra of spectral radiation intensity fluctuations — were in excellent agreement with measurements. Thus, the main impediment for applying this technology to practical nonluminous fires is the limitations of existing turbulence models concerning the necessary statistical properties of mixture fractions. Current work is focussing on measurements of mixture fraction properties in buoyant plumes as a step toward developing information on mixture fraction statistics in flame-like flows.

Analagous measurements of mixture fraction statistics in luminous flames are an active area of research; therefore, test of the stochastic methods for continuum radiation proceeded indirectly. This involved measuring the statistical properties of soot volume fractions along radiation paths in luminous acetylene and propylene flames and working through the laminar flamelet concept to obtain simultaneous simulations of soot volume fractions and temperatures along the radiation paths. A narrow-band model then yielded a time series of spectral radiation intensities in the continuum for comparison with measurements. These predictions were successful, similar to findings for the nonluminous flames, supporting use of the laminar flamelet concept for soot volume fractions for radiation predictions of luminous flames. Thus, a direct test of the flamelet concept in turbulent soot-containing flames is the main focus of current work.

Reports and Papers:

1. M.E. Kounalakis, J.P. Gore and G.M. Faeth, "Mean and Fluctuating Radiation Properties of Turbulent Nonpremixed Carbon Monoxide/Air Flames," J. Heat Transf., Vol. 111, pp. 1021-1030, 1989.

2. Y.R. Sivathanu and G.M. Faeth, "Soot Volume Fractions in the Overfire Region of Turbulent Diffusion Flames," Combust. Flame, Vol. 81, pp. 133-149, 1990.

3. Y.R. Sivathanu and G.M. Faeth, "Temperature/Soot Volume Fraction Correlations in the Fuel-Rich Region of Buoyant Turbulent Diffusion Flames," Combust. Flame, Vol. 81, pp. 150-165, 1990.

4. Y.R. Sivathanu and G.M. Faeth, "Generalized State Relationships for Scalar Properties in Nonpremixed Hydrocarbon/Air Flames," Combust. Flame, in press.

5. Y.R. Sivathanu, M.E. Kounalakis and G.M. Faeth, "Soot and Continuum Radiation Statistics of Luminous Turbulent Diffusion Flames," Twenty-Third Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, in press.

6. M.E. Kounalakis, Y.R. Sivathanu and G.M. Faeth, "Infrared Radiation Statistics of Nonluminous Turbulent Diffusion Flames," J. Heat Transf., submitted, 1990.

7. U.O. Koylu, Y.R. Sivathanu and G.M. Faeth, "Carbon Monoxide Emissions from Buoyant Turbulent Diffusion Flames," Third International Symposium on Fire Safety Science, Hemisphere Publishing Corp., Washington, submitted, 1990.

8. M.E. Kounalakis and G.M. Faeth, "Measurements of Mixture-Fraction Correlations in Turbulent Jet Diffusion Flames," Proceedings of the 22nd Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, pp. 41-1 to 41-4, 1989.

9. Y.R. Sivathanu, M.E. Kounalakis and G.M. Faeth, "Structure and Radiation Properties of Turbulent Diffusion Flames," NIST-GCR-90-570, 1990.

10. Y.R. Sivathanu, "Soot and Radiation Properties of Buoyant Turbulent Diffusion Flames," Ph.D. Thesis, The University of Michigan, 1990.

11. M.E. Kounalakis, "Turbulence/Radiation Interactions in Nonpremixed Flames," Ph.D. Thesis, The University of Michigan, 1990.

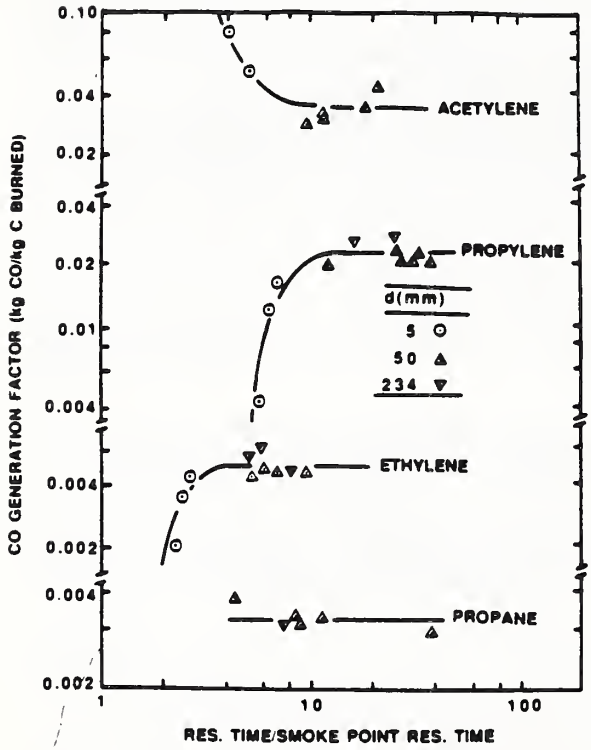

Fig. 1 CO generation factor as a function of flame residence time.

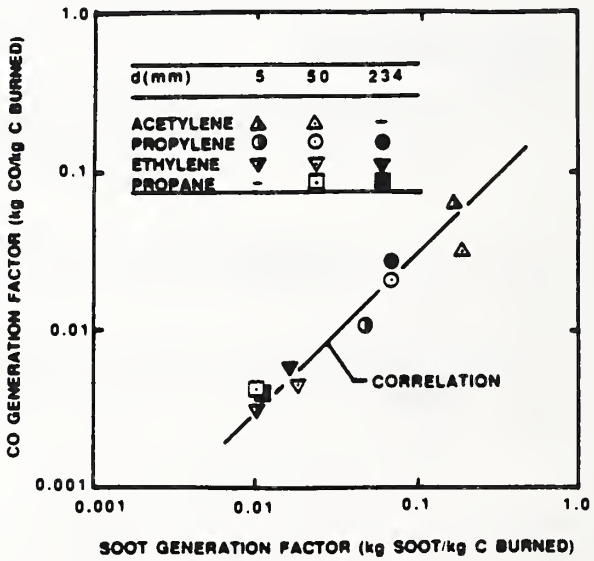

Fig. 2 Correlation between CO and soot generation factors.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: University of California, Berkeley

Grant No: 60NANB7DO737

Grant Title: Fire Propagation in Concurrent Flows

Principal Investigator: Professor A. Carlos Fernandez-Pello
Department of Mechanical Engineering
University of California
Berkeley, CA 94720

Other Professional Personnel: Liming Zhou, Doctoral Student

NIST Scientific Officer: Mr. Kenneth Steckler

Technical Abstract:

An experimental study is being conducted of the effect of gas flow turbulence on the concurrent spread of flames over the surface of a solid combustible material. Two research projects have been completed during this reporting period. They are studies of the effect of flow velocity and grid induced flow turbulence on the concurrent spread of flames over thick PMMA sheets in a floor configuration, and of the subsequent mass burning. The flame spread measurements show that the flow turbulence affects strongly the rate of flame spread, which decreases as the flow turbulence is increased due to the shortening of 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. A study is currently underway to study the turbulent concurrent spread of flames in the ceiling configuration with the objective of determining the effect of buoyancy on the process.

Concurrent Turbulent Flame Spread

An experimental study has been conducted of the influence on the spread of flames over the surface of PMMA sheets of the turbulence intensity of an air flow in the same direction of flame propagation. The experiments are carried out in a facility specifically designed to perform flame spread experiments consisting of a small scale combustion wind tunnel and supporting instrumentation. The turbulence intensity in the tunnel test section is varied by means of grids and perforated plates of different sizes placed at the exit of the tunnel converging nozzle. The velocity and turbulence intensity of the flow field are measured with a one component Laser Doppler Velocimeter. The flame spread rate is measured from the surface temperature history as given by thermocouples embedded at fixed intervals along the fuel surface. A Schlieren system is used to provide qualitative information about the effect of the flow turbulence on the flame and thermal layer structure. The fuel specimens are 6 in. wide, 12 in. long and 0.5 in. thick PMMA sheets and the oxidizing gas is air. Tests are conducted for flow velocity ranging from 1 to 4 m/sec with turbulence intensity varying from 1 to 20%.

The measurements of the flame spread rate over PMMA sheets as a function of the concurrent air flow velocity are shown in Fig. 1 for several values of the turbulence intensity. It is seen that the spread rate increases approximately linearly with the flow velocity, that it decreases as the turbulence intensity increases, and that this last effect is more pronounced for larger flow velocities. These results are very interesting and somewhat surprising since this mode of flame spread is controlled by heat transfer from the flame to the fuel, and it is well known that turbulent boundary layer heat transfer is larger than the laminar flow one. The results, which appear to be due to a strong effect of the turbulence intensity on the flame length, are very important not only because they introduce new aspects about the flame spread process not previously predicted, but because it may have significant influence in the application of flame spread formulas in models of room fire development.

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 (Saito, L., Quintiere, J. and Williams, F.A., 1st Int. Symp. Fire Safety Sci. 75, 1986).

$$v_f = q^2 \, l_f/(k\rho c \, (T_p - T_i))^2 \qquad (1)$$

where q is the surface heat flux, l_f the flame length, $k\rho c$ are the thermal properties of the solid and T_p and T_i the solid pyrolysis and initial temperatures respectively. The flow velocity and turbulence intensity can affect both q and l_f and through them the flame spread rate. Thus, it is important to determine how turbulence affects these parameters. In the present work the flame length is determined with the spread rate and the time required for the surface temperature at a thermocouple position to rise from ambient to the pyrolysis value. The surface heat flux is calculated from the time variation of the surface temperature by assuming that the fuel behaves as a semi-infinite solid. The variation of the flame length to pyrolysis length ratio with the flow velocity and turbulence intensity is presented in Fig. 2. It is seen that the dependence of the flame length on the flow velocity is different depending on the turbulence intensity. For all turbulence intensities, the flame length decreases with the turbulence intensity. The heat flux is only weakly affected by the flow turbulence, All of these results are combined in terms of a non-dimensional flame spread rate deduced from Eq. (1) and plotted versus the flow turbulence intensity. It is found that the non-dimensinal spread rate is independent of the flow velocity and turbulence intensity, which shows the validity of Eq. (1) and verifies that the effect of the flow turbulence on the flame spread rate takes place primarily through the flame length and heat flux. This again is a significant result since the prediction of flame length as a function of the problem parameters is an important factor in the development of room fires.

Turbulent Surface Burning

Measurements have been made of the PMMA burning rate dependence on the velocity and turbulence intensity of the air flow. The objective of the measurements is to provide additional information about the mechanisms that control the observed effect of flow turbulence on the flame spread rate. As it was reported above, the concurrent flame spread rate decreases as the turbulence intensity is increased due primarily to the shortening of the flame length with the turbulence intensity. Since the flame length is the result of the combustion of the excess pyrolyzate produced at the pyrolysis region, it is important to determine how the regression rate, and consequently the pyrolysis rate, depends on the flow turbulence.

The measured regression rate of the PMMA sheet for a flow velocity of 2 m/sec is shown in Fig. 3 as a function of the distance from the specimen upstream leading edge, with

the turbulence intensity as parameter. The experimental data for other flow velocities show very similar trends and are not presented here. From Fig. 3, it is seen that the regression rate becomes smaller with the distance from the upstream fuel edge, which is in agreement with the theoretical predictions for flat plate boundary layer mass burning. Since the boundary layer grows downstream, the flame moves away from the surface and the heat transferred to the solid is reduced as does the regression rate. The flow velocity effect shows that the regression rate increases as the flow velocity increases. As the external flow velocity becomes larger, the boundary layer becomes thinner, the flame gets closer to the fuel surface and, therefore, both the heat transfer and the regression rate increase. The flow turbulence affects the regression rate substantially. Fig. 3 shows that the regression rate goes up to 50% as the turbulence intensity increases from 1% to 20%. Qualitative information about the mechanisms by which turbulence affects the fuel mass burning process was obtained from Schlieren images of the reaction zone and thermal boundary layer. The images show that at low turbulence intensity, the flow is smooth and the flame is stable. The flow becomes much more violent and the mixing becomes stronger as the turbulence is raised. From the photographs, it can be inferred that more heat is transferred to the fuel surface because of the proximity of the reaction zone to the fuel surface and that this is an important factor in the observed regression rate increase with the turbulent intensity.

Because of the qualitative agreement between these results and the predictions from boundary layer analyses, it is natural to look for a dimensionless mass burning rate parameter that would correlate the experimental data in terms of the flow non-dimensional parameters; i.e. the Reynolds number and the turbulent intensity. The result is shown in Fig. 4. The non-dimensional parameter $\dot{m}''Lx/k\ (T_f - T_p)$ is equivalent to a forced flow convection Nusselt number. It is seen that when this parameter is plotted versus $(Re^{0.8}(u'/U))^{0.5}$, a linear correlation between these two non-dimensional parameters is obtained. From this correlation an explicit formula for the mass buring rate is deduced.

Reports and Papers

Zhou, L., Fernandez-Pello, A.C., and Cheng, R., "Flame Spread in an Opposed Turbulent Flow," *Combustion and Flame*, **81**:40-49 (1990).

Di Blasi, C., Crescitelli, S., Russo, G., and Fernandez-Pello, A.C., "On the Influence of the Gas Velocity Profile on the Theoretically Predicted Opposed Flow Flame Spread," *Combustion Science and Technology*, **64**, p. 289, (1989).

Zhou, L. and Fernandez-Pello, A.C., "Concurrent Turbulent Flame Spread," *Twenty-Third International Symposium on Combustion*, The Combustion Institute, (in press) (1989). Also presented at the 11th Joint Panel Meeting of the UJNR panel on Fire Research and Safety, October 19-29, 1989, U.C. Berkeley, California.

Zhou, L. and Fernandez-Pello, A.C., "Turbulent Burning of a Flat Fuel Surface," submitted to Third International Symposium on Fire Safety Science, 1990. Also presented at the Spring Joint Meeting, Western States Section and Canadian Section of the Combustion Institute, April 29-May 2, Banff, Alberta, Canada (1990).

Fernandez-Pello, A.C., "Solid Phase Combustion," Chapter 2, Combustion Treatise on Fire, G. Cox, Editor, Academic Press (in press)(1990).

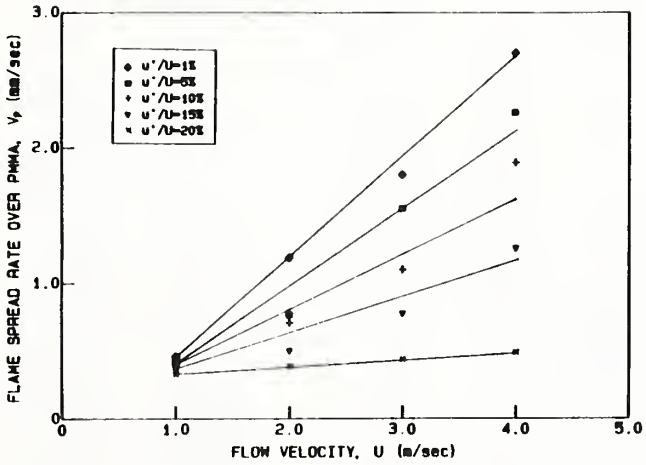

Figure 1.

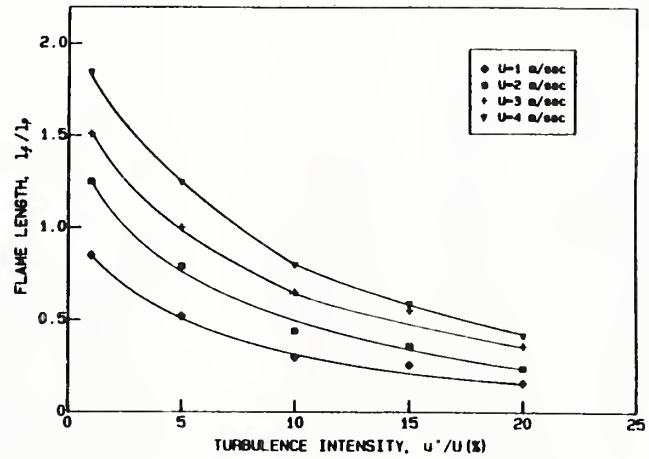

Figure 2.

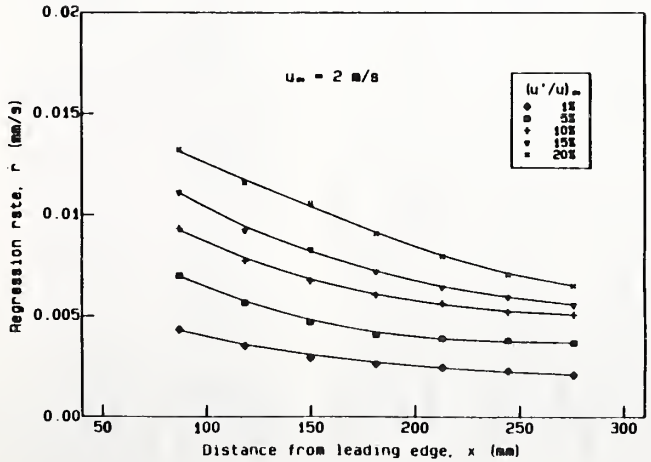

Figure 3.

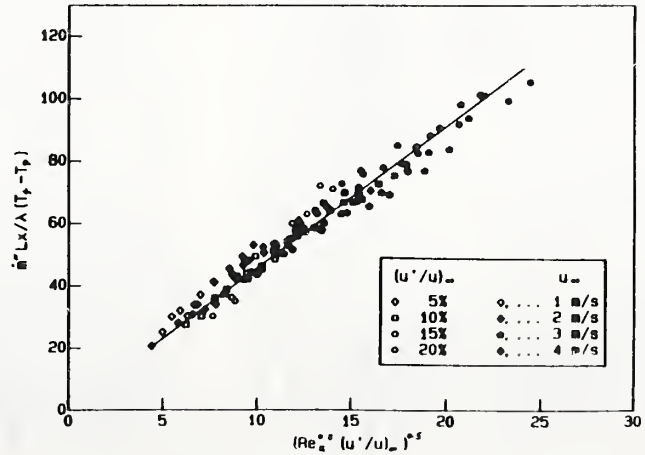

Figure 4.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	University of California at Berkeley
Grant No:	60NANB8D0848
Grant Title:	Fire Modeling
Principal Investigator:	Prof. Patrick J. Pagni Department of Mechanical Engineering University of California at Berkeley Berkeley, CA 94720
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NIST Scientific Officer:	Dr. Howard Baum

Technical Abstract:

Glass breaking in compartment fires is an important practical problem since a window acts as a wall before breaking and as a vent after breaking. If sufficient excess pyrolyzates have accumulated in the hot layer, this sudden geometric change can lead to backdraft and flashover. As Emmons explained at the First Fire Safety Science Symposium, windows break in fires due to thermal stress from the differential heating of the central portion and the shaded edge. The focus of this project is on quantifying the connection between the compartment fire and the glass temperature in order to predict the window breaking time, t_b. Techniques are presented for accurately calculating the history of the central glass temperature profile, $T(x,t)$, for any fire exposure. Two-dimensional temperature histories, $T(x,y,t)$, where x is depth and y is toward the center, and mean stress histories, $\sigma_{zz}(y,t)$, are also calculated. It is determined that breaking occurs when the mean glass temperature difference is

$$\Delta T = (\sigma_b/E\beta)(1+s/H), \tag{1}$$

where σ_b/E is the maximum glass tensile strain, β is the thermal coefficient of linear expansion and s/H is the ratio of the shaded width to the window half-width. Calculations suggest that the edge remains at its initial temperature when the shading is large, $s/L \geq 2$, and the heating is fast, $\alpha t_b/s^2 \leq 1$, where L is the glass thickness and α is the glass thermal diffusivity. A glass-breaking subroutine for use with any compartment fire model is in preparation.

HEATED GLASS TEMPERATURE HISTORY, $T(x,t)$

Consider the window shown in Fig. 1a and 1b. The goal is to calculate the temperature in the large central section of the glass as a function of depth into the glass, x, and time, t. We will show later that the appropriate ΔT is the mean temperature increase, $\frac{1}{L}\int_0^L T(x,t)dx - T_i$. The unshaded glass is uniformly heated, so $\partial/\partial y$ and $\partial/\partial z$ are zero. Then the governing equation for this system is

$$\rho c \frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} + I(t)\frac{e^{-x/l}}{l}, \tag{2}$$

where $I(t)$ is the incident radiative flux directly from the fire which is at sufficiently short wavelengths that its distributed internal absorption needs to be included and l is the decay length in the glass. The initial and boundary conditions are

$$t = 0:\ T = T_i,$$

$$x = 0:\ -k\frac{\partial T}{\partial x} = h_2(T_{2\infty}(t) - T(0,t)) + \varepsilon_\infty \sigma T_{2\infty}^4 - \varepsilon\sigma T^4(0,t) = q_2(t), \tag{3}$$

$$x = L:\ -k\frac{\partial T}{\partial x} = h_1(T(L,t) - T_{1\infty}(t)) + \varepsilon\sigma T^4(L,t) - \varepsilon_\infty \sigma T_{1\infty}^4(t) = q_1(t),$$

where side 1 is toward the ambient and side 2 is the hot layer in the compartment.

Results

Figure 2 shows the temperature history of the hot gas layer (calculated from *FIRST* for a recent full scale fire) along with surface temperatures from initiation to breakage for the two cases identified in the caption. The $I = 0$ case represents a window far from the fire; $I = 10 kW/m^2$ represents a window adjacent to the fire. The $100s$ difference in t_b, defined by $[T(0,t_b) + T(L,t_b)]/2 = \sigma_b/E\,\beta$, allows the conditions in the compartment to change dramatically, as indicated by the hot layer temperature, $T_{2\infty}(t)$. The temperature of the exposed side is sufficiently greater than that of the unexposed side to justify our concern with $T(x,t)$. Here h_2, h_1 and I are taken as constants; the compartment fire program to which our subroutine is coupled will hopefully provide these as functions of time.

GLASS TEMPERATURE PROFILES, $T(x,y,t)$

Consider now the glass pane section shown in Figure 1c. The range of interest is $-\infty < y < +\infty$, so that the temperature field under the frame can be explored and the s/L ratio at which the edge temperature increases can be determined. The origin of y is on the inside edge of the frame. Here the goal is to calculate the temperature distribution along the pane from the shaded edge to the unshaded central section. The governing equation for this system is

$$\rho c\frac{\partial T}{\partial t} = k\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right] + \frac{I(t)}{l}e^{-x/l}H_v(y), \tag{4}$$

where H_v is the Heaviside function and all other notation is standard. The initial condition and boundary conditions are

$$t{=}0:\ T = T_i;\ \ y \to \pm\infty\ \frac{\partial T}{\partial y} = 0. \tag{5}$$

$$x{=}0:\ -k\frac{\partial T}{\partial x} = q_2(t)H_v(y);\ \ x{=}L:\ -k\frac{\partial T}{\partial x} = q_1(t)H_v(y).$$

The heat fluxes, $q_2(t)$, $q_1(t)$ and $I(t)$ are assumed here to be specified *apriori*.

Results

Figure 3 shows dimensionless isotherms for for the cases listed in the figure captions at times when the dimensionless surface temperature becomes 1. The $q_1{=}0$ condition in Fig. 3a is clearly artificial, since the calculation gives $\theta(1,\tau) = 0.4$ so that significant heat loss would occur to the ambient. However it represents a useful limit where the only heat sink is at $\zeta \to -\infty$, so the thermal penetration under the window frame is maximized. Fig. 3b shows another example of that limit at a later time with gentler heating. Fig. 3c shows the effect of significant cooling at $\xi{=}1$. Figs. 3 b and c represent conditions similar to Fig. 2. The slow fire in Fig. 3d produces a larger thermal penetration than 3b or 3c because of its longer duration. In none of these examples does $\theta(-2,\tau)$ exceed 1%. This suggests that

$$T(-s,t) = T_i \ \text{ if } s/L \geq 2 \text{ and } \alpha t_b/s^2 \leq 1. \tag{6}$$

STRESS FIELD

It is assumed that the temperature field is unaffected by the stress field and that the stresses instantaneously accomodate to changes in the temperature field. Since there are no z temperature gradients, changes in stresses with z are neglected. Let σ_{zz} and σ_{yy} be normal stresses in the z and y directions and σ_{zy} and σ_{yz} be the shear stresses on the z and y planes. All stresses are normalized on the tensile strength σ_b, $\psi = \sigma/\sigma_b$ and temperature is non-dimensionalized as $\theta = (T - T_i)/(\sigma_b/\beta E)$. To avoid a three dimensional stress analysis, we integrate over x and define the following dimensionless mean stresses and dimensionless mean temperature

$$N_{zz} = \int_0^1 \psi_{zz}\, d\xi\ ;\quad N_{yy} = \int_0^1 \psi_{yy}\, d\xi;\quad N_{yz} = N_{zy} = \int_0^1 \psi_{yz}\, d\xi = \int_0^1 \psi_{zy}\, d\xi;\quad N_T = \int_0^1 \theta\, d\xi. \tag{7}$$

The local force balances in the z and y directions respectively are

$$\frac{\partial N_{zz}}{\partial \mu} + \frac{\partial N_{zy}}{\partial \zeta} = 0\ ;\quad \frac{\partial N_{yz}}{\partial \mu} + \frac{\partial N_{yy}}{\partial \zeta} = 0. \tag{8}$$

The boundary conditions are no external forces and a constant limit

$$\int_{-s/L}^{H/L} N_{zz}\, d\zeta = 0;\quad \zeta \to \infty:\ \frac{dN_{zz}}{d\zeta} = 0. \tag{9}$$

The stress field is related to the temperature field by the compatibility relations which simplify to

$$\frac{d^2}{d\zeta^2}\left[N_{zz} + N_T\right] = 0. \tag{10}$$

Integrating Eq. (10) twice and applying the boundary conditions, gives the stress throughout the range $-s/L < \zeta < H/L$, which by symmetry represents the entire window,

$$N_{zz}(\zeta,\tau) = -N_T(\zeta,\tau) + \frac{L}{H+s}\int_{-s/L}^{H/L} N_T(\zeta,\tau)\, d\zeta. \tag{11}$$

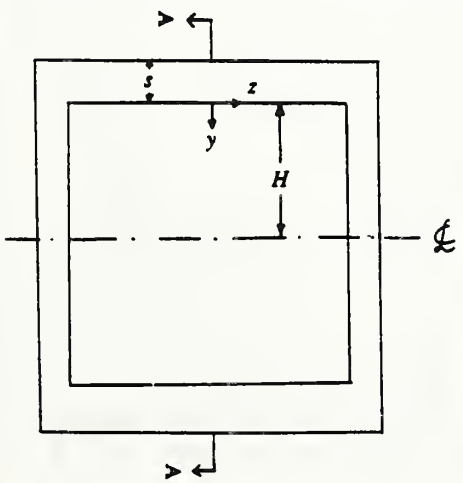
Results

Figure 4 presents the mean stress from Eq.(11) as a function of ζ for the temperature fields given in Figure 3. For this case $s/L = 3.0$ and $s/H = 0.02$. The tensile(+) stress at the edge of the shaded region is large and drops to a small compressive(-) stress in the unshaded region. In the limit that N_T=0 for ζ<0 and 1 for ζ>0 Eq. (11) shows that N_{zz} becomes $1/(1+s/H)$ for ζ<0 and $-s/H\,(1+s/H)$ for ζ>0. This provides the factor $(1+s/H)$ on the right of Eq. (1) to account for compression in the central section of the glass. Equation (11) also shows that it is the mean temperature, N_T, not the surface temperature, $\theta(0,\tau)$, is required in Eq.(1).

Reports and Papers

Joshi, A. and Pagni, P. J., "Thermal Analysis of Effect of a Compartment Fire on Window Glass", NIST-GCR-90-579, 1990.

Pagni, P. J. and Joshi, A., "Glass Breaking in Fires", submitted to the Third International Symposium on Fire Safety Science, Edinburgh, Scotland, July 8-12, 1991.



1(a)

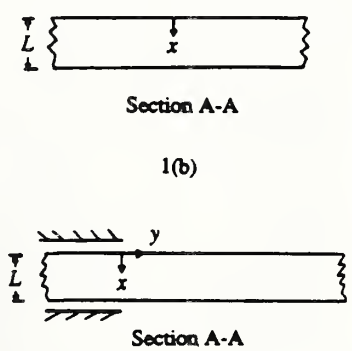


Figure 1. Window Schematics

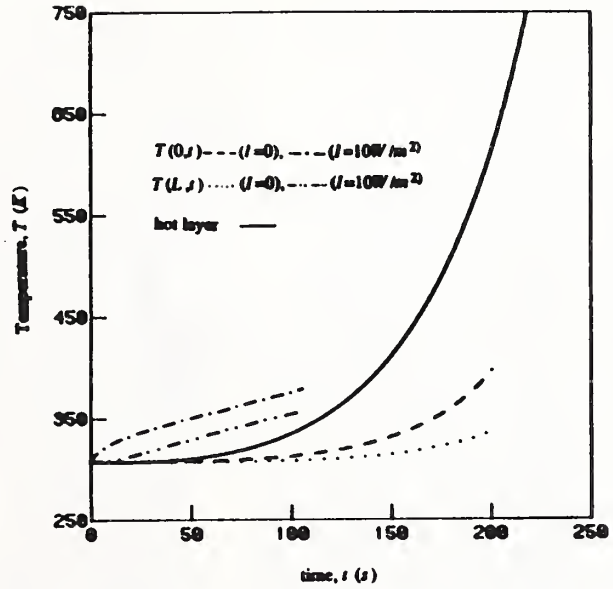


Figure 2. Temperature history of hot gas-layer and surface temperatures for $I(t) = 0$ and $10 W/m^2$ with $h_2 = 50 W/m^2\text{-}K$ and $h_1 = 10 W/m^2\text{-}K$. The initial and ambient temperature is set equal to 307K.

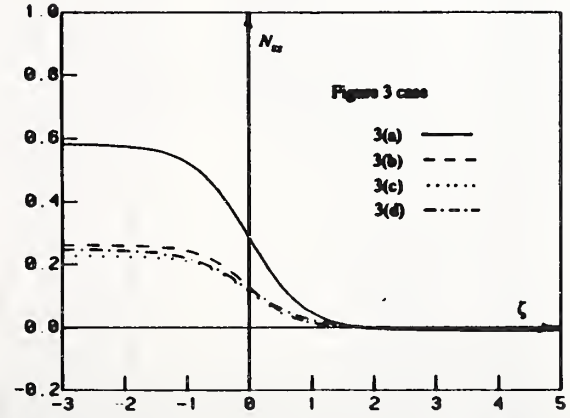


Figure 4. Stress fields corresponding to the temperature fields in Fig.3.

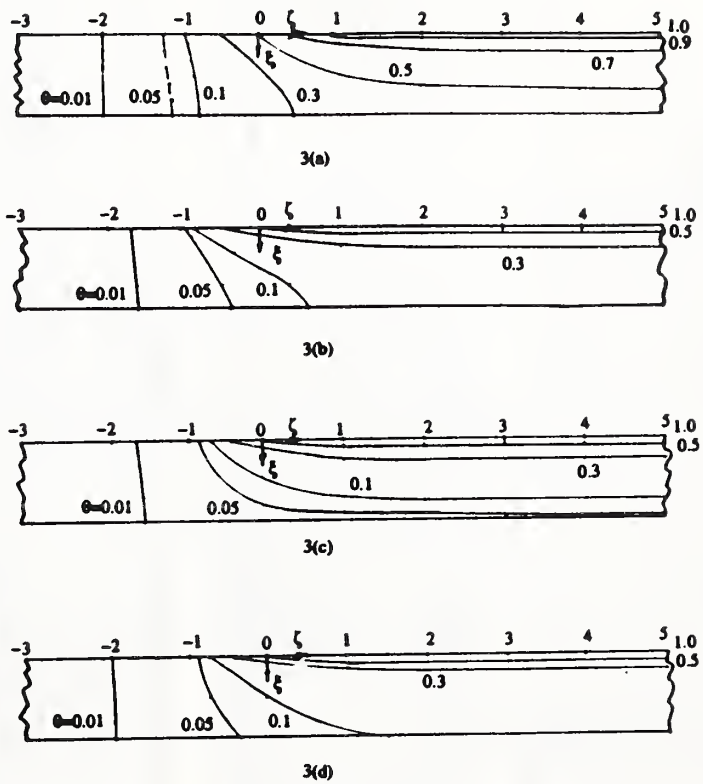


Figure 3a. This represents a fast fire next to the window with, $\tau_b = 0.66$. Here $q_1 = 0$, $I = 5kW/m^2$ and $q_2 = 1\ kW/m^2\ exp(t/30s)$.

Figure 3b. This is a medium spread fire away from the window with $\tau_b = 1.40$, with $q_1 = 0$; $I = 100\ W/m^2\ exp(t/30s)$ and $q_2 = 200\ W/m^2\ exp(t/30s)$.

Figure 3c. This is the same as 3b, except for $q_1 0$, with $\tau_b = 1.42$, with $q_1 = 0$ from 0 to 30 seconds, and $100\ W/m^2\ exp((t-30s)/30s)$; $I = 100\ W/m^2\ exp(t/30s)$ and $q_2 = 200\ W/m^2\ exp(t/30s)$.

Figure 3d. This is a window in a room away from the fire, with $\tau_b = 3.17$, with $q_1 = 0$ from 0 to 30 seconds, and $10\ W/m^2\ exp((t-30s)/60s)$; $I = 0$; and $q_2 = 100\ W/m^2(t/60s)$.

B. SOOT FORMANTION

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

SOOT FORMATION AND EVOLUTION

Professional Staff

Kermit C. Smyth, Project Leader
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Project Objectives

Develop scientifically sound principles, metrology, data, and predictive methods for the formation and evolution of smoke components in flames for use in understanding and modeling general fire phenomena.

Scope

This work embraces broad areas underpinning CFR programs with focussed study in the areas 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 hydrocarbon 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 combustion efficiency in furnaces and 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 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 proce.. 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 characterized. 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. Detailed flame structure measurements (species concentrations, temperature, and velocity) have been made in a laminar methane/air diffusion flame using a variety of laser-based optical techniques as well as mass spectrometric sampling. By using all of these data, the species profiles have been analyzed to determine production and destruction rates of intermediate hydrocarbons.

Recently we have made the first quantitative OH· concentration measurements in a hydrocarbon diffusion flame, as well as relative profile measurements of H atom, O atom, and CH· concentrations. These data are the first detailed measurements of radical species in hydrocarbon diffusion flames. The results have enabled us to carry out a partial equilibrium analysis of the radical pool species (OH·, H·, and O:) and also perform a reaction path analysis of the fastest routes for the formation of the vinyl and ethynyl radicals, which are thought to be key precursors in chemical growth.

For our multiphoton ionization measurements of H-atom concentrations we have been able to devise a novel approach which enables one to place the highly sensitive profile data on an accurate relative concentration basis by calibrating the electron detection sensitivity as a function of flame position. The new experimental findings on CH· fluorescence should be very useful for interpretation of current imaging work on turbulent diffusion flames, where CH· has often been interpreted as a marker of the primary reaction zone. We have also carried out a reaction path analysis for the CH· production and destruction reactions, as well as a steady-state analysis - both for the first time in a diffusion flame. Our current emphasis is to establish reduced chemical mechanisms for hydrocarbon oxidation and growth processes using these new measurements of radical concentrations.

2. Smoke Agglomerates

A combined experimental and theoretical effort is focussed on the characterization of the optical properties of smoke agglomerates. The theoretical effort has consisted of generating simulated smoke agglomerates of various sizes and then computing the light scattered by the agglomerates using Rayleigh-Debye scattering theory. The most noteworthy result of this analysis is the prospect of inferring information about the concentration and size of the soot from the scattering measurements. It is shown that from the scattering measurements one can infer the overall size of the agglomerate,

the size of the primary units in the agglomerate, the number of primary units in the agglomerate, and the number concentration of agglomerates.

To study the optical properties of smoke, a combined transmission cell-reciprocal nephelometer has been developed. This device allows the simultaneous measurement of the extinction coefficient and the total scattering coefficient of smoke. These are the key quantities needed for studying radiation transport through a smoke cloud. From the difference of these two quantities, the absorption coefficient of smoke can be determined. During the past year a radiometric model has been developed for the transmission cell reciprocal nephelometer (TCRN). The model involves the computation of the light scattered from an infinitesimal element of the laser beam within the TCRN to an infinitesimal element of the cosine sensor. Integrating over the surface of the senor and along the laser beam yields the total flux of light reaching the cosine sensor. Calculations were carried out for smoke agglomerates by using the theory of fractal optics and for spheres by using Mie theory. The cluster size was varied from 10 spheres to 10^8 spheres for the fractal calculation and the sphere size was varied from 0.02 μm to 8 μm for the Mie scattering. Key issues in the analysis included the effect of the finite size of the detector and the finite length of the TCRN on the predicted total scattering. It is expected that as the size of the soot cluster or sphere increases the TCRN would underestimate the total scattering, since the light scattered at small angles increases as the particle size increases. The TCRN collects light over the range 7° to 173°. Preliminary results indicate that the TCRN will underestimate the total scattering by at least 15% for agglomerates with more than 10,000 primary spheres of size 30 nm and fractal dimension of 1.9 and for spheres (refractive index=1.588, the value for the calibration particles made of polystyrene) with diameters greater than 2 μm.

The specific extinction area, σ_e, was computed for smoke agglomerates based on Mie theory and on three different models for the optics of fractal soot: Berry-Percival Model (first publication of optics of fractal agglomerates), Nelson's Mean Field Theory, and the Dobbins-Megaridis Polydisperse Model. The calculations were performed for agglomerate sizes varying from 80 to 3200 primary spheres to compare with the previous years experimental study of the effect of agglomeration on the optical properties of crude oil smoke. The experimentally observed constancy of σ_e is consistent with the fractal models but not with Mie theory. The predictions by the fractal models were found to be sensitive to the prefactor in the relation between the number of primary spheres and the radius of gyration and to the nature of the cut-off function for the pair correlation function. It was also found that the value of the refractive index needed for agreement between the measured and predicted value of σ_e appears to be inconsistent with the measured refractive index.

Publications

P. J. H. Tjossem and K. C. Smyth, Journal of Chemical Physics, 91, 2041 (1989). Multiphoton Excitation Spectroscopy of the $B^1\Sigma^+$ and $C^1\Sigma^+$ Rydberg States of CO.

K. C. Smyth, P. J. H. Tjossem, A. Hamins, and J. H. Miller, Combustion and Flame, 79, 366 (1990). Concentration Measurements of OH· and Equilibrium Analysis in a Laminar Methane/Air Diffusion Flame.

K. C. Smyth and P. J. H. Tjossem, Applied Physics B 50, 499 (1990); special issue on Laser Diagnostics in Combustion. Radical Concentration Measurements in Hydrocarbon Diffusion Flames.

A. Hamins, D. T. Anderson, and J. H. Miller, Combustion Science and Technology 71, 175 (1990). Mechanistic Studies of Toluene Destruction in Diffusion Flames.

K. C. Smyth and P. J. H. Tjossem, Twenty-Third Symposium (International) on Combustion (in press). Relative H-Atom and O-Atom Concentration Measurements in a Laminar, Methane/Air Diffusion Flame.

J. H. Miller, Twenty-Third Symposium (International) on Combustion (in press). The Kinetics of Polynuclear Aromatic Hydrocarbon Agglomeration in Flames.

K. C. Smyth and P. J. H. Tjossem, Applied Optics (in press). Signal Detection Efficiency in Multiphoton Ionization Flame Measurements.

T. S. Norton and K. C. Smyth, submitted to Combustion Science and Technology. Laser-Induced Fluorescence of CH· in a Laminar CH_4/Air Diffusion Flame: Implications for Diagnostic Measurements and Analysis of Chemical Rates.

P. Meakin, B. Donn, and G.W. Mulholland, Langmuir, 5, 510 (1989). Collision between Point Masses and Fractal Aggregates.

B.A. Benner, N.P. Bryner, S.A. Wise, and G.W. Mulholland, Environmental Science and Technology (in press). Polycyclic Aromatic Hydrocarbon Emissions from the Combustion of Crude Oil on Water.

N.P. Bryner and G.W. Mulholland, Atmospheric Environment (accepted). Smoke Emission and Burning Rates for Urban Structures.

T. Cleary, R. Fletcher, L. Ives, G.W. Mulholland, and J. Gentry, submitted to Aerosol Science and Technology. Ultrafine Combustion Aerosol Generator.

Related Grants

1. Soot Morphology and Radiation in Turbulent Flames,
   Richard A. Dobbins, Brown University.

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

3. Simplifications of Diffusion Flame Chemistry: A Theoretical and Experimental Study of the Structure of Laminar Diffusion Flames,
   J. Houston Miller, George Washington University.

4. Fundamental Mechanisms for CO and Soot Formation in Diffusion Flames,
   Robert J. Santoro, Pennsylvania State University.

5. A Study on the Scavenging and In-Cloud Processing of Combustion Aerosols,
   Donald Hagen, University of Missouri, Rolla.

CENTER FOR FIRE RESEARCH
NATIIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: Brown University

Grant No.: 60NANB9D0975

Grant Title: "Soot Morphology in Buoyancy Dominated Flames"

Principal Investigator: Prof. R. A. Dobbins
Division of Engineering
Brown University
Providence, RI 02912

Professional Personel: H. Subrumaniasivam, Graduate Student
W. D. Lilly, Senior Technical Assistant

NIST Scientific Officer: Dr. G. W. Mulholland

Technical Abstract:

I. Experimental - Thermophoretic Sampling of the Soot Formed The Buoyancy-Dominated Flame.
Previous use of the thermophoretic sampling procedure was dedicated to the study of the coannular laminar ethene flame. In the past year we have applied this technique to the unsteady buoyancy-dominated ethene flame which is formed when the flow rate is increased to 50 cm^3/s. The burner i.d. is 1.11 cm and a coannular air flow is provided. This flame, which is well described in the literature, displays a periodic oscillation of 12 - 13 hertz which is amplified into an irregular, roughly toroidal vortex at 15 cm above the burner. The vortex is shed periodically and breaks into a turbulent flame brush that extends to $z \approx 40$ cm above the burner mouth. The strong flickering of radiant intensity that is characteristic of many unsteady flames is displayed. An important finding low in this flame, where unsteady effects are absent, is the region in which isolated, nascent, primary particles are found to coexist with the aggregates. The smaller isolated particles have a diffuse circular border, are polydisperse, and range in size up to about 8 nm. The ratio of isolated particles to aggregates is very high near the burner mouth and decreases with increasing height. We conclude that the isolated particles contribute to the surface growth of the monomers within the aggregates. In Fig. 1 we show a micrograph taken at a height of 1 cm above the burner mouth that shows the coexisting isolated particles and the aggregates. The coexistence of these two particle types is an indication that particle inception is present.

In the vortex there is a very low population of solitary particles. Primary particles in the vortex have achieved the maximum size of about 35 nm, and are quite monodisperse apparently as a result of sustained surface growth. Even though the vortex is highly unsteady, the particle morphology is essentially independent of time in this region.

Higher in the flame the aggregates essentially each consist of monodisperse primary particles with some a variability of the primary particle sizes from aggregate-to-aggregate. This variabilty is probably as the result of differing amounts of oxidation in the upper portion of the flame. No isolated particles are observed in this portion of the flame.

II. Theoretical - Optical Cross Sections of Soot Aggregates. Our formulation of the optical cross sections of polydisperse aggregates has been presented[1,2] and is scheduled for publication[3]. This formulation has applications in explaining the extinction properties of smoke of various origins. The most important of these measurements is the aging smoke tests of conducted at the CFR. In these tests the optical extinction per unit mass was found to be independent of time as is consistent with our formulation of the aggregate optical cross sections. This comparison was discussed at a recent meeting[4] and shows important progress in the ablility to predict the optical properties of smoke from fires and to use these properties with greater confidence and reliability in experiments relating to fire research. A more critical test is the use of these cross sections in the analysis of the scattering/extinction data described below.

At the 23rd Symposium[5] we presented the results of the analysis of the scattering/extinction tests previously analyzed using Rayleigh theory for spherical particles. More recently we have been examined the improved scattering/extinction data of Santoro, Puri and Richardson for the same nonsooting, laminar, coanular ethene flame. The results of this analysis, see Fig. 2, strongly confirm trends found previously, viz., a) the aggregate number concentration decreases monotonically with height or residence time, b) the soot volume fraction increases by surface growth to a maximum near the midflame height and then decreases due to oxidation, and c) the number of primary particles per unit volume remains approximately constant throughout the upper portion of the flame. These results are in agreement with our interpretation that in these flames the following sequence occurs: Low in the laminar flame there exists intense particle inception combined with early aggregate formation and creating a perscribed number concentration of primary particles which remains constant along along a given soot particle path. Above this region the primary particles grow by surface reactions, and later contract by oxidation. Cluster-cluster aggregation is sustained throughout the flame. There is thus a regional partitioning of the soot aerosol processes within the laminar flame.

III. Commentary On The Interaction of The Scattering/Extinction and the Thermophoretic Sampling Experiments.
These contrasting experiments have proven to be highly informative. With the aggregate morphology found via the sampling process, it becomes possible to formulate the optical cross sections. Optical tests then permit the internally consistent measurement of the soot concentration and soot aggregate properties, and they lead to an interpretation of the soot aerosol dynamic processes. The soot inception zone is detectable only in micrographs that show the coexistence of both isolated and aggregated particles. The aggregates would dominate the scattering and would mask the presence of the smaller nascent particles in scattering/extinction tests.

Reports and Publications:

1. Dobbins, R. A. and Megaridis, C. M., "Absorption and Scattering of Light by Polydisperse Fractal Aggregates", 2nd International Congress On Optical Particle Sizing, Tempe, March 1990.

2. Dobbins, R. A., "Optical Cross Sections of Flame-Generated Aggregates", Invited paper, fall meeting of the Eastern States Section of the Combustion Institute, Albany, October 1989.

3. Dobbins, R. A., and Megaridis, C. M., "Absorption and Scattering of Light by Polydisperse Aggregates", to appear in Applied Optics.

4. Dobbins, R. A., Bryner, N. P. and Mulholland, G. W., "The Extinction of Light by Soot Aggregates", Abstract of paper presented at the Sixth Annual Meeting of the AAAR, Philadelphia, June 1990.

5. Dobbins, R. A., Santoro, R. J., and Semerjian, H. G., "Analysis of Light Scattering for Soot Using Optical Cross Sections for Aggregates", 23rd Symposium (International) On Combustion, 1990.

6. Megaridis, C. M., and Dobbins, R. A. "Morphological Description of Flame Generated Materials", Comb. Sci. and Tech. 71, 95 (1990).

7. Megaridis, C. M. and Dobbins, R. A., "A Bimodal Integral Solution of the Dynamic Equation for an Aerosol Undergoing Simultaneous Particle Inception and Coagulation", Aerosol Science and Technology 12, 240 (1990).

8. Dobbins, R. A., "Data Inversion of Laser Scattering From Pyrogenic Aggregates" Abstract of paper presented at the Fifth Annual Meeting the AAAR, Reno 1990.

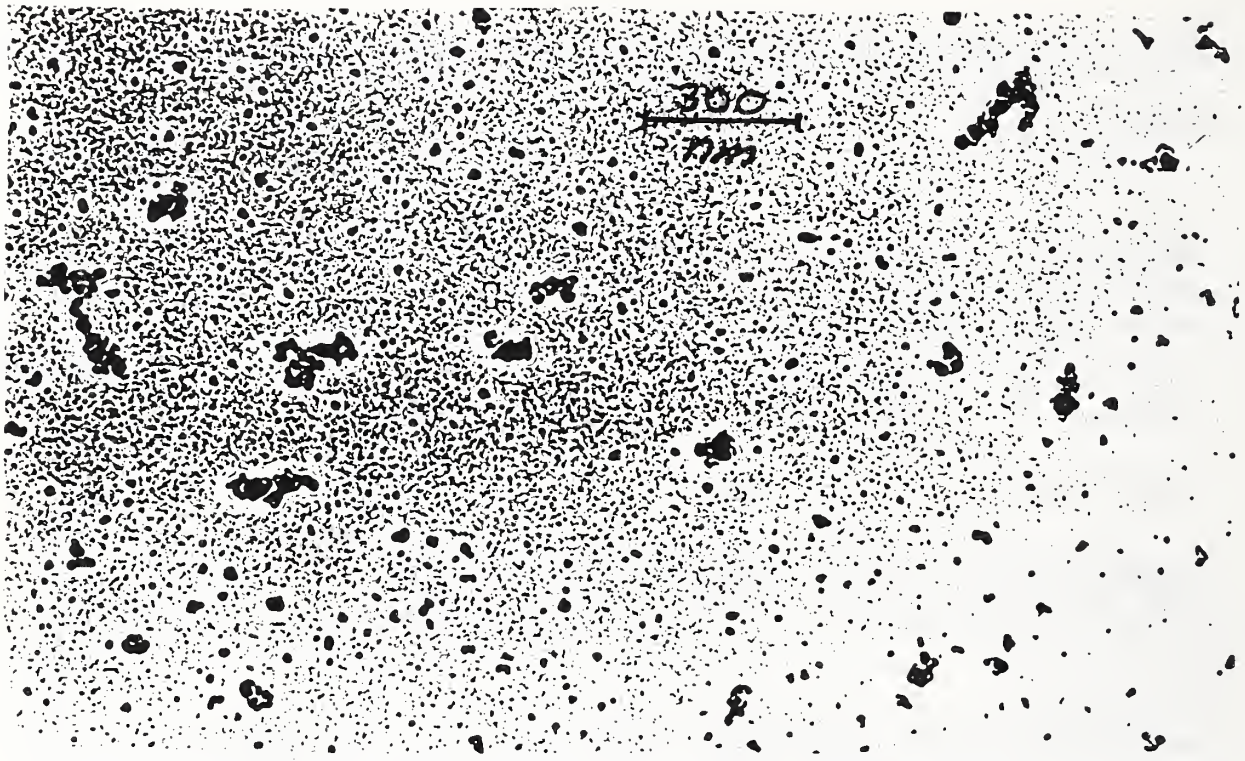

Fig 1. Micrograph of Particle Inception and Cluster Growth Low in the Buoyancy Dominated Ethene Flame, Q = 50 cm^3/s.

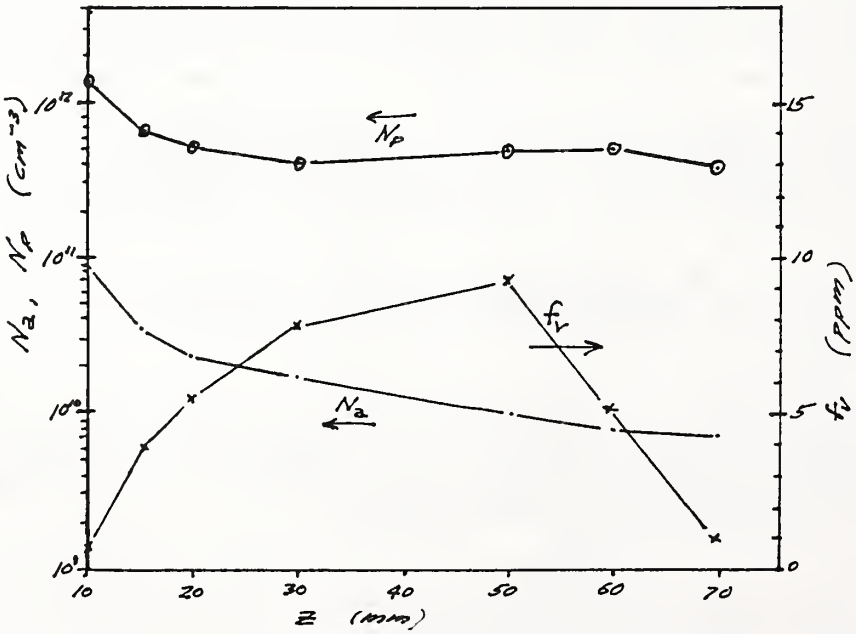

Fig 2. Graph of Soot Volume Fraction f_v, Aggregate Number Concentration N_a, and Primary Particle Concentration N_p. Laminar Ethene Flame, Q = 3.85 cm^3/s.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	University of California Davis
Grant No.:	
Grant Title:	Modelling Soot Formation in Diffusion Flames
Principal Investigator:	Dr. Ian M. Kennedy Dept. of Mechanical Aeronautical and Materials Engineering, University of California Davis, Davis, CA. 95616
Other Professional Personnel:	Prof. W. Kollmann
NIST Scientific Officer:	Dr. Kermit C. Smyth

Technical Abstract:

Introduction The formation of soot in flames has been a subject of extensive research for many years. In the last decade laser measurement techniques have provided valuable insights into the physics of soot formation which is now seen as a fourfold process viz., particle inception, surface growth, coagulation or agglomeration, and finally oxidation. Most combustion that is of practical interest occurs in non-premixed or diffusion flames; the formation of soot in these flows is affected greatly by the flowfield itself. In fact, there is strong coupling between the flowfield and the production or burnout of soot as a result of the significant heat loss from the flames. The heat loss arises from the luminous radiation of the soot particles. Temperatures may be reduced many hundreds of degrees below their adiabatic values.

Although we have a better understanding of some of the fundamental processes which lead to the formation of soot there have been few attempts to utilize the existing information in a predictive model. Ideally such a model would incorporate the appropriate physics and chemistry for the basic processes (as far as we understand them) into a calculation of the flowfield with radiation. Furthermore, it must be borne in mind that most flames of practical importance are turbulent and, therefore, any model should be sufficiently simple that it can be incorporated eventually into a turbulent flame code.

Soot Modelling

A brief recapitulation of our current approach is offered here in order to point out some of the weakness and uncertainties in the model. The basic approach has been to rely upon experimentally determined growth rates and number densities as inputs to the soot growth model. The primary source has been laser light scattering and extinction measurements in a counterflow Tsuji type diffusion flame on a porous cylinder. This flame configuration is useful in that it provides a very well defined flow field for measuring the rates of surface growth along a streamline. In addition, it is well suited to the application of the conventional laser extinction technique for the measurement of soot volume fractions because of the uniformity of the soot aerosol along the optical path.

The growth model is based upon the kinetics of Harris and Weiner who assume a growth rate that is proportional to soot surface area and a specific surface growth rate. The latter quantity was derived in our model from the laser measurements in the Tsuji flame. This data is, of course, fuel specific. We have found that the inclusion of an equation for the particle number density was not necessary in order to achieve reasonable results; an average number density was used.

The specific surface growth rate is expected to depend upon a concentration of available growth species, the temperature and the reactivity of the particles. The first effect is accounted for via a correlation of measured specific growth rates with the so-called mixture fraction in the flame. This quantity is widely used in the theoretical description of diffusion flames and is a measure of the mixing of fuel and air in a two stream mixing flow. The temperature is determined through the calculation of an energy equation (enthalpy) with an assumption of constrained equilibrium chemistry. radiation was calculated by invoking the optically thin assumption. The specific surface growth rates which are used in the program are adjusted by the ratio of the calculated temperature to the measured temperature with an assumed activation energy to give the correct temperature sensitivity. The particle reactivity is not accounted for explicitly.

Oxidation in the soot model has been calculated as a function of the OH concentration on the rich side of the flame and as a function of the temperature on the air side of the flame with the Nagle Strickland-Constable formula. The OH oxidation rate is estimated from the collision rates of soot and OH with a reaction probability taken from the work of Neoh et al. However, the concentration of OH which is obtained from the constrained equilibrium chemistry is much different to the levels predicted by a detailed computation of an ethylene air counterflow diffusion flame with the code of Miller et al. The latter set of data was found to give more satisfactory predictions of OH oxidation than the equilibrium calculation. Furthermore, it was assumed that the temperature on the air side of the flame at the location where the O_2 reaction was turned on was sufficiently low that the oxidation rate of Nagle and Strickland-Constable was independent of O_2 concentrations.

A somewhat surprising result from these calculations of axisymmetric diffusion flames and, in fact, from earlier modelling of counterflow diffusion flames is the insensitivity of the soot production to the particle inception rate. In contrast, the soot volume fractions were quite sensitive to the specific rates of surface growth that we used in the models. These findings contradict the widely held view that particle inception controls ultimate soot loadings and that specific surface growth rates are essentially similar in most flames. Our computer modelling suggests, in fact, that the situation may be somewhat more complex, in that lightly sooting flames may depend on particle inception rates but heavily sooting flames may exhibit a greater sensitivity to growth rates.

Planned Research

In the coming year we plan to concentrate almost exclusively on the numerical modelling of laminar diffusion flames. Any fundamental difficulties or gaps in the available database for the various processes which are incorporated in our model may need to be investigated in later years.

All our modelling to date has been done for ethylene flames. In this year our research plan is to develop suitable correlations for surface growth with mixture fraction and temperature for a number of different fuels or fuel blends by using available information in the literature as far as possible. This requires laser extinction and scattering measurements and velocity measurements in sooty laminar diffusion flames from which

area specific surface growth rates may be inferred. The ideal configuration is the counterflow diffusion flame which has been used by Vandsburger et al ,Hura and Glassman and Axelbaum et al. Results are available from these flames for propane and ethylene although the former data contain some uncertainty due to the low soot loading.

Other measurements of soot growth rates and surface areas are available in axisymmetric diffusion flames of blends of methane and C4 hydrocarbons. Unfortunately, these data sets do not include gas composition measurements from which the mixture fraction may be deduced. However, it is possible to develop a reasonable prediction of mixture fraction in these flows with existing numerical codes. These predicted profiles of mixture fraction can then be used for a correlation with the local specific surface growth rate. With this information the soot model as it stands now can be evaluated for a range of fuels with the aim of predicting global properties such as the sooting height and the soot yield. An important aspect of the project will be to develop information that is related to the sensitivity of the sooting process to the various sub-models such as inception rates, growth rates and oxidation rates.

CENTER FOR FIRE RESEARCH
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FY 90

Institution:	The George Washington University
Grant Number:	60NANB9DO963
Grant Title:	Products of Incomplete Combustion: Formation and Emission from Diffusion Flames
Principal Investigator:	Professor J. Houston Miller Department of Chemistry The George Washington University Washington, DC 20052 (202) 994-7474
Other Personnel:	Mr. Parviz Hassanzadeh, Doctoral Student Mr. Bijon Ahzani, Doctoral Student Ms. Salma Elreedy, Research Assistant
NIST Scientific Officer:	Dr. Kermit C. Smyth

Technical Abstract:

Reduced Chemistry Description of Diffusion Flame Structure

The earliest mathematical treatment of diffusion flame structure was that of Burke and Schumann [1]. Since the time of this pioneering work, several improvements to the Burke/Schumann model have been made. However, it was not until relatively recently that a new, more realistic approach to thinking about diffusion flame structure has evolved. This can be traced to two improvements over the capabilities available earlier this century: the development of powerful computers and the development of the conserved scalar description for flame structures.

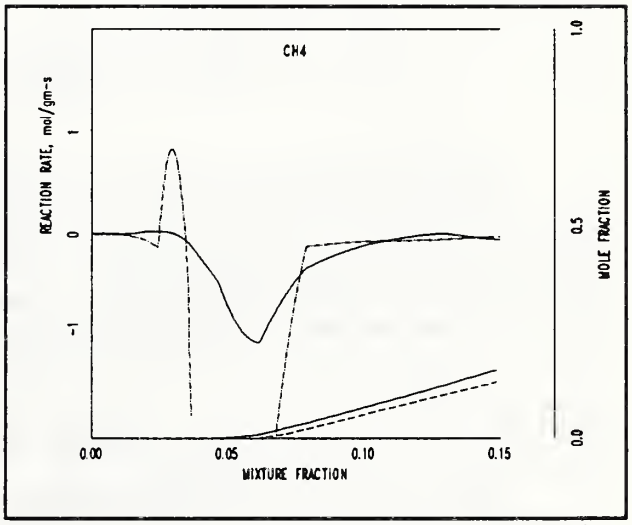

Figure 1: Comparison of experimental and calculated methane concentration and net chemical production rate.

In general, to describe the structure of a diffusion flame requires the solution of both energy and species conservation equations. With modern computers, these equations have now been solved for methane/air diffusion flames in both counterflow and in coflowing, axially symmetric flames

[2,3,4]. However, the codes required for these computations are still much too large to be applied to non-laminar diffusion flames.

Prof. Robert Bilger's group at the University of Sydney has stimulated the efforts aimed at simplifying the analysis of diffusion flame structure. Bilger has been responsible for the methodology of calculating chemical rates from mixture fraction gradients [5], using this to predict carbon monoxide concentrations in diffusion flames [6], and developing reduced mechanisms for diffusion flame chemistry [7,8]. Our extensive data set provides a unique opportunity for the validation of reduced mechanisms, and these comparisons were one of the goals of our recent collaboration with the Sydney combustion community.

Using a 16 species, 58 reaction mechanism, Prof. Mitch Smooke of Yale University calculated chemical composition, temperature, and velocity profiles for a one dimensional, opposed flow, methane/air diffusion flame burning at atmospheric pressure. Bilger's group has analyzed Smooke's mechanism to identify the fastest reactions, and then looked for species whose concentrations were partially equilibrated with other flame species (H atom) and those species for which a steady state analysis was appropriate (O: and CH_3•) [8]. With these simplifications, the following reduced mechanism was derived:

$$CH_4 + 2H\bullet + H_2O \rightarrow CO + 4H_2 \quad \text{(I)}$$
$$CO + H_2O \rightleftarrows CO_2 + H_2 \quad \text{(II)}$$
$$2H_2 + O_2 \rightarrow 2H_2O \quad \text{(III)}$$
$$3H_2 + O_2 \rightleftarrows 2H_2O + 2H\bullet \quad \text{(IV)}$$

For this mechanism, the rates of individual reactions are composites of rates from the original mechanism. For example, the rate of Reaction I is determined by the rates of methyl radical reaction with both atomic and molecular oxygen. Therefore, the rate of disappearance of methane can be written as:

$$\frac{d[CH_4]}{dt} \approx -k_{13}\cdot[CH_3\cdot][O:] - k_{18}\cdot[CH_3\cdot][O_2] \quad (1)$$

Figure 1 compares our results for methane concentration (___) with the full 58 step mechanism (_ _) and for net rate of destruction with the prediction of the Sydney reduced mechanism (_._). The disagreement of the methane destruction rate may be attributable to the uncertainty in the methyl radical concentration estimate. One of the goals of our tunable diode laser diagnostic program (described below) is improved methyl measurements.

Tunable Diode Laser Diagnostics for Diffusion Flames

During the past year a Tunable Diode Laser (TDL) Spectrometer System was obtained through a grant from the National Science Foundation. We have done many preliminary experiments in low pressure cells with CO, CO_2, NO_2, C_2H_2, and CH_4. A copy of the Wolfhard-Parker slot burner was constructed in the GWU shops and was in use by mid May. In addition to some preliminary profile measurements for methane in the flame, we have also done extensive profile measurements for carbon monoxide.

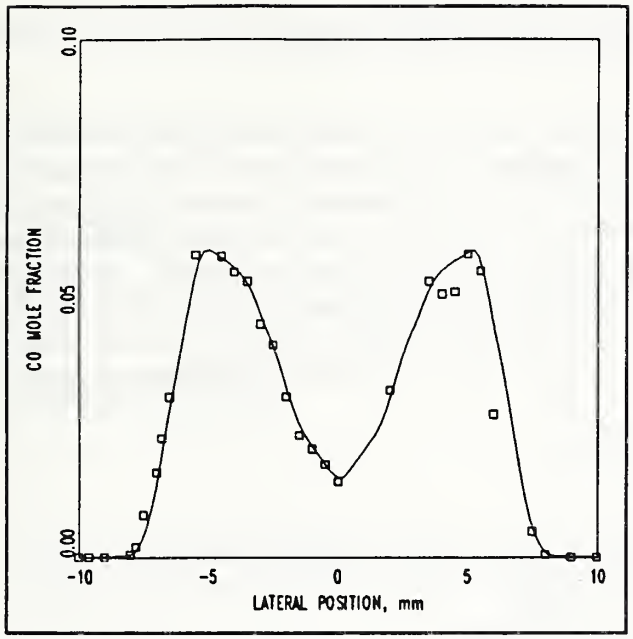

Figure 2: Profile of carbon monoxide concentrations at 9 mm above the burner surface. Each data point was derived from a spectral sweep through the P(8) rotational transition of CO.

Figure 2 shows data concentration data for CO at 9 mm above the burner surface in our methane/air flame. For each data point (□), a spectral sweep across the P(8) rotational line was recorded. A Lorentzian line shape approximation to the data was made with a four parameter fit which included variable line center position, baseline level, line width, and carbon dioxide partial pressure. Similar results were obtained with other CO ro-vibrational transitions.

Estimation of the Kinetic Parameters for PAH Agglomeration in Flames

Chemical growth reactions which occur during hydrocarbon combustion lead to the formation of polycyclic aromatic hydrocarbons (PAH) and carbonaceous soot particles. In large scale fires, thermal radiation associated with soot dominates the energy transfer processes which control flame spread, the rate of fuel pyrolysis, and the temperature field within the flame. In addition, the rate of soot particle formation is associated with the smoke generated by a fire. Because of the importance of soot in fire related phenomena, any useful fire model must contain a predictive capability for soot particle generation.

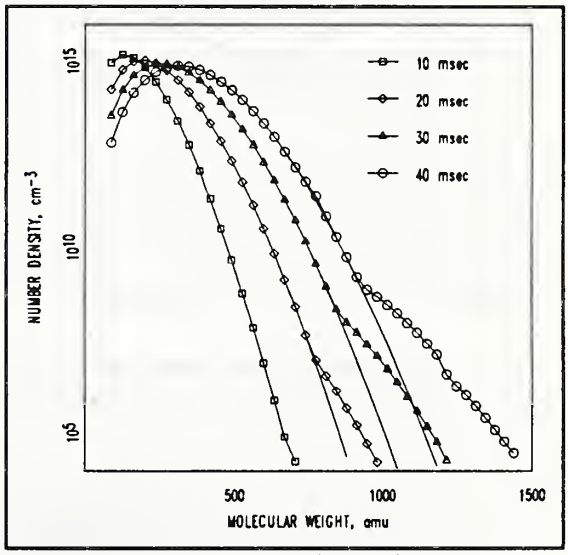

Figure 3: Results of simulation of PAH growth for a model which includes chemistry alone (the solid lines) and the same model with the inclusion of PAH agglomeration (the lines with symbols).

PAH have often been invoked as important intermediates in the chemical processes which lead from hydrocarbon fuels to soot particles. These species, which are found in all sooting, hydrocarbon flames, have structures similar to the graphitic morphology which has been observed in the final particles, and possess carbon to hydrogen ratios in between typical fuels ($<\approx 1$) and soot particles (>5). In recent years models which were developed to follow the chemical transformations of simple fuels into multiple ring structures have been reasonably successful at predicting aromatic concentration profiles in both shock tubes and premixed flames.

However, there remains a conceptual gap in our understanding of particle formation: how do large planar PAH form into three dimensional particles?

To examine the role of agglomeration in PAH growth, we recently developed a model which combines a mechanism for chemical growth with agglomeration. The results of a simulation of PAH growth is shown in Figure 3. This data show that growth is dominated by chemistry at short times before appreciable concentrations of heavy PAH have accumulated. Later in time, dimers of heavy PAH are formed which survive long enough to serve as nuclei for continued growth. At this point an enhancement in the growth rate occurs and a bimodal size distribution is evident. The departure of the model which includes agglomeration from that with chemistry alone occurs only when the reduced mass of the colliding pair is greater than $\approx$ 400 amu (or when the PAH mass reaches 800 amu).

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Publications during this reporting period:

1) "Mechanistic Destruction of Toluene in Diffusion Flames", A. Hamins, D. Anderson, and J.H. Miller, **Combustion Science and Technology 71**, 175 (1990).

2) "Concentration Measurements and Production Rate Analysis of OH· in a Laminar Methane/Air Diffusion Flame", K.C. Smyth, P.J.H. Tjossem, A. Hamins, and J.H. Miller, poster session, **Combustion and Flame 79**, 366 (1990).

3) "The Kinetics of Polynuclear Aromatic Hydrocarbon Agglomeration in Flames", J.H. Miller, **The Twenty-third International Symposium on Combustion**, in press.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	The Pennsylvania State University
Grant No.:	60NANB01035
Grant Title:	Fundamental Mechanisms of CO and Soot Formation in Diffusion Flames
Principal Investigator:	Dr. Robert J. Santoro Department of Mechanical Engineering 130 Research Building (East) University Park, PA 16802
Other Professional Personnel:	T. F. Richardson, Doctoral Student R. Puri, Doctoral Student
NIST Scientific Officer:	Dr. Kermit C. Smyth

Technical Abstract:

Introduction The occurrence and growth of a fire is characterized by a complex set of phenomena involving the interaction between combustion and fluid mechanical processes. Over the past decade an extensive effort has been undertaken to understand these basic processes and their relationship to fire protection. With the major objective to limit the loss of life and property, an emphasis has been given to developing a better understanding of the manner in which fires propagate and the impact of the species produced in a fire. Through the incorporation of this understanding into suitable fire modelling efforts, systematic design and assessment tools have been developed and continue to evolve. Clearly, improved performance of these modelling approaches relies on continued development of our understanding of the basic phenomena involved in fire situations.

In recent years numerous investigations [1-7] have focussed on carbon monoxide (CO) production and emission from fires since CO is widely recognized as the most serious combustion product resulting from fires. High concentrations of CO as well as soot characterize typical fire situations [5,6] and it has also been recognized that there may be a relationship between the CO and soot concentrations observed in fires. In order to avoid the need for detailed chemical kinetic modelling of CO and soot formation and destruction processes in these complex reacting flows, several workers have pursued approaches emphasizing correlations. While some workers [4] have tried to directly correlate their CO and soot data, others [1,2,7-12] have used the conserved scalar approach to correlate CO production with the local equivalence ratio (these relations are referred to as state relationships). However, since the quantity of soot formed in a fire has been shown to be a function of scale [5], the correlation of CO with soot implies that the CO state relationship depends on scale (i.e. residence time) as well and therefore may not be useful over a wide range of conditions. Recent work by Faeth and co-workers have extensively investigated the effects of flame size and residence time on the soot concentration from a state relationship viewpoint for both the underfire (fuel rich) and overfire (fuel lean) regions of buoyant, turbulent flames [8-12]. These studies have shown that, for reasonably long residence times, approximate state relationships can be formulated for soot concentration which allow good predictions of radiation from turbulent diffusion flames characteristic of fires [9,13].

These previous studies have not attempted to examine from a fundamental viewpoint the relationship between soot formation and CO in diffusion flames. In the present study, a more fundamental understanding of the nature of the interaction between CO and soot is sought. Two possible mechanisms that could affect the concentration of CO in the presence of soot, namely radiative quenching and competition for oxidizer species, are examined. Since soot accounts for upwards of 80% of the radiation heat loss from hydrocarbon flames, the resulting lower temperatures in flames containing soot would reduce CO oxidation rates and consequently enhance CO emission. Additionally, soot particles could compete for oxidative species such as hydroxyl radicals (OH) [14], which have a major role in converting CO to CO_2 in the temperature range of interest for fires. The copious amounts of soot present in a typical fire environment could very well result in soot oxidizing faster than CO, resulting in higher concentrations of CO, since soot oxidizes to produce CO.

In the present work, a systematic study of the effects of soot formation on the production of carbon monoxide (CO) in laminar diffusion flames has been conducted. Increased amounts of soot have been observed to result in larger CO mole fractions in the higher regions of the flames. Comparisons of CO state relationships as a function of local equivalence ratio show distinct effects as the local soot volume fraction is varied. Fuel rich regions exhibit lower CO mole fractions as soot concentration increases, whereas higher CO mole fractions are observed under fuel lean conditions. An analysis of the likely mechanisms responsible for these effects has been conducted to explain the observations as well as to identify future research directions.

Technical Accomplishments In order to examine the relationship between CO and soot under well controlled conditions, bench scale laminar diffusion flames have been selected for this study. A fuel mixture approach is adopted to systematically vary the soot concentration in three laminar diffusion flames in which the total carbon flow rate is held constant. Diffusion flames burning pure methane, as well as methane-butane and methene-butene mixtures, have been used to vary the soot concentration. Axial (centerline) measurements of major species concentration and the temperature field in these flames have been carried out. Concentrations of OH at the measured temperature and local equivalence ratio are estimated based on chemical equilibrium. Data on soot concentration and velocity measurements in identical flames have been obtained from the work of Richardson and Santoro [15]. Table I presents the results for the temperature, CO concentrations, CO oxidation rates and soot volume fraction as a function of equivalence ratio (ER) for the three flames studied.

Profiles of the CO mole fraction as a function of time are shown in Figure 1 for the three flames. These profiles were obtained from sampling probe measurements made along the axis of the flame along with appropriate velocity measurements to convert the spatial profiles to temporal profiles. The methane-butene flame, which produces the most soot, has the smallest CO gradient and temperatures. Similar distinctions regarding the importance of soot on the CO mole fractions are observed if the results are compared on an equivalence ratio basis (see Figure 2). Opposite effects are observed in the fuel rich and fuel lean regions with smaller CO mole fractions observed in the fuel rich region as the sooting propensity increases (methane-butene > methane-butane > methane) while the converse is observed in fuel lean regions. Similar results have been observed in larger scale fire studies [1,5], lending interest to a better understanding of the mechanisms responsible for these observations.

To assess the potential importance of temperature and competition for OH resulting from soot oxidation, calculations of the appropriate CO [16] and soot oxidation [14] rates by OH have been evaluated. For CO oxidation, temperature affects the magnitude of the reaction rate constant as well as the OH concentration. The present analysis indicates that the OH concentrations are more significantly affected for the temperature variations observed in these flames, while effects on the reaction rate constant are small by comparison. Furthermore, these OH concentration variations appear to be significant enough to account for the observed

differences in the fuel lean regions of the flame as soot concentration is varied. However, in the fuel rich region, no direct correlation between the equilibrium OH concentration and the variation in the CO oxidation rate was observed. Thus, the mechanism responsible for the behavior in the fuel rich region remains unresolved at this time.

A similar analysis for the soot oxidation rate indicates the competition for OH by oxidizing soot particles can represent a viable mechanism for accounting for the lower CO oxidation rates observed as soot concentration increases. This analysis held for both fuel rich and fuel lean regions. However, present uncertainties in the OH reaction efficiency and the actual soot surface area have precluded a quantitative evaluation of the relative importance of this mechanism as compared to the previously discussed temperature effect.

Summary Competition between soot and CO for OH is a plausible mechanism that can contribute to higher CO emission from fires. Radiative quenching, resulting in lower temperatures, appears to be important in fuel lean regions, but does not account for the observations in the fuel rich regions. Further work in better estimating soot oxidation rates is needed. Specifically, measurements of OH, soot surface area and OH collision efficiency at lower temperatures are required.

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2. Puri, R. and Santoro, R.J., "The Role of Soot Particle Formation on the Production of Carbon Monoxide in Fires", submitted to Third International Symposium on Fire Safety Science.

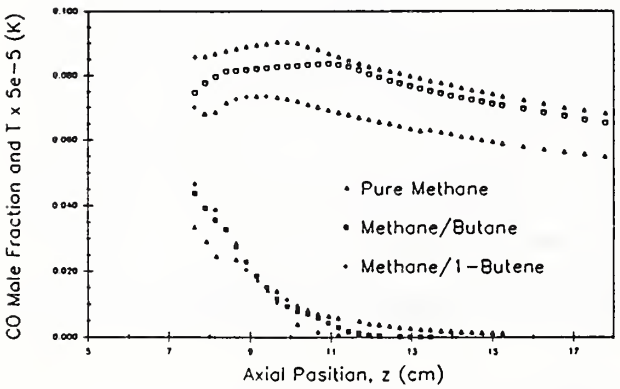

Figure 1. Axial centerline profiles of CO mole fraction (solid symbols) and radiation corrected temperatures (hollow symbols).

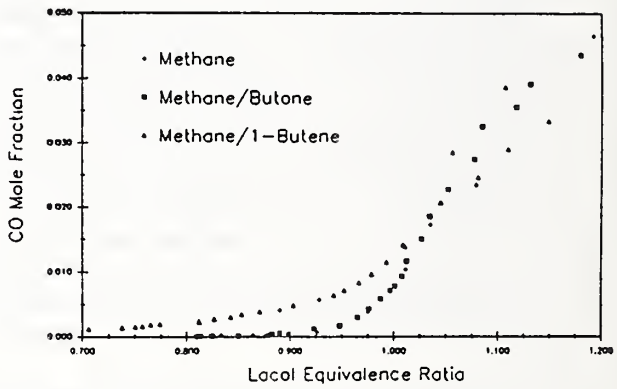

Figure 2. Plots of CO mole fraction along flame centerline as functions of local equivalence ratio - CO State Relationships.

Table I: Comparison of soot volume fraction (f_v), temperature (K), CO concentration (moles/cm^3) and normalized reaction rate of CO, R_{CO} (1/S), at various equivalence ratios in the three flames.

	FLAME A (CH_4 : 9.8 cm^3/S)				FLAME B (CH_4 : 5.6 cm^3/s / C_4H_{10} : 1.05 cm^3/s)				FLAME C (CH_4 : 5.6 cm^3/s / C_4H_8 : 1.05 cm^3/s)			
ER	f_v x10^6	T	[CO] x10^4	R_{CO}	f_v x10^6	T	[CO] x10^4	R_{CO}	f_v x10^6	T	[CO] x10^4	R_{CO}
1.15	0.52	1722	3.015	-98.7	1.74	1529	3.260	-111.5	3.68	1403	2.910	-102.0
1.10	0.56	1736	2.611	-122.4	1.91	1609	2.581	-119.1	3.86	1364	2.463	-105.0
1.05	0.57	1770	1.743	-175.8	2.00	1635	1.663	-147.1	4.09	1467	1.749	-105.4
1.00	0.38	1801	0.559	-383.0	1.68	1661	0.566	-235.0	4.22	1457	1.036	-119.3
0.95	--	1758	0.109	-736.0	0.54	1655	0.140	-390.6	4.31	1397	0.604	-131.9
0.90	--	1673	0.029	-332.2	--	1616	0.059	-574.8	4.33	1334	0.423	-107.0
0.85	--	1624	0.015	-363.7	--	1549	0.012	-201.6	4.34	1293	0.308	-91.6

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	University of Missouri-Rolla
Grant No.:	60NANB9D0953
Grant Title:	A study on the scavenging and in-cloud processing of combustion aerosols
Principal Investigator:	Dr. Donald E. Hagen Dept. of Physics G-7 Norwood Hall University of Missouri-Rolla Rolla, MO 65401
Other Professional Personnel:	M.B. Trueblood, Sr. Research Aide A.R. Hopkins, Research Engr. D.R. White, Assoc Prof Basic Engr & Cloud Physics J. Podzimek, Prof Mech & Aero Engr J. Schmitt, Assoc Prof Physics J. Carstens, Prof Physics
NIST Scientific Officer:	Dr. George Mulholland

Technical Abstract:

Introduction The behavior and evolution of combustion aerosol in the atmosphere is an important problem in atmospheric science. Much effort has been put into the development of numerical models to simulate this aerosol evolution. Here we are undertaking laboratory studies into the fundamental microphysics of several processes which control aerosol evolution. We are focusing on processes germane to the embryonic stage of cloud formation. We are using the UMR Cloud Simulation Facility to examine the scavenging and in-cloud processing of combustion aerosols. The aerosols are those resulting from the combustion of liquid fuels, such as kerosene, jet fuel, and crude oil. An existing combustion aerosol generation system has been modified to handle crude oil combustion on a laboratory scale. These studies are covering both static and time-dependent thermodynamic conditions. The experimental results will be translated into a form suitable for use as inputs into the numerical models used to describe the overall evolution of combustion aerosols in the atmosphere.

Experimental Approach A number of specialized laboratory facility refinements have been made in order to facilitate the combustion aerosol scavenging experiments: new saturators for the aerosol generation and characterization laboratory, fluorescent aerosol spectrometer, and a technique for real time correction to the expansion cloud chamber pressure profile.

The new aerosol laboratory saturators were designed to correct a problem which arose concerning the dew point of the air being put into the simulation chamber for the combustion aerosol scavenging experiments. The problem was that water vapor diffusion between the sample air and the sheath air was occurring in the EAC's used to size the two aerosols for the experiment. Our solution was to construct two simple saturators to bring the aerosols to the proper dew point before they were sent to the EAC's.

The polydispersed aerosol flows are now directed through the saturators, thus bringing their dew points up to the temperature at which the two saturators are maintained. The dew points of the two aerosol flows are so close to that of the sheath air flows that now an insignificant transfer of water vapor occurs between the two; thus the monodisperse aerosols have the desired dew points.

Dew point tests of the sample aerosol laden air being fed to the cloud simulation chamber have shown that this solution works.

Combustion aerosol scavenging experiments using a fluorescence method to detect (count) scavenging are planned; and to this end a suitable optical particle counter (spectrometer) that can detect fluorescence is under development. The following improvements have been made in this device. The optical system has been redesigned to improve the parallelism of the light passing through the interference laser blocking filter. A new notch interference filter has been obtained, one that matches the fluorescent spectrum of the fluorescent dye we use. We now find that turning on the laser, introduces "noise" only at the level of the dark current in the photomultiplier tube.

The improved device has been tested. We grew water drops on fluorescent dye and NaCl particles. For NaCl particles of all sizes we detected 0.5% as "fluorescent"; for 0.2 micron dye particles we detected 45% as fluorescent; finally at the smallest size we were able to produce water drops with in this test, for 0.05 micron dye particles we detected 6% of the drops as fluorescent. Clearly the device is functioning properly but the detection percentage must be improved.

Cloud simulation chamber operation requires the provision of two time dependent functions: wall temperature and gas pressure. Normally the temperature is calculated via thermodynamics before the experiment, and depends on several experimental parameters: e.g. initial relative humidity and temperature, aerosol size, critical supersaturation, concentration, etc. The scavenging experiments are especially sensitive to these parameters, and they are difficult to bring sufficiently close to their design values.

Here we developed a strategy to bring the various experimental parameters to values near their prescribed values, and then in real time compute a pressure profile based on their measured values. Special provisions were made by the campus computer center in order to allow us to gain high priority access to the campus mainframe computer. This allows the required computations to be done within a few minutes of wall clock time, and the results transferred into the computer attached to the cloud chamber. This gives us a considerable increase in our chamber control capability.

Technical Accomplishments The results from our first series of experiments has been completed, written up, and accepted for publication in Atmospheric Environment, and a final revised manuscript is enclosed. The title is "Combustion aerosol scavenging". A copy of the manuscript is attached. Measurements were made of scavenging rates for combustion aerosols by larger collector particles using the changes which the combustion particles induce in the scavengers when deposition occurs. The presence of the small combustion particles was found to dramatically lower the critical supersaturation of the composite particle, and this allowed us to differentiate between the large pure particles and those which collected a small one. The scavenging was found to occur at faster rates than those predicted by Brownian scavenging theory.

Considerable effort was spent expanding the effort to measure the scavenging of combustion aerosol in the size ranges 0.07, 0.09, and 0.11 μm diameters by 0.314 μm collector particles (fixed size). This work was reported at the 1990 AAAR (American Association for Aerosol Research) conference.

Laboratory experiments have been performed in order to determine to what extent the deposition of carbon (combustion aerosol) particles can affect the activation of well defined pure condensation nuclei such as sodium chloride and to study the way in which the carbon particles are distributed within the solution droplets. A significant effect was found for NaCl nuclei (dry particle diameter D=0.425μm) after several hours of exposure to the carbon aerosol (D_g=0.05 - 0.07μm) generated by a blowtorch. The critical supersaturation of sodium chloride nuclei with deposited carbon particles was slightly lowered in all samples. Analysis of electron micrographs shows that carbon particles are deposited on the droplet surface and in the core as well. A simple model of a droplet with insoluble deposited particles has been suggested. These results have been accepted for publication in Atmospheric Environment in a paper entitled "Condensation nuclei activation or deactivation by deposited insoluble particles".

C. CO PREDICTION

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

CARBON MONOXIDE PRODUCTION AND PREDICTION

Professional Personnel

William M. Pitts, Project Leader
Vytenis Babrauskas, Head, Fire Toxicity Measurement Group
Emil Braun, Physicist
Leonard Y. Cooper, Mechanical Engineer
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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 CFR models of fire behavior.

Technical Accomplishments

During FY90 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 assess 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 divided by the ratio of fuel and air required for complete combustion to water and carbon dioxide.

1. Effects of Vitiation on the Production of CO (Mulholland)

In the past it has been hypothesized by some that combustion of a fuel in the presence of vitiated air leads to the production of high concentrations of CO. Such a production mechanism could be very important for enclosure fires where combustion often occurs under vitiated conditions. During the past year the levels of CO generated during burning of gaseous and solid fuels in vitiated gases have been studied in a modified cone calorimeter. The new design features include an adjustable total flow through the chamber, variable O_2 concentration, load cell separated from combustion chamber, overpressure panel on back of cone enclosure, and a radiation shield for the specimen.

The yield (g CO produced/g fuel consumed) of CO as a function of decreasing oxygen mole fraction has been measured for two gaseous fuels--methane and propane--and four solid fuels--polymethylacrylate (PMMA), acrylonitrile-butadiene-styrene (ABS), polyethylene-surlyn (PE), and Douglas fir. Most measurements were recorded using nitrogen as diluent, but several tests were run with carbon dioxide. The results show that CO yields increase as the oxygen concentration is reduced. For methane, which generates quite low levels of CO in air, the increase is roughly a factor of 30. For all of the other fuels the increase is a factor of five or less. It is important to note that these increases in yield are negligibly small in comparison to those observed when fuels are burned in underventilated conditions.

Based on the findings of this study we conclude that burning in vitiated conditions is not sufficient to generate the high levels of CO often observed in full scale fires.

Comparison of the results for nitrogen and carbon dioxide diluents suggest that the small increases in production of carbon monoxide are correlated with flame temperature. This finding may provide important insights into the in-fire production of carbon monoxide.

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

A necessary condition for the GER concept to hold is that the layer of gases outside of and above the fire be nonreactive. For GER values less than 0.5 this is expected to be the case since very little fuel or products of incomplete combustion are present. As the GER becomes greater than $\approx$ 0.5 the upper layer composition starts to change. Experiments indicate that in addition to CO_2 and water; unreacted fuel, a variety of hydrocarbons and soot, carbon monoxide, and hydrogen are found in an upper layer in increasing amounts with increasing GER. For sufficiently high upper layer temperatures, additional chemical reaction outside of the immediate flame zone is to be expected for these rich conditions.

A modeling effort has been initiated to determine the stability of an upper layer assuming only homogeneous (i.e. gas phase) reactions are important. The role of heterogeneous reactions (e.g., those involving soot) will be the subject of a later study. Since previous experimental investigations have indicated that the upper layer molecular composition is uniform for regions outside of the fire plume, the upper layer is treated as a perfectly stirred reactor. A full kinetic code developed at Sandia National Laboratories (P. Glarborg, R. J. Kee, F. Grcar, and J. A. Miller, "PSR: A Fortran Program for Modeling Well-Stirred Reactors," SAND86-8209, July, 1987) is being used to investigate the chemical stability of gas mixtures which are typical of those observed in an upper layer when natural gas is the fuel.

Calculations are made as a function of GER, residence time in the upper layer, and the temperature of the upper layer. Early indications are that homogeneous reactions are relatively slow for temperatures less than 900 K, but that for higher temperatures, reaction channels open up and the composition of the upper layer begins to change as the residence time is increased. Most previous investigations of the GER concept have been made for conditions where the upper layer temperature is less than 900 K. It should be noted that upper layer temperatures in full scale fires often reach levels in excess of 1300 K suggesting that homogeneous reactions may be fast enough to invalidate the GER concept for certain phases of real fires. Work is continuing to characterize the conditions for which the GER concept is appropriate for characterizing CO production during underventilated burning.

3. Fabrication of a Reduced Scale Enclosure for Fire Studies (Braun)

Despite the importance of the problem, very few detailed investigations of CO production during full scale fire tests are available. The principal reason for this lack of data is the high cost associated with full scale testing. An approach which is often used is to perform experiments on a reduced scale where costs are lower and the tests are more easily manageable. A major drawback to this approach is that all the important fire parameters cannot be scaled simultaneously. Despite this, reduced scale testing has contributed immensely to the understanding of fire behavior for conditions where the effects of scaling are properly understood. A reduced scale enclosure is being fabricated here at CFR and will be used to characterize CO formation for a variety of test conditions and fuels. Once an extensive data base is available, selected full scale tests will be carried out to assess the effects of scaling.

Dimensional scaling has been used for the design of the reduced scale enclosure. The relative dimensions are based on those for the proposed ASTM Procedure "Proposed Method for Wall and Ceiling Materials and Assemblies" which includes a specification for a test room which is used in a number of laboratories for a variety of fire tests. The prescribed room is a 2.44 x 3.66 x 2.44 m^3 enclosure with a 0.76 x 2.03 m^2 doorway centered in one of the short walls. The reduced scale enclosure has dimensions corresponding to a 2/5 scale factor (i.e., 0.98 x 1.46 x 0.98 m^3). The doorway is scaled such that $Ah^{1/2} = 2/5$. This is the standard procedure for properly scaling enclosure ventilation. The reduced scale enclosure is designed in such a way that the wall containing the doorway can be replaced with ones having differently sized doorways. In this manner the ventilation factor for the room can be easily varied. Instrumentation currently includes thermocouples and a variety of NDIR concentration meters. The enclosure has been constructed. Tests are expected to commence shortly.

4. Development of a Mathematical Model for the Time Dependent Development of CO Concentration in an Enclosure (Cooper)

The experiments which have led to the development of the GER concept have all been steady state. Fires are dynamic events and the concentrations of flame gases in an upper layer are expected to change during the fire history. At early times the upper layer is likely to be lean, but as the fire grows and combustion products build up, the layer will become richer and richer with considerably higher concentrations of CO to be expected.

A general model has been developed for predicting the generation rates of oxygen, fuel, and any other products of combustion in rooms containing fires. An algorithm for implementing the model has also been prepared. During the past year the model was exercised for the special case of complete combustion. During the coming year it will be extended to cases for which products of incomplete combustion are generated.

Reports and Publications

"Long-Range Plan for a Research Project on Carbon Monoxide Production and Prediction," W. M. Pitts, National Institute of Standards and Technology Internal Report, October 1989.

"The Effect of Oxygen Concentration on CO and Smoke Produced by Flames," G. Mulholland, M. Janssens, S. Yusa, W. Twilley, and V. Babrauskas, submitted to the 3rd International Symposium on Fire Safety Science.

"A Model for Predicting the Generation Rate and Distribution of Products of Combustion in Two-Layer Fire Environments," L. Y. Cooper, National Institute of Standards and Technology Internal Report, NISTIR 90-4403, October, 1990.

"Effects of Global Density Ratio on the Centerline Mixing Behavior of Axisymmetric Turbulent Jets," W. M. Pitts, accepted for Experiments in Fluids.

"Reynolds Number Effects on The Mixing Behavior of Axisymmetric Turbulent Jets," W. M. Pitts, accepted for Experiments in Fluids.

"Large-Scale Turbulent Structures and the Stabilization of Lifted Turbulent Jet Diffusion Flames," W. M. Pitts, accepted for the Twenty-Third Symposium (International) on Combustion.

Related Grants

"Soot Particle Formation and Destruction in Diffusion Flames," Robert J. Santoro, Pennsylvania State University.

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

"Experimental Studies of the Environment and Heat Transfer in a Room Fire," Edward E. Zukoski, California Institute of Technology.

"Compartment Fire Combustion Dynamics," R. J. Roby, Virginia Polytechnic Institute and State University and C. L. Beyler, Fire Science Technologies.

"Chemical Pathways to the Formation and Emission of the Products of Incomplete Combustion in Diffusion Flames," J. H. Miller, George Washington University.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution: Virginia Polytechnic Institute & State University

Grant No.: 60NANB8D0829

Grant Title: Compartment Fire Combustion Dynamics

Principal Investigators: Richard J. Roby
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NIST Scientific Officer: Dr. William M. Pitts

Technical Abstract:

This abstract covers the second year of a project on compartment fire combustion dynamics. This program is directed toward understanding the generation and spread of toxic gases, particularly carbon monoxide, in realistic compartment fires. As most fire fatalities are the result of exposure to toxic products of combustion, it is essential that methods be devised to evaluate the toxic hazards posed by specific materials in varying building designs. While toxic products are produced during both smoldering and open combustion modes, the rate of generation of toxic products of incomplete combustion, such as carbon monoxide, is greatest under conditions where compartment flow dynamics create oxygen deficient combustion.

The current three year research effort is designed to experimentally 1) determine the effects of realistic fire flows on species generation rates and their correlation with equivalence ratio, 2) establish major toxic gas and smoke generation rates for important fuels such as PMMA, wood and TDI-based polyurethane, and 3) determine the efficiency of external flames in destroying major toxic gases produced within the compartment during oxygen deficient combustion.

Two fuels were investigated during the second year. Hexane was utilized first as an easy and chemically simple fuel to analyze followed by preliminary tests of PMMA. Measurements consisted of CO, CO_2 and O_2 concentrations, temperatures within the compartment, fuel volatilization rate and air entrainment rate. The compartment has two

ventilation paths. There is an inlet air duct at the base of the compartment in which the entrained air rate is measured with the use of a linear velocity probe. Secondly, a window style exhaust vent is sized so that there is only outflow of the combustion products. By varying the fuel surface area and the exhaust vent size different steady-state equivalence ratio fires are obtained. Overall equivalence ratio is the ratio of fuel volatilization rate to air entrainment rate normalized by the stoichiometric fuel to air ratio.

Several notable observations have been made that show the strong dependance of compartment fire characteristics on transition from overventilated (equivalence ratio less than one) to underventilated conditions. Negligible CO concentrations (less than 0.1%) exist until the overall equivalence ratio reaches a value near one. As the compartment becomes underventilated the CO concentration rises sharply reaching lethal levels as high as 3.5 percent for an equivalence ratio of 2.8. The CO_2 concentration also rises sharply and reaches a maximum within 20 seconds after the transition. The O_2 concentration in the upper layer sharply decreases to less than half a percent as the compartment becomes underventilated, reaching equivalence ratios greater than 2. The transition to underventilated conditions is also marked by continuous external burning out of the vent with flame lengths on the order of the compartment size. At the time of transition the upper layer in the compartment either has all ready reached or levels out to a steady-state temperature.

The hexane experiments show repeatable correlations between species yield and overall equivalence ratio. Yield is the grams of species produced per gram of fuel burned. The correlations between steady-state yields and overall equivalence ratio are shown in Figures 1 and 2. As can be seen the correlations are similar to Beyler's hood experiments. The CO yield correlated with the equivalence ratio exhibits a primarily two value function with a transition region between an equivalence ratio of 1 and 1.5 to 2. At equivalence ratios greater than 1.5 a leveling off of CO yield is observed at approximately 0.19. Figure 1 shows an offset between Beyler's rise in CO yield to the results of these tests. This offset is believed to be the result of Beyler's use of an upper layer equivalence ratio rather than an overall equivalence ratio based on the air entrained. Zukoski has discussed this equivalence ratio difference and has presented a correlation for CH_4 in agreement with the results presented here. The O_2 yield is the grams of O_2 consumed per gram of fuel burned.

Hexane fires with steady-state equivalence ratios of 2 or greater exhibit transient yield to equivalence ratio correlations similar to the steady-state correlations. The transient correlation is obtained from the transient data of one fire where as the steady-state correlation is obtained by using the steady-state value from each fire. A transient correlation is shown in Figure 3 for a fire with a steady-state equivalence ratio of 2.85. Comparing Figure 3 to Figure 1 one can see the close comparison between the transient and the steady-state correlations. The CO yield rises sharply at equivalence ratio of 1.1 and begins to level out an equivalence ratio of 2.

As the fire progresses, a layer of hot combustion products is formed in the top of the compartment and is noted as the upper layer. The lower layer is ambient air which is preheated prior to being consumed in the fire. Figure 4 shows temperature profiles in the compartment at three different times during a fire with a steady-state equivalence ratio of 1.3. Temperature measurements are made with a tree of eight aspirating thermocouples located in the front corner of the compartment. As the fire progresses the upper layer grows and moves further down in the compartment and reaches a steady state depth of 24 inches. The upper layer is well mixed as shown by the uniform temperature profile. Additionally, species concentration measurements verify the uniform layer assumption. A large temperature gradient indicates the thermal layer interface. The layer interface is not able to be seen during an experiment but is assumed to be steady with little mixing. Transient temperature plots of the thermocouples bordering the large temperature

gradient show no fluctuation in temperature and, therefore, suggests that any mixing of the upper and lower layers occurs in an interface less than the thermocouple spacing of four inches. A narrow window will be installed down the side of the compartment in order to make visual observations of the layer during an experiment.

PMMA samples burned consisted of 3/16 inch and 3/4 inch thick 8x8 and 12x12 inch squares. The initial PMMA tests repeat several of the conclusions observed from the hexane tests: temperature profiles show the establishment of a two layer system and overventilated fires show no CO and no external burning. Oxygen concentrations of 9 to 17 percent have been observed for the tests performed. In order to reach underventilated conditions larger size PMMA sheets will be burned.

Future work

Future work includes completing PMMA and wood studies and determining the efficiency of external flames in destroying major toxic gases produced within the compartment during oxygen deficient combustion. Attempts will be made to destroy the two layer system in order to test the robustness of the yield to equivalence ratio correlation. Two configurations will be used to examine the effect of external flames on ultimate species yields. One configuration will simulate a window vent where the flame will be allowed to flow up the side of the outside wall. This configuration should allow for high rates of entrainment of outside air. A second configuration will use a "ceiling" outside the vent to force the flame to flow horizontally. This configuration, similar to the flame issuing into a corridor, should allow for much lower rates of entrainment of outside air. Total hydrocarbon measurements will be made upon the addition of an FID analyzer. A soot measurement device will also be added.

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 under fuel-rich compartment fire conditions. In addition, through the experiments involving external flames, it will provide information about the spread of toxic species from the compartment of fire origin. Since the spread of toxics 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. This knowledge will allow for informed decisions concerning the regulation of materials and the design of firesafe buildings. Based on the emerging understanding of the effects of chemical structure of fuels on the toxic species produced, this work may ultimately allow the development of new materials with better fire properties. By providing detailed information of compartment fire dynamics under well controlled and documented conditions, this work directly supports the development of computer fire models. These models will ultimately be used for the design and evaluation of buildings for fire safety.

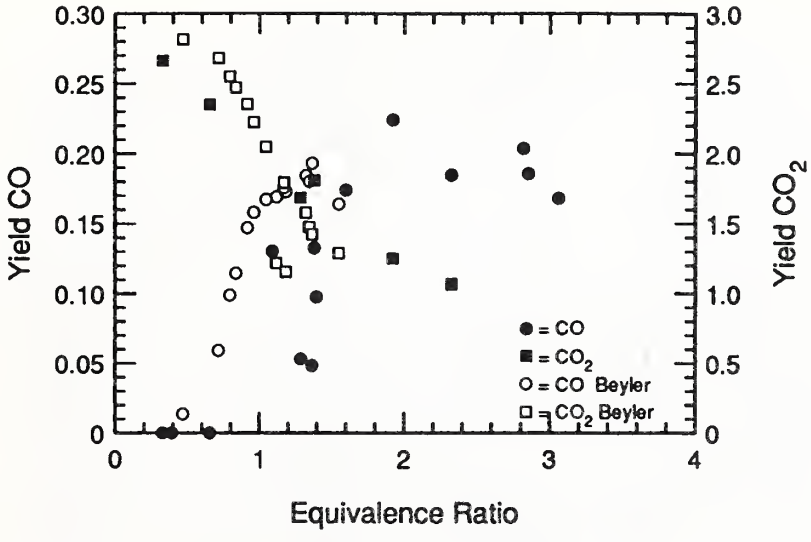

Figure 1.

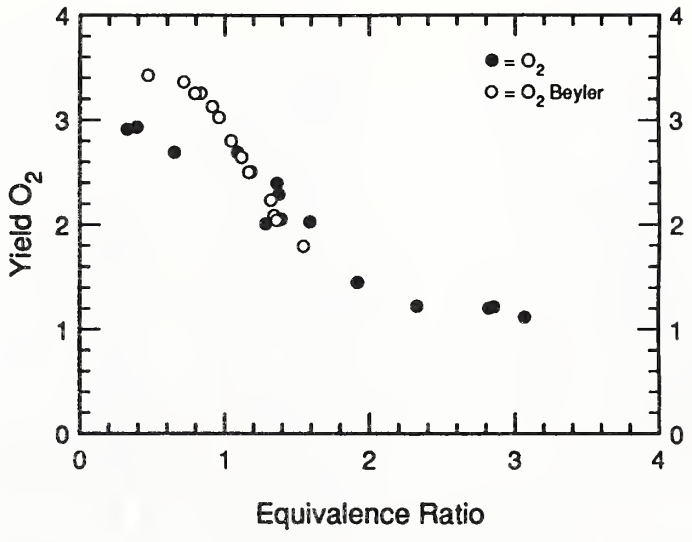

Figure 2.

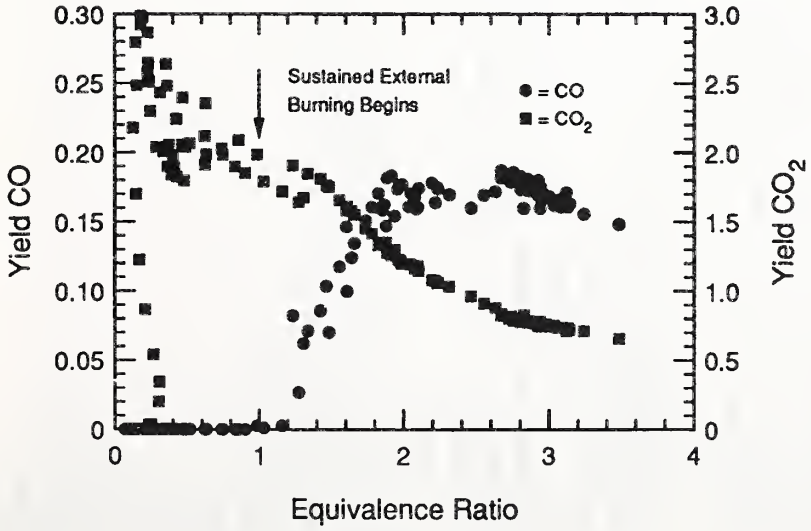

Figure 3.

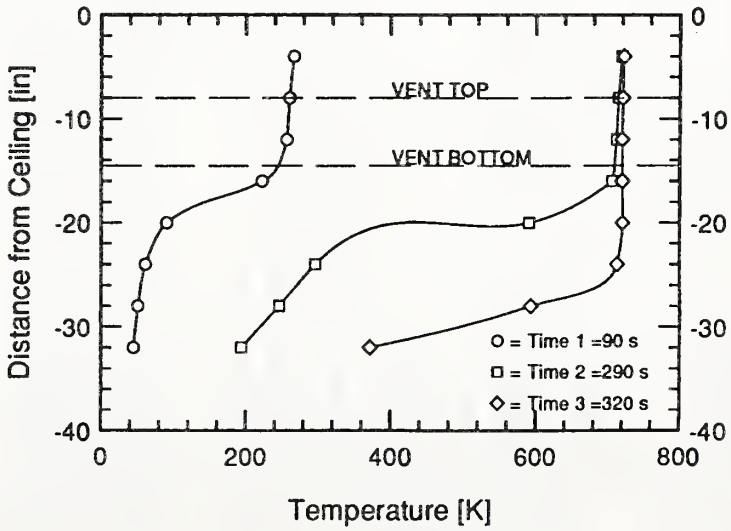

Figure 4.

CENTER FOR FIRE RESEARCH

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

FY 1990

Institution:	California Institute of Technology
Grant Number:	60NANB9D0958
Grant Title:	Experimental Study of Heat Transfer and the Environment of a Room Fire
Principal Investigator:	E. E. Zukoski 301-46 California Institute of Technology Pasadena, California 91125
Other Professional Personnel:	T. Kubota, Professor Emeritus J. H. Morehart, Doctoral Student R. Chan, Doctoral Student R. McGuffin, Doctoral Student
NIST Scientific Officer:	Dr. Leonard Cooper

TECHNICAL ABSTRACT:

INTRODUCTION The products of combustion produced in various situations in accidental fires and the flow of gravity currents in hallways are under investigation in an experimental program. The first subject will be discussed here and progress in the latter area will be described at a subsequent meeting.

The composition of the gas surrounding large diffusion flames, characteristic of unwanted fires, can have a profound effect on the structure of the flame and the composition of the gases produced in the flame. We are studying three possible situations or *modes* of combustion.

During the development of the fire in an enclosure, a stratified and homogeneous layer may be formed at the ceiling which is composed of a mixture of products of combustion and air, called here a *vitiated* gas. Very early in the history of the fire, the flame is surrounded by undiluted air at room pressure and temperature, and the flame is defined to be in the first mode. If the ventilation

of the enclosure is restricted, the thickness of this vitiated layer will grow in time. The flame is defined to be in the second mode when the region of flaming combustion intrudes into this vitiated gas layer so that part of the flame entrains pure air and part, vitiated gas. The third mode is reached when the vitiated ceiling layer descends below the base of the fire so that the entire flame is immersed in vitiated gas and only vitiated gas is entrained into the fire plume.

In the first mode, the generation of incomplete combustion products is very small. In the second mode, substantial amounts of carbon monoxide and products of incomplete combustion are produced when the equivalence ratio of the gas in the upper layer increases above one. The species produced in this mode have been investigated for ethylene and propylene fuels during the past year and these measurements supplement earlier results obtained with natural gas[1-3]. Other measurements[3,4], also completed during the past year, have been made of the characteristics of ethylene, propylene and natural gas flames burning in mode three and these will also be discussed here.

The aim of the work reported here is to obtain the understanding of the combustion and accompanying fluid dynamic processes which is required to make possible the development of computer based numerical models of species production and mass transfer rates in accidental fires.

EXPERIMENTAL METHOD In these experiments, the hot gas layer is contained within a bare-metal hood measuring 1.83 m square by 1.83 m tall and the oxygen mass fraction of the gas within the hood is controlled by injecting air into the top of the hood through a network of 2.54 cm diameter copper supply lines with 365 evenly spaced 1.6 mm diameter holes on 2.54 cm centers. Excess combustion products mixed with the added air are allowed to spill out beneath the bottom edges of the hood and produce a well-defined interface between the recirculating hot, vitiated gas inside the hood and the cool uncontaminated room air. In these experiments, burners with diameters of 8.9, 19 and 50 cm were used and the the fire was stabilized on a 5 cm deep porous bed of 6.3 mm diameter spherical glass beads. The burner surface is held 5 to 15 cm below the bottom of the hood for the mode-two combustion and is located at least 30 cm above the bottom edge of the hood for mode-three combustion.

Gas samples are continuously withdrawn through a 9.5 mm diameter stainless steel tube inserted into the upper layer at an elevation roughly in the middle of the hood and are fed into the sample loop of a gas chromatograph for analysis. In all experiments, measurements were made after holding flow conditions constant for at least 20 minutes.

MODE TWO RESULTS Experiments concerning the production of incomplete products of combustion in flames burning in mode 2 have been carried

out with propylene and ethylene fuels. These experiments are quite similar to those described in the past several years[1] in which natural gas was used as the fuel and air was added to the upper layer. This arrangement allows the equivalence ratio of the upper layer and the gas entering the layer though the fire plume to be different and thus allows this steady state experiment to model the processes which occur during the transient development of the upper layer in a room fire.

The principal results, described in a paper[1] and in more detail in a thesis[3], are also similar to those found with natural gas:

1) The generation of incomplete combustion products is a strong function of the equivalence ratio of the upper layer and is almost independent of the equivalence ratio of the gas in the fire plume at the interface. Carbon monoxide, unburnt fuel and fuel fragments begin to be formed in appreciable amounts when equivalence ratio of the upper layer rises above 0.75 and rise to large values for fuel-rich upper layers. For example, mass fractions of carbon monoxide as high as 0.025 (yields of 24 %) are observed when the equivalence ratio of the upper layer is close to 2 and natural gas was the fuel.

2) The production rates of carbon monoxide and incomplete products of combustion depend in detail on the structure of the fuel molecule but have the same general characteristics.

3) When the equivalence ratio of the upper layer is greater than 0.9, the oxygen mass fraction remaining in the upper layer depends weakly on the temperature of the layer for temperatures in the 100 to 400 C range.

3) Computations show that reaction rates in the upper layer gases are negligible for periods greater than several hundred seconds when the temperature of the gas in the hood is below 700 K.

MODE THREE RESULTS The effects of reducing the oxygen concentration in the ambinet atmosphere on diffusion flames have been the subject of a number of small scale and a few large scale experiments discussed elsewhere[3,4] in this context. The current work differs in the use of large scale and of vitiation to reduce oxygen mole fraction, and in the measurement of the composition of the product gas and flame lengths. Natural gas and ethylene data are presented here.

In these experiments air was supplied to the top of the hood at a steady rate, gaseous fuel was supplied at a fixed rate to a burner flame, and burnt gas was removed from the hood at least 30 cm below the level of the burner surface. After the properties of the gas within the hood reached a steady condition, which required at most 15 minutes, the composition of the gas within the hood and the flame length are measured. The air flow rate was then decreased slightly, to reduce the oxygen mass fraction and increase the degree of vitiation, and the measurements were made again. This process was continued until the flammability limit was defined to within an uncertainty of about 0.005 in the oxygen mass fraction.

Flame lengths, based on a 50 % intermittency level, first increased and then decreased a few per cent as vitiation was increased from zero to a value close to the flame extinction limit. Very close to the limit, radiation from soot in the flame became imperceptible, leaving only a weakly-luminous blue flame which frequently lifted above the surface of the burner. To within the accuracy of the measurements, the hydrocarbon fuels were completely oxidized to water and carbon dioxide, even near the extinction condition, and concentrations of carbon monoxide and other products of incomplete combustion were present at levels below the measurement limit of our instrumentation, about 250 ppm.

Oxygen concentrations measured at the flame extinction limit and calculated values of the limiting flame temperatures for these conditions are in good agreement with values obtained in previous experiments[3,4] despite widely varying experimental techniques and scales of apparatus. Small scale experiments in which vitiation is modeled by adding nitrogen to air appear to give reasonable estimates of the extinction condition for the larger burners.

The application of these results to the extinction of full scale accidental fires depends critically on the motion of the interface past the surface of the burner. In a room fire situation, ventilation parameters and the feedback between the rate of pyrolysis of fuel, the heat release rate of the fire, the heat losses from the layer to the walls and ceiling, and the motion of the interface often prevent the clear cut passage of the interface past the base of the fire. Hence, the combustion process can be left in mode-2 in which the production of undesirable species can be large.

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1. Zukoski, E. E., Morehart, J. H., Kubota, T., and Toner, S. J., Combustion Processes in Two-Layered Configurations, Second Symp on Fire Safety Sci., Tokyo (1988).
2. Zukoski, E. E., Morehart, J. H., Kubota, T., and Toner, S. J., Species Production and Heat Release Rates in Two-Layered Natural Gas Fires, to be published in *Comb. and Fl.* (1990).
3. Morehart, J. H., Species Production in Fires Burning in Two-Layered and Homogeneous, Vitiated Environments, Ph.D. Thesis, California Institute of Technology, 1990.
4. Morehart, J. H., Zukoski, E. E. and Kubota, T., Chemical Species Produced in Fires Near the Limit of Flammability, submitted to *Fire Safety J.* (1990).

D. POLYMER GASIFICATION

Center for Fire Research
Priority Project - 1990

BURNING RATE

Professional Personnel:

T. Kashiwagi, Project Leader
J. Brown, Chemist
S. Fisher, NRC Post Doctoral Fellow
A. Hamins, Mechanical Engineer
H. Nanbu, Guest Researcher
K. Steckler, Physicist

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 models for each component 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 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. Experiment

An experimental apparatus for studying transient gasification of materials exposed to radiant heating in a nitrogen atmosphere was designed. Most components have been purchased or fabricated. These include the 0.6 m diameter X 1.5 m high stainless-steel, water-cooled chamber, pneumatic lift for inserting the sample assembly into the chamber, precision mass balance, and heating elements and controls. Measurements will include temperature profiles within the sample, depth of bubble layer in the sample, and mass of the sample as a function of time.

2. Gasification Rate Model

An analytical surface-absorption model for the one-dimensional gasification of a noncharring thermoplastic material subjected to a specified, time-dependent external radiant heat flux was developed. The model assumes a well-defined vaporization temperature and heat of gasification. Comparisons between the model and experimental results for PMMA at two levels of external heat flux (17 and 40 kW/m^2) show better agreement between theory and experiment at the higher flux level than at the lower flux level. Under the latter condition, sub-surface absorption and degradation processes play a significant role but are not yet represented in the model. Results for the higher flux are presented in Fig. 1. The experimental surface-temperature data (not shown) suggest a vaporization temperature, T_v, of approximately 390 C for this flux.

The next step is to develop a partial differential equation gasification model which accounts for sub-surface absorption and degradation processes.

II. Pool Burning

1. Experiments

Experiments are conducted in a 30 cm diameter water-cooled pool burning apparatus which consists of four concentric rings. Each ring is fed independently to monitor burning rates and to maintain the liquid level close to the burner rim. Experiments have been conducted with a number of liquid fuels including heptane, methyl methacrylate, toluene, and methanol. Figure 2 shows total energy feedback rates determined from measured burning rates and takes into account the energy required to heat the fuel from ambient temperature to the boiling point as well as the energy required to vaporize the fuel. All fuels have highest heat feedback rates at the inner-most ring (Ring 1). Large differences are noted for different fuels.

Transmission measurements through pool flames using a black body source (1200K) and flame radiance measurements using a wide angle radiometer are conducted at a series of radial locations across the pool flame and for a number of heights above the fuel surface. Effective radiation temperatures and gray body absorption-emission coefficients are calculated from this data using an Abel inversion technique.

Flame radiance measurements and mass burning rate data are used to calculate the fraction of idealized combustion energy radiated to the surroundings. These measurements are made for a series of pool flame diameters. A method to estimate the radiative fraction using a single location radiometer measurement was determined.

Experimental measurements of radiative feedback as a function of incoming angle to a series of pool surface locations using a nitrogen purged, water jacketed narrow view angle radiometer are

jacketed narrow view angle radiometer are currently underway. Experiments using oxygen calorimetry to ascertain combustion efficiency as a function of pool diameter and fuel type are being prepared. Additional flame radiance measurements are planned for larger sized pool flames (diameter ≈ 1 meter).

2. Burning Rate Model

A global mass burning rate model based on a mean beam length radiative transfer approximation was developed. A cylindrical flame shape is assumed. Flame temperatures are calculated taking into account radiative losses and combustion efficiency. Gray body absorption-emission coefficients are calculated from a mean beam length approximation and data on the fraction of idealized combustion energy radiated to flame surroundings. Predictions of burning rates are accurate to within a factor of two for luminous flames, but the calculated gray body absorption-emission coefficients are inconsistent with those experimentally determined.

Publications:

Steckler, K.D., Kashiwagi, T., Baum, H.R., and Kanemaru, K., Analytical Model for Transient Gasification of Noncharring Thermoplastic Materials, submitted to the Third International Symposium on Fire Safety Science, Edinburgh, Scotland, July 1991.

Kashiwagi, T., Omori, A., and Nanbu, H., Effects of Melt Viscosity and Thermal Stability on Polymer Gasification, Combustion and Flame **81**, 188-201 (1990).

Hamins, A., Kashiwagi, T., Gore, J., and Klassen, M., Estimate of Flame Radiance via a Single Location Measurement, submitted to Combustion Science and Technology.

Gore, J., Klassen, M., Hamins, A., and Kashiwagi, T., Fuel Property Effects on Burning Rate and Radiative Transfer from Liquid Pool Flames, submitted to the Third International Symposium on Fire Safety Science, Edinburgh, Scotland, July 1991.

Related Grants:

"Flame Radiation", Chang-Lin Tien, University of California at Berkeley.

"The Behavior of Charring Materials in Simulated Fire Environments", Eric Suuberg, Brown University.

"The Structure and Radiation Properties of Pool Fires", J.P. Gore, University of Maryland.

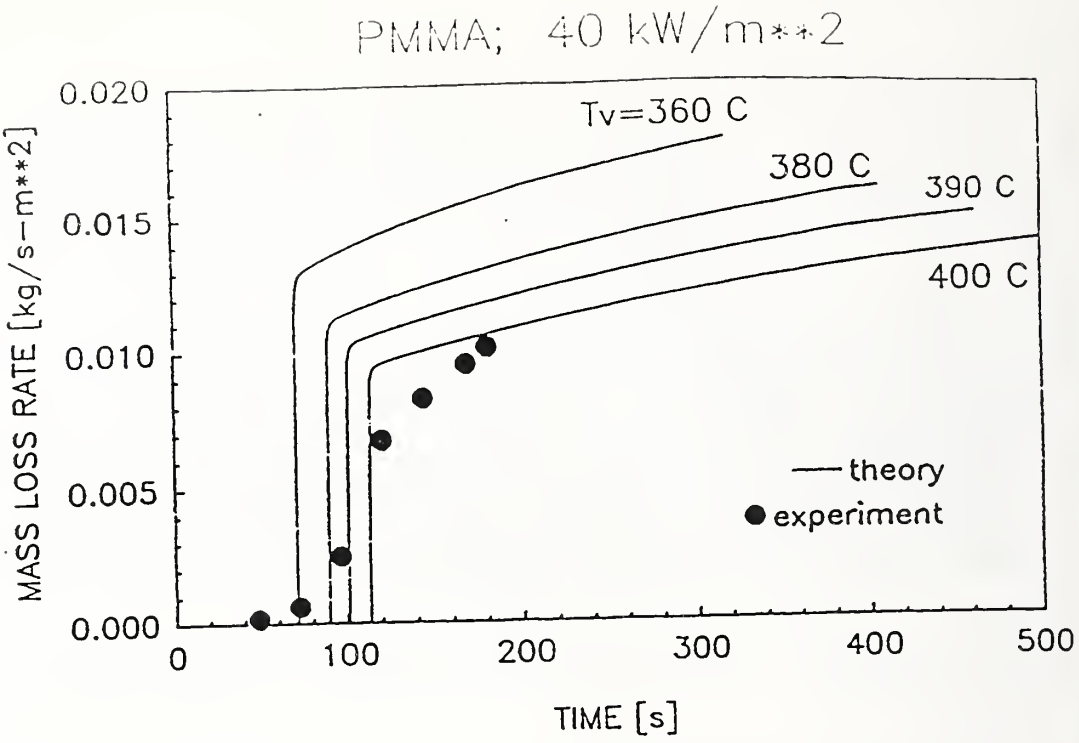

Fig. 1. Mass loss rate of PMMA exposed to 40 kW/m^2 incident heat flux.

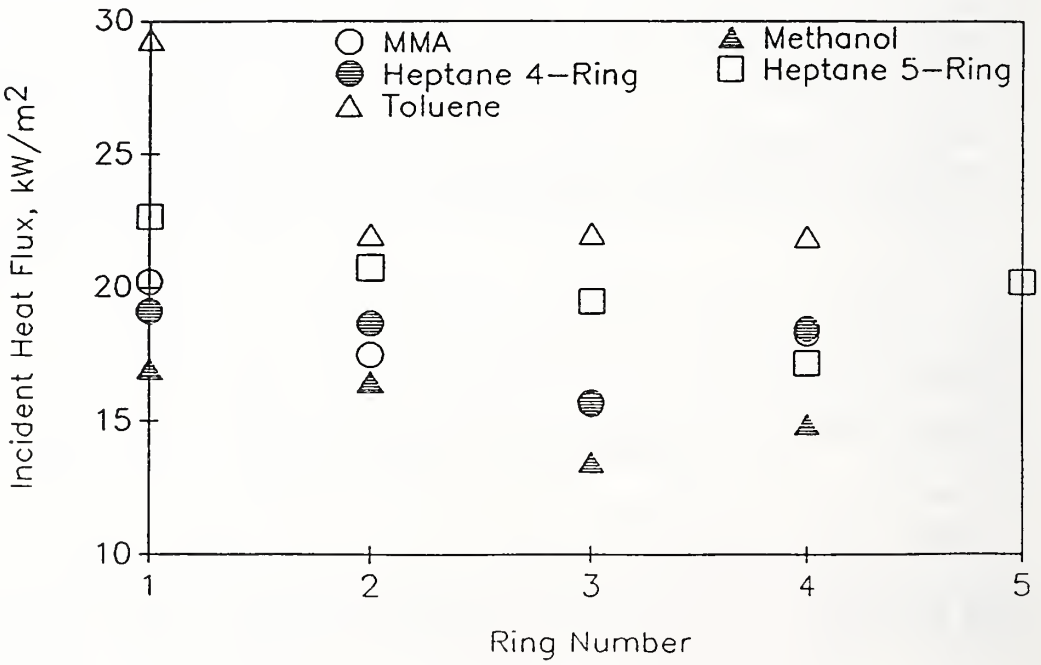

Fig. 2. Incident heat flux on the fuel surface as a function of ring number for various fuels in a pool fire apparatus.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution:	University of California--Berkeley/Irvine
Grant No.:	60NANB4D0827
Grant Title:	Flame Radiation
Principal Investigator:	Dr. Chang-Lin Tien A. Martin Berlin Professor Department of Mechanical Engineering University of California Berkeley, California 94720
Other Professional Personnel:	S. H. Park, Doctoral Student A. Tuntomo, Doctoral Student T. Q. Qiu, Doctoral Student
NIST Scientific Officer:	Dr. Takashi Kashiwagi

Technical Abstract:

Introduction The goal of this research program is to establish a simple analytical framework for the accurate predictions of thermal radiation phenomena in fires, while retaining the fundamental physics of the problem. The products are approximate formulations from careful experimental and theoretical investigations, which simplify the analysis and calculations to a great extent. The thrust of the research was focused on three primary topics: (1) experimental and theoretical determination of the infrared radiation properties of hydrocarbon gases evolved from condensed fuels; (2) development of an accurate radiation model for large pool; and (3) investigation of the effects of the gas-phase radiation absorption on the ignition mechanism of solid plastics.

Radiation Properties of Hydrocarbon Gases. The infrared radiation properties of the evolved gases are important in the prediction of thermal radiation feedback and combustion of large-scale fires. Since current information about the radiation properties of hydrocarbon species is quite limited, a combined analytic and experimental research has been directed at the determination of the radiation characteristics of several gas species common in plastic fires.

The infrared radiation properties of ethylene (C_2H_4), which is one of the important pyrolysates in plastic fires, have recently been determined experimentally [1]. The spectral absorptivities for each of the four infrared-active bands of ethylene have been measured at low resolution for temperature between 300K and 700K. With the aid of narrow-band and wide-band models, the measured data have been correlated to produce spectral, band and total properties. The total emissivity of ethylene is presented in Fig. 1 as a function of temperature for various optical pathlengths. The wide-band parameters have been further employed to develop Planck mean absorption coefficients. Figure 2 compares the Planck mean absorption coefficients of ethylene with those of other gaseous combustion products. These results are useful for the calculation of radiation heat transfer in multiple gas systems as well as single gas systems.

Thermal Radiation in Large Pool Fires. The two-zone model proposed by Brosmer and Tien[1] can accurately estimates the global pyrolysis rate and radiation heat losses from PMMA fires, but falls short of the predictions of external radiative heat fluxes. For more accurate predictions of the external fluxes, a fluctuating cone has been developed [2]. The study shows that extensive numerical computations for the randomized cone movement are not necessary, and only the three cone positions presented are sufficient to estimate the extreme and mean values of the radiant heat flux to the fuel surface.

In addition, the structural-averaging scheme as an improved technique for providing mean property and temperature distributions to accurately calculate radiant heat losses from a fluctuating geometry, such as a fire or plume, has been introduced [3]. It is based on spatial averaging of its instantaneous shapes as opposed to conventional time-averaging or stochastic methods. This structural averaging technique has been applied to improve predictions of radiation heat flux from moderate-sized PMMA pool fires.

Radiation Induced Ignition of Solid Plastics. A comprehensive numerical analysis on the radiation induced ignition of solid and porous fuel has been carried out, which includes the effects of the absorption of incident radiation by pyrolyzed gases and the natural convection over a vertical fuel surface [4,5]. The study reveals that the radiation absorption in the gas phase is one of the major mechanisms inducing the ignition of plastics. Moreover, for less favorable physical and chemical conditions, ignition is mainly governed by radiation absorption by pyrolyzed gases from plastic solid surfaces. In general, the ignition delay times for absorbing gases are shorter than those for non-absorbing gases. As shown in Fig. 3, transmittance curves of the incident radiation calculated at the fuel surface indicate that a significance amount of the incident radiation is attenuated by the gas phase for the case of vertical surfaces as well as for the zero gravity case. In this simulation, the spectral absorption coefficient of MMA vapor at 10.6 mm wavelength was used.

Reports and Papers:

1. Tuntomo, A., Park, S.H., and Tien, C.L., "Infrared Radiation Properties of Ethylene," *Experimental Heat Transfer*, vol. 2, pp. 91-103 (1989).

2. Stretton, A.J., Park, S.H., and Tien, C.L., "Fluctuating Cone Model for Large Pool Fires," (to be submitted).

3. Stretton, A.J., Park, S.H., and Tien, C.L., "A Structural-Averaging Scheme for Calculating Radiation Heat Transfer in Fires," submitted for publication.

4. Park, S.H. and Tien, C.L., "Radiation Induced Ignition of Solid Fuels," *Int. J. Heat Mass Transfer*, vol. 33, pp. 1511-1520 (1990).

5. Park, S.H. and Tien, C.L., "Radiation Induced Ignition of Porous Fuels," *Comb. Sci. Tech.*(to appear).

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[1] Brosmer, M.A. and Tien, C.L., "Radiative Energy Blockage in Large Pool Fires," *Comb. Sci. Tech.*, vol. 51, pp. 21-37 (1987).

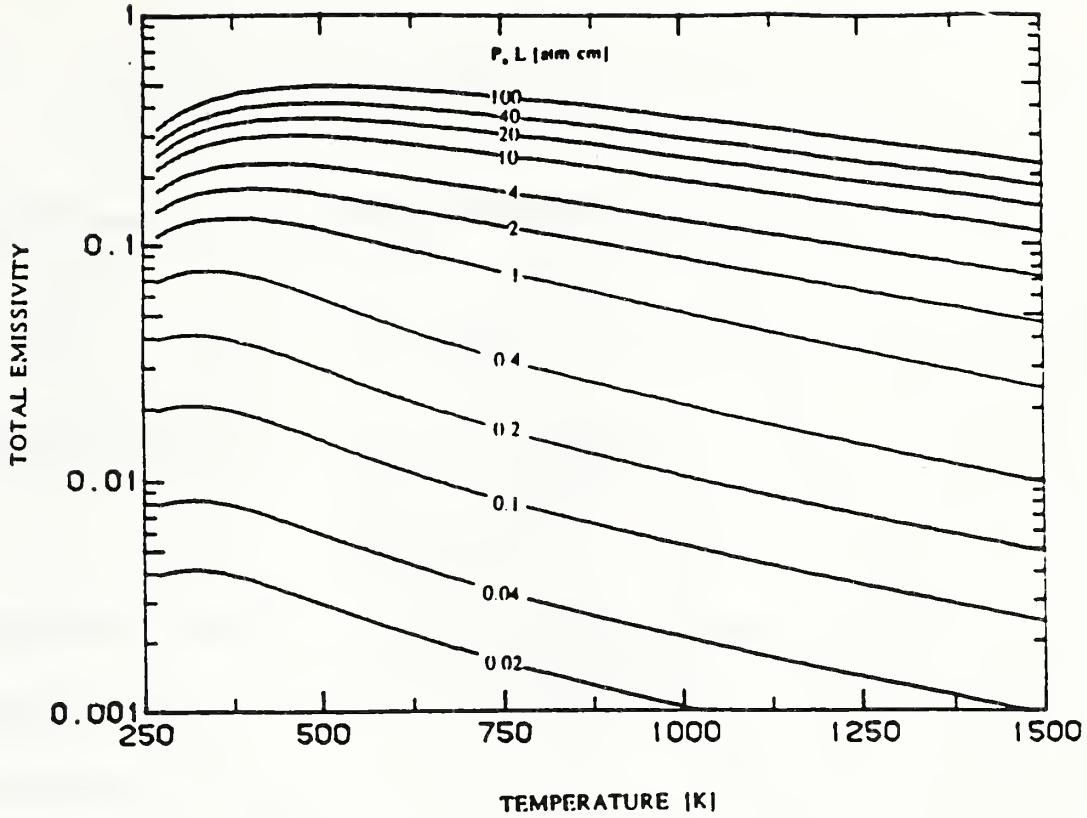

Fig. 1 Total emissivity for ethylene

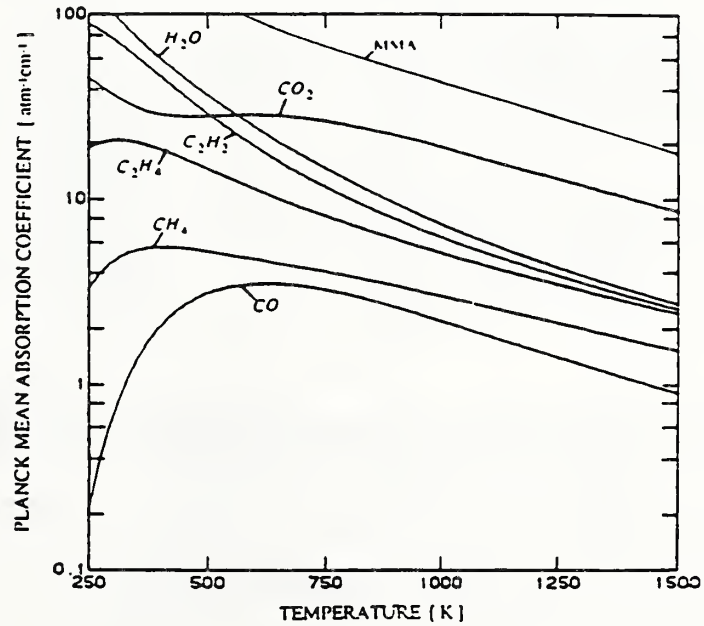

Fig. 2 Planck mean absorption coefficient of various gases

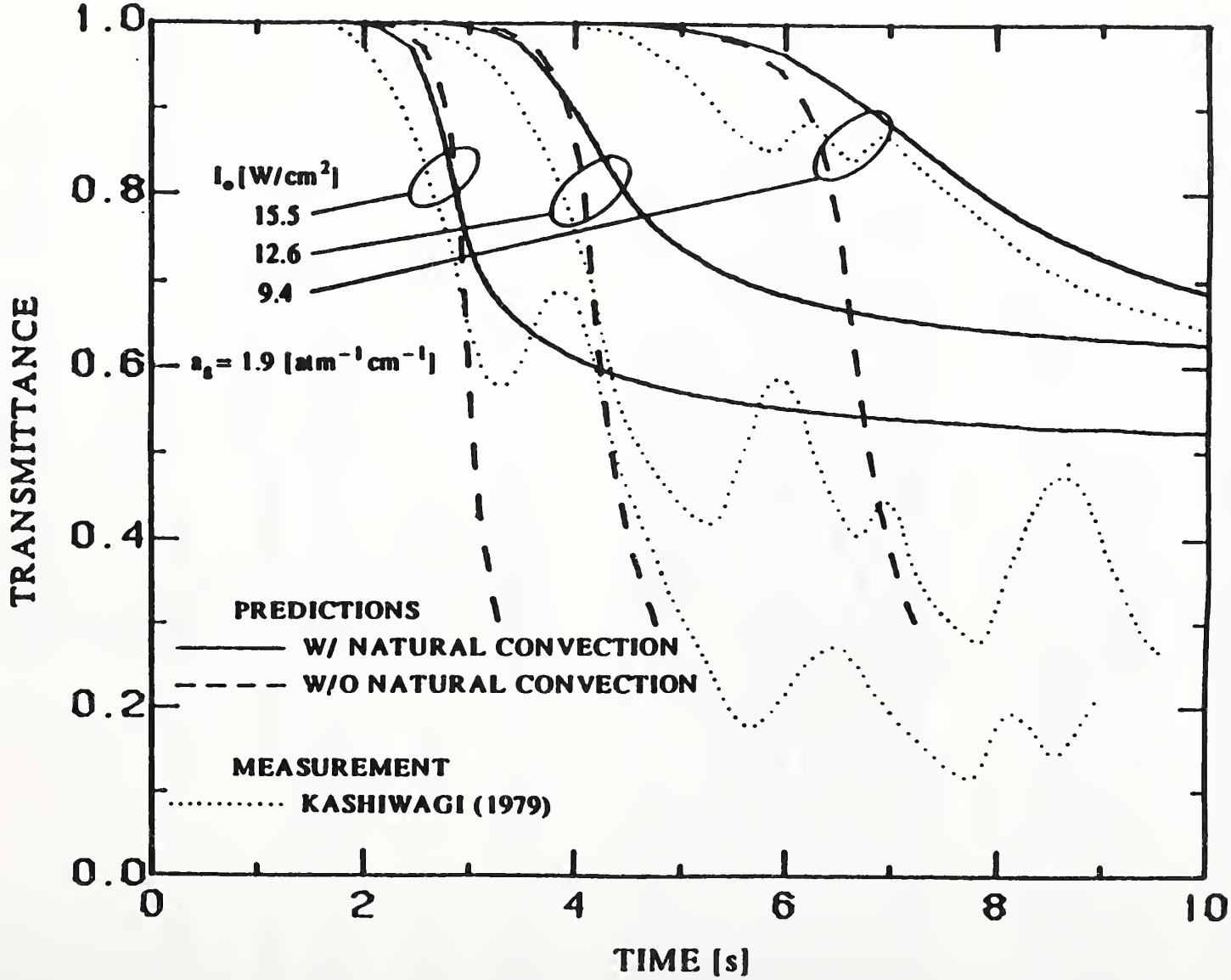

Fig. 3 Transmittance of the incident radiation at the fuel surface

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	Brown University
Grant Number:	60NANB0D1042
Grant Title:	The Behavior of Charring Materials in Simulated Fire Environments
Principsl 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. Steven Floyd, Student
NIST Scientific Officer:	Dr. Thomas Ohlemiller

Technical Abstract:

Introduction. The complicated interplay of chemistry, heat and mass transfer serves to make the study of combustion phenomena generally quite difficult, particularly when a solid phase is also involved. 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.

The general phenomena that govern fire behavior are qualitatively understood, and in some cases a reasonable quantitative understanding is also emerging. Still, there are major unanswered questions in many areas, particularly some related to fire chemistry. Six areas were recently highlighted as in need of significant further elucidation (R.Friedman, in Proc. First Int. Conf. Fire Sci., p349, 1986). These included:

1. The rates of pyrolysis of solids. It was recognized that detailed kinetic models would not be soon developed for most cases of practical interest, so the recommendation was that focus be turned to approximate methods that capture the essence of the processes.
2. The rates of release of toxicants.
3. Characterization of fire luminosity and smoke generation.
4. Fire retardation.
5. Flammability characteristics of the hot gas layer.
6. The chemistry of fire extinguishing agents.

The particular focus of this study involves the behavior of charring solids in fire situations, and the work relates to items 1, 2 and 3 most directly, with primary emphasis in area 1. Any study of fire phenomena that involves the study of chemistry in an environment that is removed from that encountered in actual fire situations runs a significant risk of producing results that do not accurately model actual fire behavior. This is not to deny the value of model studies, for these are undoubtedly of great value in advancing fundamental understanding of many aspects of the problem; the concern is in our ability to predict a priori the key variables that must be controlled in order to accurately simulate conditions of relevance. For example, studies of pyrolysis of organic solids have been performed under an enormous variety of conditions, and

the question in the fire literature has been often raised as to which if any of the studies are of relevance to fire modeling? If the heating rate of the solid in controlled laboratory experiments were orders of magnitude different from that encountered in the fire situation, would the same products of pyrolysis obtain? It seems wise in situations in which the entire variable set that might affect fire chemistry behavior has not been well established, to employ an approach that combines the examination of behavior in real fire situations with more controlled laboratory experimentation. This is the guiding philosophy of the present study.

The actual focus of the present work is on the behavior of charring solids during combustion in a fire environment. Wood and many synthetic polymers, particularly those that are crosslinked, fall into this class of materials. Obviously this is a class of some significant practical interest. It has been reported that the char forming tendency of organic materials may be predicted from a knowledge of their chemical structures (e.g. Van Krevelen, Polymer, 16, 615 [1975]), and that this char forming tendency is correlated with the limiting oxygen index (LOI). There are of course some significant questions about the relevance of the LOI itself as an indicator of fire behavior, but still the possibility of predicting features of some relevance to the behavior of the material in a fire environment from chemical structure alone is significant, and a theme that will be explored in this work. There should be no illusions about how straightforward such a task will be. It should be remembered that the char forming tendency of a material may be affected by factors other than the chemical structure of the polymer itself. The yield of char in cellulose pyrolysis has, for example, been reported to be a function of heating rate, although recent work in this laboratory has revealed only a minor effect of this variable in the range of heating rates of relevance in fires, in the absence of transport limitations. Also, the important role of both impurities as well as deliberately added retardants must be recognized.

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 certain reactions of volatiles. It can catalyze 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 CO_2 or H_2O and the char temperature is high enough, some gasification reactions may occur, resulting in release of H_2 and/or CO 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. This aspect of the problem will receive attention in this work.

Experimental Approach The tendency of organic solids to form chars during pyrolysis is well established. Earlier work on predicting the yield of char from the chemical structure of a polymer has been cited above. Extensive tabulations of char yields from pyrolysis of polymers have been reported (Hilado and Casey, J.Fire and Flamm., 10, 140,227 [1979]). At present, the conclusion from these studies is that in pure pyrolysis of polymers at heating rates comparable to those in fires, the chemical structure of the starting material is the primary factor in determining char yield. The addition of retardants can of course modify the char forming tendency significantly.

The above cited studies were however not conducted under actual fire conditions. The tests were often performed in inert gas environments, and the samples were quite small. The presence of oxygen is in certain cases able to change the pathway of the degradation process.

Samples that are small in size may not reveal the importance of mass transfer effects in bulk materials that are of relevance in fire situations. Also, the overall configuration of the sample and the flow patterns near its surface may be important. In at least one test, the char yields depended to some extent upon the flowrate of air across the surface of the sample, as it was held in a boat in a tube furnace.

Thus there is a need to tie the impressive progress that has been made in measuring and predicting char yields from pyrolyzing organic solids under laboratory conditions to predicting the yield under actual fire conditions. This work will address this issue explicitly as part of a larger study of the behavior of charring polymers under simulated fire conditions. The particular approach proposed here involves the use of equipment that has been developed to simulate the environment of real wall fires. The device was actually extensively utilized in Center for Fire Research supported work on the determination of combustion properties and behavior of pure and fire retarded cellulose, under the direction of Professor M. Sibulkin of Brown University. The actual device is shown schematically in Fig.1. It can be seen to have some general 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. Heating of the sample is accomplished by radiant quartz heaters which can provide a flux of up to about 100kW/m^2, which should cover the range of relevance in fire situations (somewhere around 40kW/m^2 will be a "standard" condition).

The windows of the system are designed to permit the radiant heating of the sample as well as viewing of the sample, photography of the surface in real time, and pyrometric determination of the surface temperature of the sample. The sample itself can be instrumented within its interior with thermocouples, to provide a temperature profile, but the surface temperature itself is better measured optically because of questions about effective contacting of surface thermocouples. We can determine the emissivity of the char in-house, using diffuse reflectance techniques on a FTIR spectrometer.

The yield of volatiles is of course provided by the data on mass loss of the sample. The The analysis of the volatiles is provided by either gas chromatography, as in the configuration used by Sibulkin and coworkers, or by mass spectrometry. The system is presently set up to provide analysis of the volatiles escaping the surface. The analysis by GC of course provides information only on the gaseous species, and the tars must be either separately collected by condensation, or determined by difference. The apparatus will be set up to provide the possibility of withdrawing volatile samples from within the pyrolyzing polymer sample, in order to permit directly addressing the question of whether there is a significant change in volatiles composition on passage through the char layer. This can be accomplished by withdrawing the samples through small diameter tubes inserted from the back face of the sample to various depths from the front face.

The fact that the present apparatus simulates a real fire environment will allow assessing the extent to which the pyrolysis environment is actually a significant consideration in modeling of fire behavior of different materials. We will perform a limited number of flaming combustion studies in an identical configuration, but with necessary modification of the apparatus. These benchmark experiments will be designed to produce char under actual flaming combustion conditions, such as we are attempting to simulate in the normal experiments.

In addition to the equipment described above, this laboratory also has available a separate pyrolysis reactor system that permits the examination of pyrolysis behavior of thin samples at heating rates that may be varied between 1°C/min and 1000°C/sec. This device has the advantage of providing the ability to examine the charring behavior in an environment free of mass transfer limitations. It has been previously used in a Center for Fire Research supported program that established that the kinetics of pyrolysis of cellulose and PMMA, as determined by ordinary TGA methods, apply over a broad range of heating rates, provided that mass transfer limitations are absent. The pyrolysis is actually performed in a wire gauze which serves as both sample holder and electrical resistance heating element. The gauze is contained within a chamber in which the gaseous environment can be controlled. The heating rate of the sample is controlled by a thermocouple sensor-computer controller circuit. This device will provide a benchmark value of char yield and volatile product composition, against which to compare the results from the fire simulation experiments.

The materials for study will include the cellulosics, phenolic resins, polycarbonates, polyimides, NOMEX (poly-m-phenylene isophthalate), to name but a few.

Technical Accomplishments As of the date of preparation of this summary, the project has been active for only one month. The activities to date have included preparing and modifying the equipment that will be used in this study.

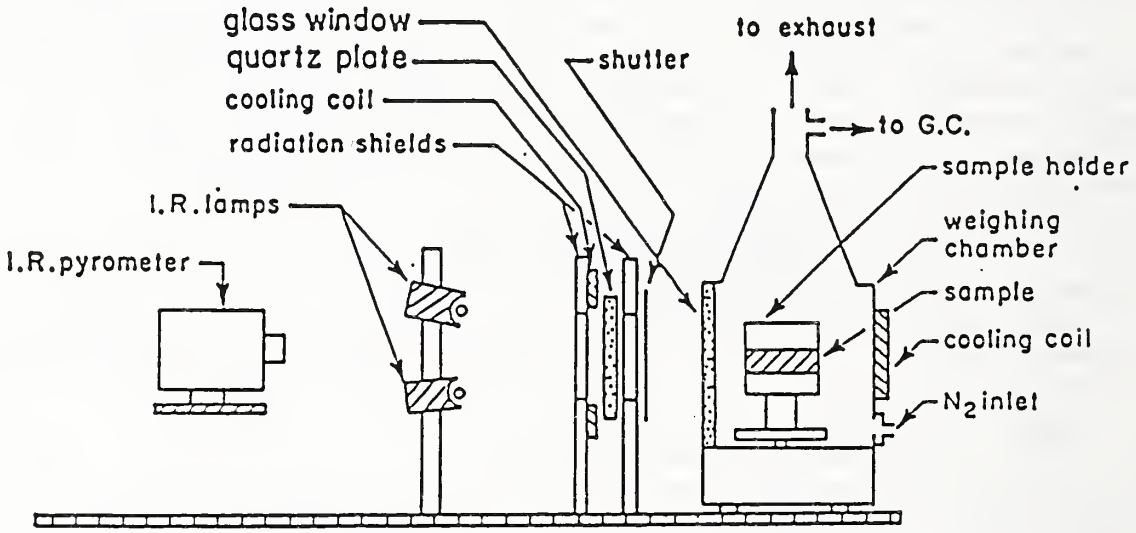

Figure 1. Schematics of the simulated fire environment pyrolysis chamber. Top -- overall system view. Bottom -- details of the pyrolysis chamber and radiative heating system.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: University of Maryland, College Park

Grant No.: 60NANB8D0944

Grant Title: Structure and Radiation Properties of Pool Fires

Principal Investigator: Professor J. P. Gore
Mechanical Engineering Department
University of Maryland
College Park, MD 20742
Telephone: (301) 405-5288

Other Professional Personnel: M. Klassen (Ph. D. Candidate)
Dr. Y. R. Sivathanu (Research Associate)

N. I. S. T. Scientific Officer: Dr. Takashi Kashiwagi

Technical Abstract:

In large scale fires, radiative feedback from the flames to the fuel determines the burning rate. Radiation to surroundings is also important for the determination of hazard to personnel and spread-rates. The objective of this research is to improve our understanding of the radiative feedback from pool flames and its effects on the burning rates. Particular emphasis is on the effects of: (1) fuel structure (including sooting tendency and flame temperatures) and (2) large scale and small scale turbulent fluctuations. Measurements completed during the past year involve burning rates and radiative heat loss fractions for seventeen flames. Two of these flames are selected to measure transmittances based on two line emission and single line absorption to understand the variation of burning rates and radiative loss fractions with sooting tendency.

Measurements of burning rates and radiative heat loss fractions have been completed for pool fires burning a variety of fuels. These include heptane, toluene, styrene, methyl methacrylate-MMA, methanol, ethanol and hexanol. Three pool sizes (4.6, 7.1 and 30 cm) have been considered. The 4.6 and 7.1 cm pools were uncooled pyrex containers and the 30 cm pool was a stainless steel pan water-cooled at the bottom. The lip height in all cases was controlled at 3 mm using a thermocouple and a flow controller. The burning rates were measured using a load cell. Radiative heat fluxes parallel to the axis of the fires and in the plane of the fuel surface were measured using a calibrated wide angle radiometer. These were integrated over the semiinfinite cylinder to estimate the total energy radiated to the surroundings. The radiative heat loss fractions were obtained from these data by taking a ratio with the ideal heat release rates obtained from the burning rates.

New measurements with different fuels and a larger pool confirmed the previous findings concerning X_R for the different flames. The X_R for the three alcohols is around 0.2 for all three burners. For the soot containing fuels, X_R is around 0.3 irrespective of sooting tendency. In order to investigate the lack of sensitivity to sooting tendency, heptane and toluene flames burning in the 7.1 cm pool were selected for further study using radiation temperature and absorption and emission transmittance measurements.

Fig. 1 shows a sketch of the instrument used for obtaining these data. A 632 nm He-Ne laser beam was passed through a sending purged tube through the fire at various axial and radial positions into a receiving purged tube. The light leaving the receiving purged tube consists of emission from the flame and the transmitted laser beam. This light was split into three parts and the intensity at 632 nm (the laser wavelength) was measured using a laser power meter. Intensities at 900 nm and 1000 nm were measured simultaneously.

The ratio of the transmitted to incident laser intensity is related to the soot volume fraction along the measurement path (in the Rayleigh limit) as follows:

$$\frac{I_\lambda}{I_{o\lambda}} = e^{-\frac{K_\lambda}{\lambda}\int_0^s f_v ds^*} = \tau_{\lambda a} \qquad (1)$$

where k_λ is a constant related to the refractive index of soot at wavelength λ and f_v is the soot volume fraction at location s^*. Absorption measurements for chord-like paths at a given height were deconvoluted to obtain local soot volume fractions.

The emission intensity at the two wavelengths is related to the local temperature and soot volume fractions along the path as follows:

$$I_\lambda = \int_o^{\tau_\lambda(S)} \frac{2C_1}{\lambda^5 (e^{C_2/\lambda T} - 1)} d\tau_\lambda(s^*) \qquad (2)$$

where τ_λ is the local transmittance defined similar to eq. (1). and T is the local temperature. The remaining terms in eq. (2) are constants. An emission transmittance and an equivalent radiation temperature for the fire is defined similar to past practice as:

$$I_\lambda = (1 - \tau_{\lambda e}(S)) \frac{2C_1}{\lambda^5 (e^{C_2/\lambda T_e} - 1)} \qquad (3)$$

It is noted that assuming a reciprocal wavelength dependence of the absorption coefficient of soot, eqs. (3) can be solved for the radiation temperature T_e and the equivalent transmittance $\tau_{\lambda e}$ since measurements at two different wavelengths are obtained. When the signal drops below the sensitivity of the present emission detectors, the temperature is set to 300 K.

Figure 2 shows the measurements of soot volume fractions along the axis of the 7.1 cm heptane and toluene flames obtained from deconvolution of transmittance data along chord-like paths. As expected flames burning toluene contain approximately factor of 20 higher soot (peak f_v = 14 PPM) than those burning heptane (peak f_v = 0.6 PPM).

In view of the identical radiative heat loss fractions for the two fuels, the T_e profiles are examined. It is noted that T_e is approximately equal to the peak temperature along the radiation path. Before the flame tip, the peak temperature depends on the adiabatic flame temperature, the combustion efficiency and the radiative heat loss fraction. If the local radiative heat loss fraction for the two fuels is identical then for 100 % combustion efficiency, the temperature in the toluene flames would be 50 K higher than that in the heptane flames. Figure 3 shows the measurements of T_e obtained in the present study. The temperatures for the two fuels are somewhat similar near the liquid surface. However, the temperatures in the toluene flames decrease rapidly and are generally 250 K lower than those in the heptane flames. The temperatures decrease rapidly beyond x/H_f of 0.5 since intensities are often below the present detection limit. The overall low temperatures in the toluene flames help explain part of the insensitivity of X_R to sooting tendency.

A study of the measured $\tau_{\lambda e}$ and $\tau_{\lambda a}$, for the flames, shown in Fig. 4 helps explain the insensitivity of X_R to sooting tendency. The emission transmittance is approximately 4 times higher than the absorption transmittance for toluene flames over most of the height while the difference between the two transmittances is approximately 20 % for the heptane flames. It is noted that the two transmittances are identical for an isothermal path. The large difference between the two for the toluene flames suggests that bulk of the soot observed by the laser absorption probe is at relatively low temperatures resulting in its deweighting by the Planck's function in eq. (2). Presence of large quantities of relatively cold soot should be accounted for in estimating radiation from flames burning heavily sooting fuels.

Reports and Papers:
J. P. Gore, M. Klassen, A. Hamins and T. Kashiwagi, 1990, "Fuel Property Effects on Burning Rate and Radiative Transfer from Liquid Pool Flames," Third International Symposium on Fire Safety Science, Scotland, UK, submitted.
J. P. Gore, M. Klassen and Y. R. Sivathanu, 1990, "Radiative Heat Feedback of Heptane and Toluene Pool Flames," Comb. Flame, submitted.
J. P. Gore, S. M. Skinner and R. J. Gettings, 1989, "Fuel Property Effects on the Radiation Properties of Laminar Diffusion Flames," Proceedings of the Twenty Second Fall Technical Meeting, Eastern States Section of the Combustion Institute, Albany, NY, pp. 52.1-52.4

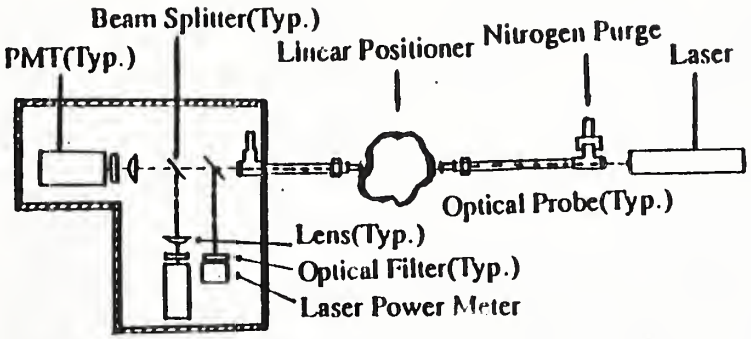

Fig.1: A Sketch of the Three Line Emission Absorption Probe

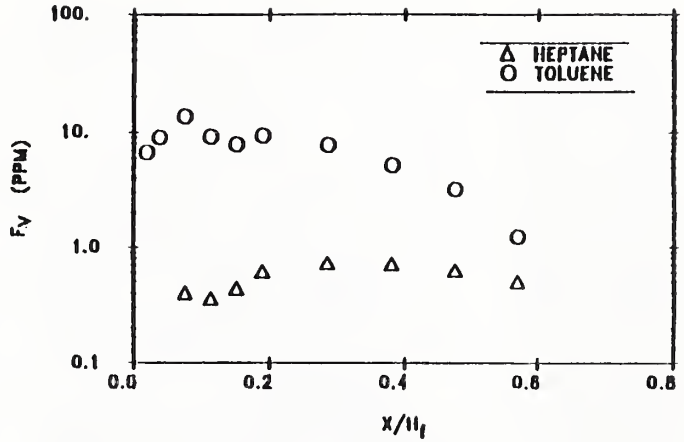

Fig.2: Mean Soot Volume Fractions in Heptane and Toluene Flames

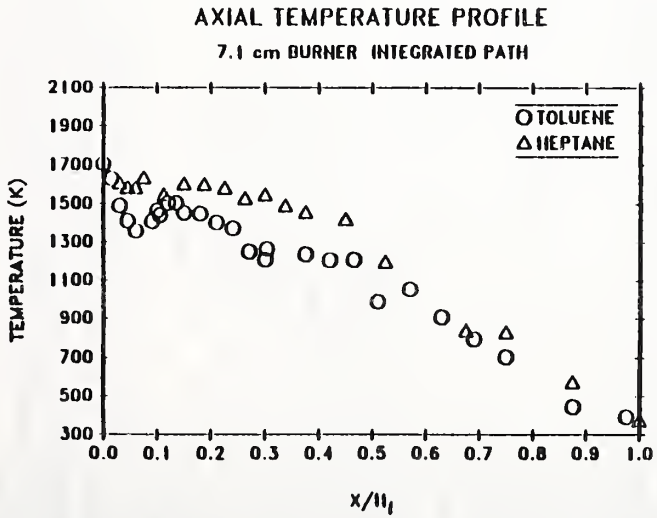

Fig.3: Mean Radiation Temperature in Heptane and Toluene Flames

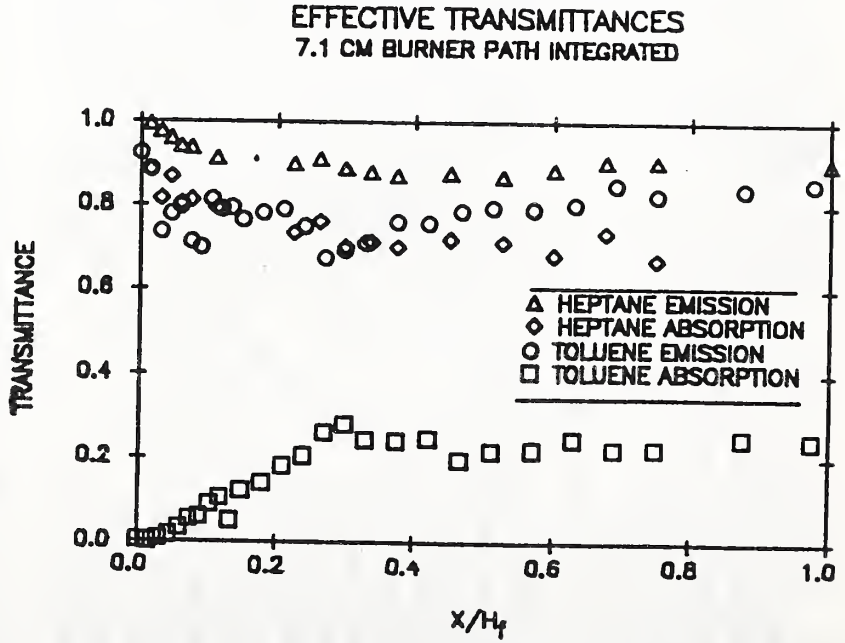

Fig.4: Absorption and Emission Transmittance in Heptane and Toluene Flames

E. FLAME SPREAD

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

WALL FIRE SPREAD

Professional Personnel

H.E. Mitler, Project Leader
K.D. Steckler, Physicist
W.J. Parker, Physicist
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A. Perez-Gerena, D. Alvord,
W.D. Davis, Programmers

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 in different configurations including flat walls, corners and ceilings will be completed and experimentally verified by the end of FY 92.

Scope

This project addresses the problem of upward fire growth in enclosures, the kind 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. Ultimately every aspect of wall fire growth will be considered, including growth on flat walls, corners, and ceilings. The burning materials will be arbitrary: from simple, uniform, isotropic, subliming solids to heterogenous, nonisotropic, charring, melting, laminated, and composite materials. Lateral and downward creeping spread will also be covered, as well as spread under a variety of external conditions, including burning in a hot, oxygen-vitiated atmosphere.

Technical Accomplishments

I. Pyrolysis model

A new pyrolysis model has been devised, which is intended to applly for any arbitrary material. If a sample of material is exposed to a heating flux (say, in the Cone Calorimeter), then we define its heat of gasisfication as

$$h_g \equiv \phi_{net}/\dot{m}'' \qquad (1)$$

where $$\phi_{net} \equiv \phi_{in} - \phi_{rr} \qquad (2)$$

that is, the incoming flux minus the reradiated flux. Evidently this can (and generaly does) vary with time. However, we expect that (within limits) the heat of gasification will be only weakly dependent on the impinging flux, and will be characteristic of the material. For example, the measured heat of gasification of untreated Douglas fir plywood, exposed to two different radiant fluxes, are shown in Fig.1. The agreement between the two curves is

seen to be fair. Note that this approach automatically takes transent effects into account.

Rather than take $\dot{m}''$ and h_g to be fuctions of t (time), as was done before, it is more physically meaningful to take the mass lost (per unit area) as the independent variable. Thus measurements of mass loss rate are made with some prescribed external flux, yielding $h_g(\Delta m'')$ through Eq.(1); then the mass-loss rate for any <u>other</u> flux history will be given, as a function of time, by

$$\dot{m}''(t) = \phi_{net}(t)/h_g(\Delta m'') \tag{3}$$

where $\Delta m''$ is the total mass lost by time t. That is,

$$\Delta m'' = \Delta m''(t) = \int_0^t \dot{m}''(t')dt' \tag{4}$$

II. Transient pyrolysis

Although the new pyrolysis module, described above, automatically takes any transient effects in pyrolysis into account in some approximation, the original pyrolysis module does not. A simplified theoretical calculation of transient pyrolysis has been made, including the effects of finite slab thickness, using an integral approach. A calculation of the burning rate of a thin PMMA sheet was made using the theory, and this was compared to an experimental measurement of $\dot{m}''(t)$. The results of this comparison are shown in Fig.2.

III. Lateral spread

The program SPREAD is being generalized to predict not only upward spread, but the simultaneous lateral spread of the burning zone. This is calculated using the expression

$$v_s = \Phi/[k\rho c(T_{ig} - T_s)^2] \tag{5}$$

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. There is a small logistical problem, therefore, which arises from the fact that the layer height changes with time. This is handled by making small adjustments to v_s such that the instantaneous total pyrolyzing area remains invariant with layer height.

IV. Burnthrough

Once ignition has occurred at a node, the surface must regress, as it loses mass. The regression rate is $\dot{m}''/\rho$, so the thickness removed at node i (at the height x_i above the bottom of the pyrolysis zone) in the time interval Δt_s is

$$r_i^s = \frac{1}{\rho}\int_{t_{s-1}}^{t_s} \dot{m}_i''(x_i,t)dt \simeq (\dot{m}_i''/\rho)\Delta t_s . \tag{6}$$

When $\Sigma r_i^s \geq \theta_i$ (the thickness of the slab at i), burnthrough has taken place at that node. When a section burns through, the pyrolyzing area decreases (or increases more slowly), so that the power output goes down, the flame height is smaller, and the spread rate goes down. For the case of a thin textile,

this effect will generally result in a constant (rather than an increasing) upward burning rate. In the most recent version of the program, we note that it is only necessary to consider the incremental mass losses $\Delta m"(t_s)$, rather than the actual thicknesses. Then burnthrough will have occurred when $\Sigma\Delta m" \geq m"_o$. This approach avoids having to deal with the otherwise intrinsically complicated case which arises when the density varies with depth (as it does, for example, for particle-board).

Programming of both lateral spread and of burnthrough are essentialy complete; the next task is validation.

V. Flame heights

Evidence has recently appeared that the heights of wall flames are perhaps better characterized by a square-root dependence on the power output, than by the "classical" two-thirds power. The former would imply that the rate of growth on a PMMA surface is asymptotically independent of the power output of the igniting burner, whereas the latter implies a definite dependence. This issue was tested experimentally, with the results shown in Fig.3. The experimental points do indeed appear to indicate a dependence. The solid curves in this figure are the theoretical calculations made by the program SPREAD.

VI. Experimental

In order to find h_g, the heat of gasification, it is necessary to measure the reradiation flux. The standard Cone Calorimeter does not have a provision for this measurement, and therefore some thermocouples and a radiometer were used in addition to the usual instrumentation, in order to make this measurement and to calibrate the instruments. The results have been reasonably satisfactory (see Fig.1); in order to avoid the cumbersome thermocouple, we are planning on using a two-color pyrometer for this measurement, in the future. A number of upward-spread-rate tests with significant external radiation are being carried out at the new BRI facility in Japan. This will provide valuable data for validation of the upward spread model.

Reports and Publications

Kulkarni, A.K., Kim, C.I., and Mitler, H.E. (1990) "Time-dependent local mass loss rate of finite-thickness burning walls," submitted for the Third International Symposium on Fire Safety Science

Mitler, H.E. (1988), "Algorithm for the Mass-Loss Rate of a Burning Wall", Fire Safety Science - Proceedings of the Second International Symposium (Eds., C.E. Grant and P.J. Pagni); Hemisphere Publishing Corp., p.179

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

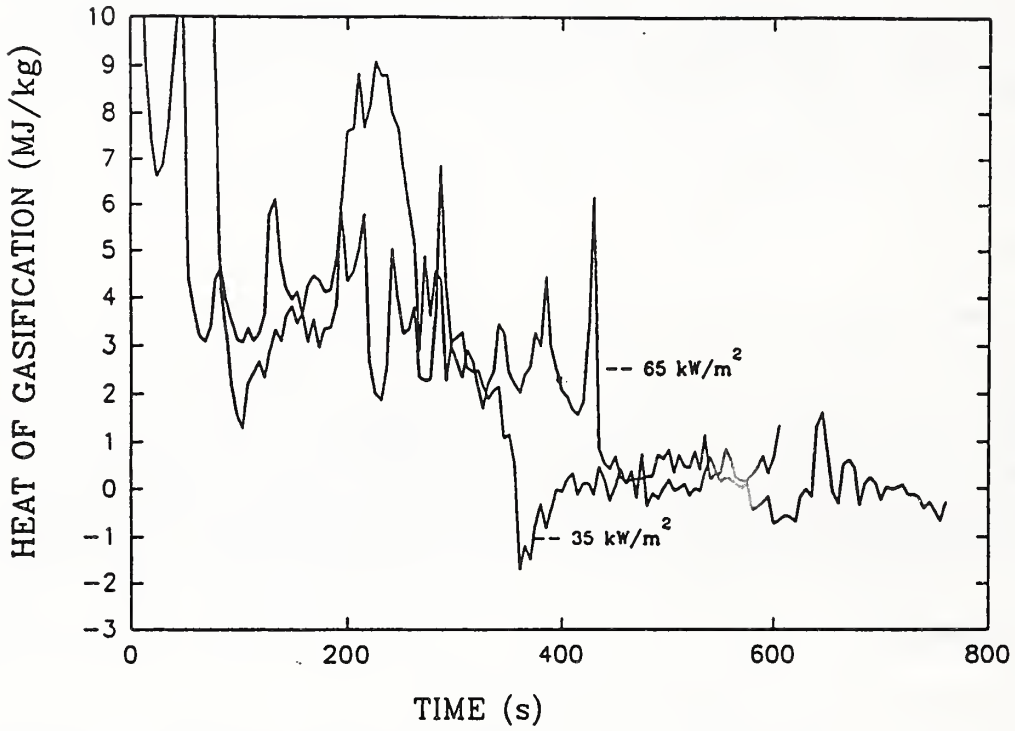
Related Grants

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

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

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

HEAT OF GASIFICATION FOR UNTREATED DOUGLAS FIR PLYWOOD AT 35 AND 65 kW/m^2 INC. FLUX



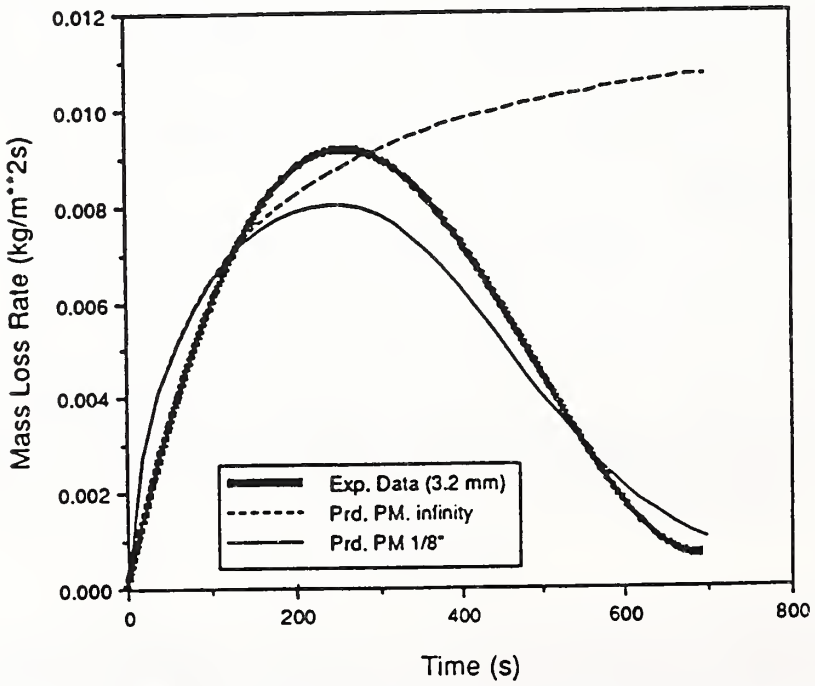
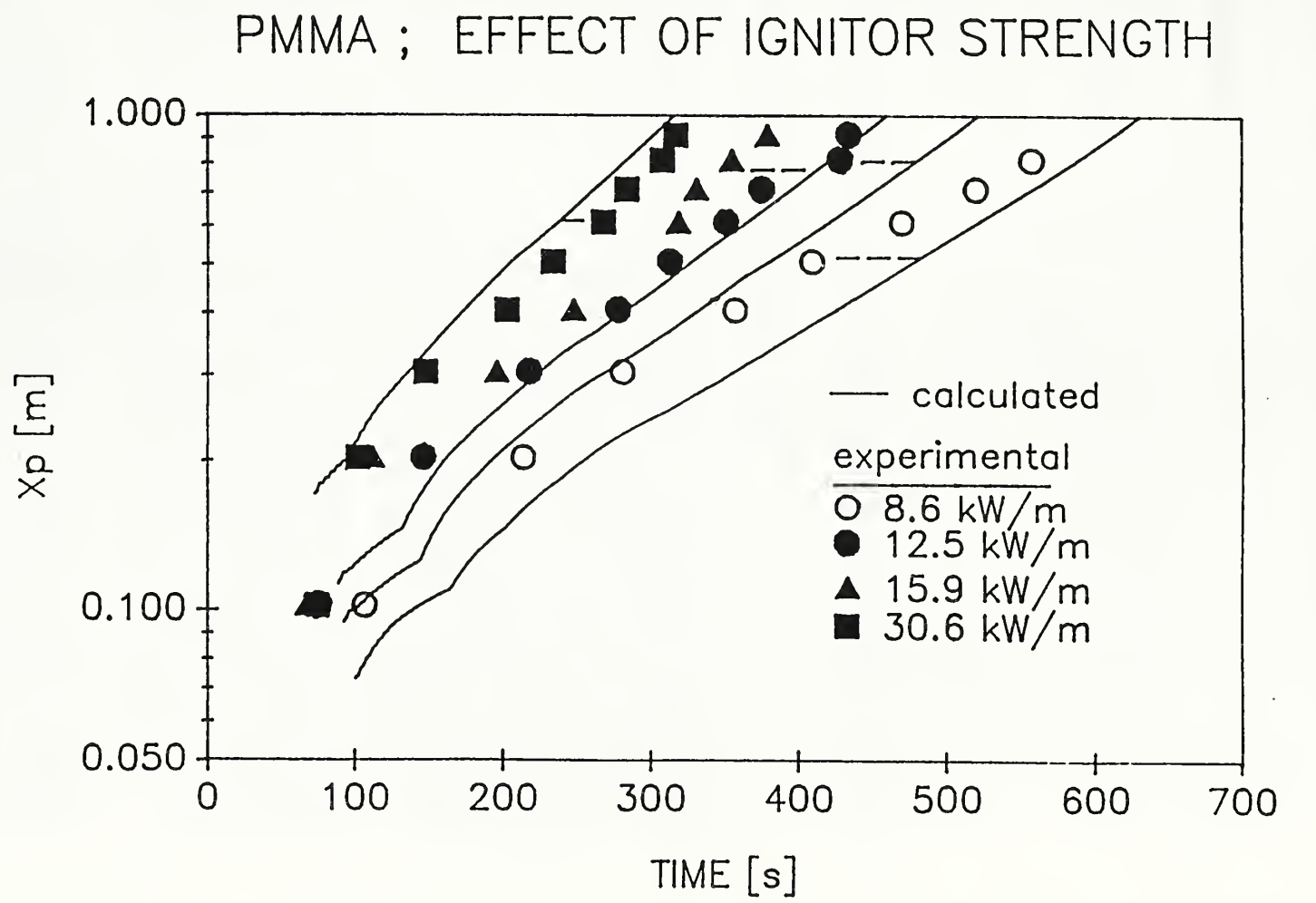


Figure 4. Comparison of measured (thick line) and predicted (thin solid line) values of local mass loss rate for 3.2 mm thick PMMA; Also shown is prediction for semi-infinite PMMA Slab.


PMMA ; EFFECT OF IGNITOR STRENGTH
1.000
0.100
0.050
Xp [m]
0
100
200
300
400
500
600
700
TIME [s]
calculated
experimental
8.6 kW/m
12.5 kW/m
15.9 kW/m
30.6 kW/m
ignit3.gra

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: Factory Mutual Research Corporation

Grant No.: 60NANB8D0845

Grant Title: Prediction of Fire Dynamics

Principal Investigators: Ronald L. Alpert and John de Ris

Other Professional Personnel: M.A. Delichatsios
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)
Please see a separate summary under this title.

Task 2. Fire Radiation and Toxic Product Release - Two papers that are based on studies in this task are nearly completed. The papers respectively describe: 1) an experimental correlation which allows one to predict the turbulent flame radiant fraction, χ_R, over a range of stoichiometric oxidizer to fuel mass ratios, S, and adiabatic flame temperatures, T_F, based on a single measurement of the fuel's smoke point. The correlation is established for seven hydrocarbon fuels with S>=12; 2) a global model for predicting χ_R for buoyant, turbulent-jet flames. The model considers both the gaseous and soot thermal radiation, as well as the influence of incompleteness of combustion and radiant heat loss on the effective radiation temperature. The advantage of the global model is its relative simplicity, ease of application and focus on the fuel smoke point as a "fundamental" material flammability property.

We have performed a careful analysis of the available data on the peak soot volume fractions in both laminar smoke-point diffusion flames and turbulent diffusion flames of corresponding fuels, with the view of incorporating the results in our global flame radiation model. Our results suggest that the laminar smoke-point data requires: 1) an orifice correction factor, which influences the results for very sooty fuels, and 2) a gaseous radiation correction factor, which influences the results for less sooty fuels. A combined correction formula was developed and incorporated in the model.

Figure 1 compares the global radiation model predictions with experiment for a wide range of fuels burning in slightly vitiated air such that the adiabatic flame temperature, T_{ad}=2200K and S=15. The rather good agreement suggests that we are beginning to have a reasonably good scientific understanding of turbulent flame radiation, at least globally for axisymmetric buoyant turbulent diffusion flames. The model introduces only two turbulence adjustment factors to achieve this agreement (a proportionality factor for turbulent soot formation, and a mean flame temperature correction for

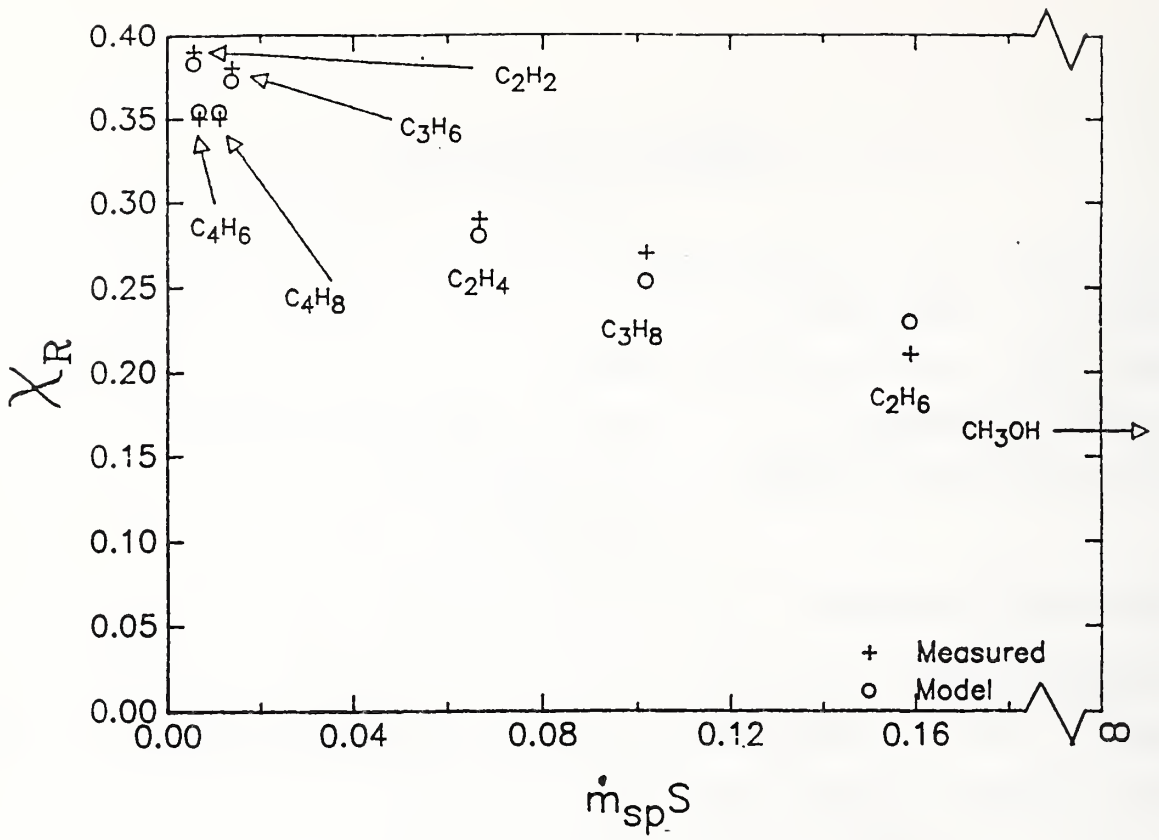


FIGURE 1

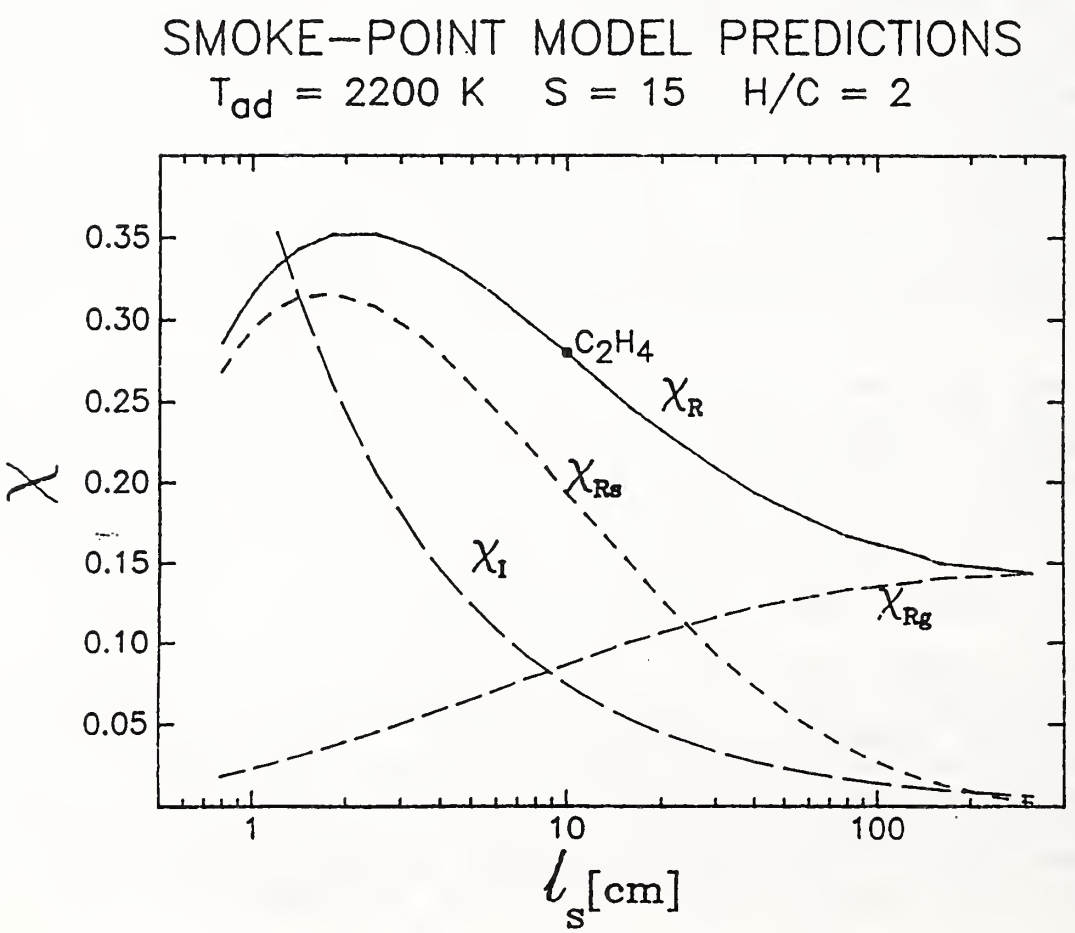


FIGURE 2

diffusion of hot products of combustion into cold reactants). Figure 2 shows the model predictions for the influence of the smoke point on the relative soot, χ_{RS}, and gaseous, χ_{Rg}, contributions to the radiant fraction, χ_R, as well as the incompleteness of combustion, χ_I, obtained from empirical correlations.

Further information on combustion incompleteness over a range of ambient atmospheres is needed in order to extend the scope of the global model. A fiber optic soot measurement system is being constructed for our turbulent-jet flame enclosure to measure soot and gaseous species production for various hydrocarbon fuels and ambient O_2 concentrations. We will also need to find the maximum conversion of fuel carbon into soot for various sized flames.

The accuracy and scope of the global model is being further enhanced by development of a full turbulent-flame soot combustion model. We have prepared an experimental design for mapping soot volume fractions and soot radiation temperatures throughout an axisymmetric turbulent flame. The design includes a charge-coupled device (CCD) for rapid lateral radiation scans of the flame. This instrumentation will permit at least two orders of magnitude more data than was possible when PMMA flames were similarly mapped several years ago.

Task 3. Models for Wall Fire Flame Radiation - The objectives are to extend previously established relationships for fire radiation to the case of vertical wall burning and to compare results with analyses of wall burning. As in other related work the significance of studies of fire radiation rests on the fact that in hazardous fires energy transfer from the flame to the fuel and to the surroundings occurs predominantly by thermal radiation. The rate of fire growth and the spread of fire to new fuel elements depends critically on this radiant energy transfer, and its quantitative assessment is thus essential for predicting fire behavior.

In the present task, wall fires of solid fuels are simulated by burning gaseous hydrocarbon fuels on a water-cooled vertical porous metal surface under steady-state conditions. The burner of 380 mm width is subdivided into a number of panels of equal height (132 mm), so that the simulated pyrolysis height can be varied by the choice of the number of fuel-supplying panels. The current burner configuration consists of ten panels topped by a water-cooled heat transfer plate, providing an overall height of 2.2 m. Water-cooled sidewalls are attached to the burner to obtain two-dimensional flame structure.

The instrumentation includes a wide-view-angle radiometer for measuring the total radiant emission from the flames, and a scanning slit radiometer for obtaining the vertical distribution of radiant power per unit height emitted by narrow horizontal slices across the flames. The scan is obtained by an electromagnetically deflected plane front surface mirror operated in a linear ramp mode. Both instruments employ spectrally flat sensors. In addition, differential thermocouples imbedded in the water-cooling ducts of the burner panels and the heat transfer plate provide measurements of the total heat flux from the flame to the wall at 132 mm vertical intervals.

Before the measurements on porous-metal wall-burner flames now underway, the same radiometers were used to study flames issuing from a slot burner placed at the base of a heat-transfer plate, providing the limiting case of

zero pyrolysis height. For comparison, the slot burner was also placed in the open between water-cooled sidewalls to obtain free-burning two-dimensional slot-burner flames, and additional runs were performed with buoyant turbulent fuel-jet flames. To cover a sufficiently wide range of sooting tendency, the four fuels, methane, ethane, ethylene and propylene, were selected for the present study. In this first phase of the work, theoretical heat-release rates were varied over the range of about 10 to 60 kW. Results have been presented[1,2] and a Technical report containing additional information has been issued.

The main conclusions are as follows:

1. Radiative fractions of total heat-release rate were nearly equal for jet flames and for free-burning slot-burner flames, except for methane flames at low heat-release rates, but were significantly reduced by placing the slot burner adjacent to a water-cooled wall. The reductions, which ranged from about 18 to 36 percent, increased with fuel sooting tendency but decreased with heat release rate.

2. The trend of radiative fraction with fuel sooting tendency was not altered by the wall-effect reductions.

3. Profiles of radiant emission per unit height differed considerably for the three-flame configurations. Placing the slot burner adjacent to the wall reduced the rate of rise and the peak values of radiant emission to about 2/5th and the rate of decay to about 1/6th of the free-burning case. The heights of peak emission remained unchanged, but the flame heights were nearly doubled by the wall effect.

4. Dimensionless correlations of radiant emission vs. height, independent of heat-release rate, were obtained by introducing a radiation flame length proportional to the standard deviation of the distribution of radiant emission. The radiation flame length varied roughly with the 1/3 power of heat-release rate for jet flames and with about 1/2 power for slot-burner flames.

5. The observed 1/3 and 1/2 powers suggest that the flame heights are controlled by a radiant cooling mechanism rather than the conventionally proposed turbulent mixing mechanism, and imply a mean volumetric heat release rate independent of fire size.

6. Analytic function fits to the dimensionless correlations were obtained by matching skewness and kurtosis parameters.

After completion of the slot-burner runs, work with the porous-metal burner was initiated with a five-panel configuration. A set of runs with the four fuels mentioned earlier, varying the number of burner panels from one to five and the total heat release rate from about 10 to 60 kW, has been completed. As expected, the results have shown that the similarity relationship established for slot-burner flames seems applicable to the over-fire region, but clearly does not hold in the pyrolysis region. To establish reliable scaling laws for the pyrolysis region, we have doubled the number of burner panels to ten. Initial runs with this configuration have shown that we must also at least double the overall fire heat release rate to achieve a high enough convective B-number.

In addition to radiant emission, the sum of radiative and convective heat transfer to the wall is also being measured within each 132 mm high panel. Results obtained thus far have shown that maximum total heat fluxes are relatively insensitive to fuel sooting tendency and mass flux, increasing from 25 to 35 kW/m^2 for small fires. We expect higher values for our forthcoming larger fires.

Separation of the total heat flux into radiative and convective components requires a knowledge of flame thickness for the correct computation of radiative flux. The convective flux, derived as the difference of total and radiative flux, is needed for computing the convective B number. In addition, measurement of flame thickness is also of general interest for understanding the structure of wall flames. Although several alternative methods for measuring flame thickness are being considered, it appears most likely that a combined lateral absorption-emission measurement, yielding not only thickness but also temperature data, will be used. An electronic line-scan camera employing an array sensor was recently purchased by the current NIST grant and will be adopted for this proposed work. Finally, the results on radiant emission, radiative and convective heat transfer, flame thickness and temperature will be used to predict the heat transfer components in terms of normal combustion parameters plus fuel smoke-point values.

Publications

1. Markstein, G.H. and de Ris, J.: "Wall-Fire Radiant Emission," International Joint Conference of the Australia/New Zealand and Japanese Sections of the Combustion Institute, Sept. 24-27, 1989, Sydney, Australia.

2. Markstein, G.H. and de Ris, J.: "Wall-Fire Radiant Emission. Part 1. Slot-Burner Flames, Comparison with Jet Flames," 23rd International Symposium on Combustion, Orléans, France, July 22-27, 1990; FMRC Technical Report, RC90-BT-2, August 1990.

Task 4. Transient Pyrolysis, Flame Radiation and Sooting Properties of Solid Materials -

During the last year we have made the following progress:

a) A report[1] has been issued and submitted to NIST on predicting surface temperature histories of materials when significant losses (such as reradiation) are present. The results from this work have led to the development of a methodology for reliably predicting the thermal inertial and the critical heat flux from piloted time-to-ignition data. These results can also be used for reinterpreting the lateral flame spread experiments in the LIFT apparatus, as we plan to show in the future. A paper on time-to-ignition has also been accepted for publication.[2]

b) The analysis of material flammability properties for non-charring (e.g. PMMA) materials is complete. As a part of this analysis, we have demonstrated that an integral model for transient heat-up and pyrolysis reproduces well (error less than 2% for extreme cases) the exact complete physical equations.[3] In addition, we have shown that even for a non-charring material, transient pyrolysis significantly affects flame spread rates,[4] by using an Upward Flame Spread and Growth (UFSG) code developed at FMRC. Such transient pyrolysis effects explain some recent results on wind-assisted flame spread.[5,6]

c) We have recently made progress in the analysis of the pyrolysis data for charring materials by 1) developing, coding and validating an integral model for pyrolysis of charring materials, and 2) identifying the key material flammability properties required for upward flame spread.[7] Table I summarizes these key flammability properties and how they could be obtained from existing flammability apparatus.

d) One important parameter for large-scale fires[7] is the radiant fraction, χ_R (see Table I), in various geometric configurations (jet fires, wall fires, pool fires). The radiant fraction in turbulent flames depends on the following parameters: 1) the volume of the flame, 2) cooling of the flame by radiation or convection (e.g. to walls) which determines an effective radiation temperature[8], 3) the intrinsic chemistry of soot formation for a given fuel, which also may be affected by the mass transfer number, B, (wall fires, pool fires).

The intrinsic chemistry of soot formation may be characterized by the smoke-point heat release rate (see Task 2). For this reason we have designed and are currently testing an apparatus for measuring the smoke-point heat release rate for charring and non-charring solid fuels. Standard smoke-point apparatus exist for gaseous and liquid fuels.

References

1.* Panagiotou, Th., and Delichatsios, M.A.: "A Numerical Solution for the Surface Temperature Rise History of a Material Including Surface Reradiation Losses," Technical Report, FMRC J.I. 0Q0J1.BU, December 1989.

2.* Delichatsios, M.A., Panagiotou, Th., and Kiley, F.: "The Use of Time to Ignition Data for Characterizing the Thermal Inertia and the Minimum (Critical) Energy for Ignition or Pyrolysis," Submitted for publication in Combustion and Flame, March 1990.

3. Delichatsios, M.M.: "Testing the Integral Model for Heat-up," FMRC Technical Memorandum, December 1989.

4. Delichatsios, M.M. and Delichatsios, M.A.: "Effects of Transient Pyrolysis on Wind Assisted and Upward Flame Spread," for Presentation at the ASME/JSME Heat Transfer Meeting, March 17-22, 1991.

5. Atreya, A.: "Wind Assisted Flame Spread," 23rd International Symposium on Combustion, 1990.

6. Zhou, L. and Fernandez-Pello, A.C.: "Concurrent Turbulent Flame Spread," 23rd International Symposium on Combustion, 1990.

7.* Delichatsios, M.A. and Saito, K.: "Upward Fire Spread: Key Flammability Properties, Similarity Solutions and Flammability Indices," in preparation, August 1990.

8.* Delichatsios, M.A., Orloff, L. and Delichatsios, M.M.: "The Effects of Fuel Sooting Tendency and the Flow on Flame Radiation in Luminous Turbulent Jet Flames," to be published in CST, 1990.

*Partially supported by NIST as part of the present program

TABLE I

KEY FLAMMABILITY PROPERTIES

NON-CHARRING	CHARRING	METHOD OF MEASUREMENT
	Heat-up and Ignition	
K, ρ, C_p	$k_v, \rho_v, C_{p,v}$	Time to Ignition[1,2]
T_p	T_p	Surface Temperature Histories[3]
*	*	
	Transient Pyrolysis	
$\Delta H_v, \rho$	$L, \rho_v, C_{p,v}, \rho_c$	Weight Loss Histories
$\Delta H_v = L + C_p (T_p - T_o)$	$d_c = \frac{k_c(T_p)T_p}{\sigma T_p^4} = \frac{k_c T_p}{\dot{q}''_{cr}}$ (charring conductance depth)	
	Gaseous Combustion	
X_A	X_A	Collecting Hood Gas Analysis
ΔH_c	ΔH_c	
X_R	X_R	
T_f, S	T_f, S	

Notes:

a) Subscript v = virgin fuel, c = char layer

b) Critical Heat Flux = $\sigma (T_p^4 - T_o^4) = \dot{q}''_{cr}$

* (Other effects such as reflectivity, in-depth radiation absorption are not currently evaluated.)

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution:	Factory Mutual Research Corporation
Grant No.:	60NANB8D0845
Title:	Prediction of Fire Dynamics: Task 1, Prediction of Fires in Buildings
Principal Investigator:	Howard W. Emmons
NIST Scientific Officer:	Dr. Henri Mitler

Technical Abstract:

There were four projects completed during this year, of which only the last will be described in detail.

1. The previously reported theory of the heat transfer from a transient ceiling jet has been completed and is ready to be written as a technical paper. It clarified the conditions under which the use of the adiabatic temperature distribution may be advantageous. It also shows the conditions in which the ceiling jet temperature falls to the point that the jet is no longer stable at the ceiling against miscellaneous air currents and lower layer return flow into the fire.

2. A paper on "Progress in Fire Modeling" was prepared for a conference on "Recent Advances in Flame Retardancy of Polymeric Materials" held in Stanford, Connecticut on May 15-17, 1990. Papers of this type help to acquaint fire engineers with the progress and understanding of fire science and its application.

3. The four reports on the development and use of CCFM was studied as an external reviewer. Many suggestions for improvement were prepared and sent to the authors for their consideration. The reports have now been issued by NIST.

4. Transient ceiling jet knowledge is needed in fire models to predict the time of operation of fire detectors and sprinklers. Empirical formulas are currently adequate for this purpose. However, the development of fire models for performance code predictive purposes must be accurate for long as well as short times. This requires a compromise ceiling jet theory of sufficient accuracy somewhere between the field modeling theories and purely empirical results.

A study has been completed on the use of top hat profile ceiling jets. The general equations for the steady ceiling jet have been written with friction, entrainment, and heat transfer.

The effect of friction alone has been solved analytically and shows that the flow proceeds toward critical (Richardson Number = 1) at the open end of a corridor. This case is well known from hydraulic channel flow.

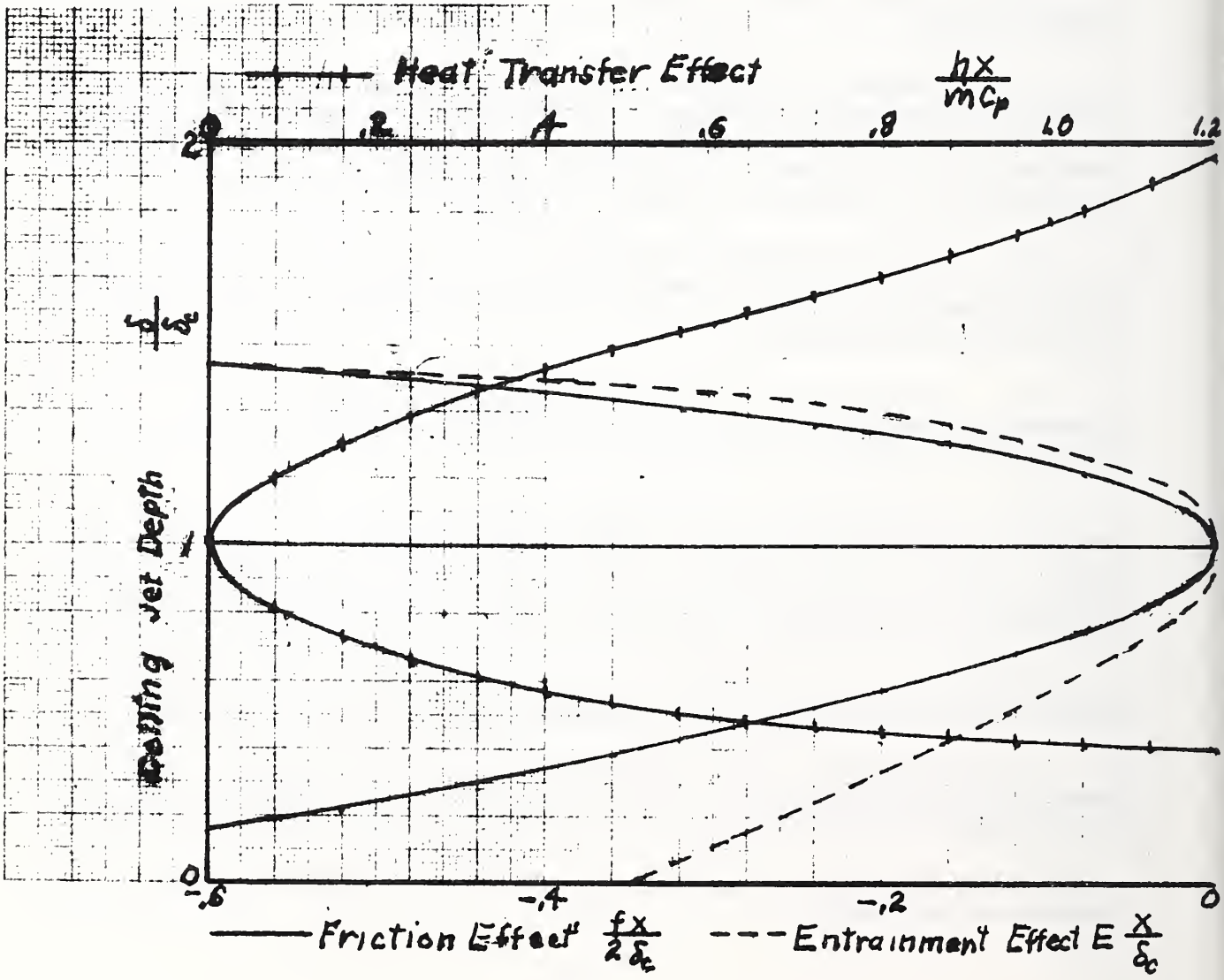
The effect of entrainment alone is qualitatively identical to friction. A common special case is again solved analytically.

Heat transfer alone has the opposite effect from friction and entrainment in the sense that the ceiling jet moves away from critical as it proceeds (see attached figure). Again, an analytical solution has been found. The flow cannot satisfy the condition of critical flow at the open end of a corridor. New experimental and theoretical studies of the end effect is needed.

When friction and heat transfer are both present (as always in fact), valid solutions exist, if dominated by friction; and no solutions exist, if dominated by heat transfer.

Careful measurements have been made at the California Institute of Technology by M. V. Chobotov as his Ph.D. thesis study. He also made a more complete theory than top hat, using realistic temperaure and velocity profiles. He was unable to find a solution agreeing with his data. The top hat theory has shown why, i.e., no suitable solutions exist. He got fair agreement with his data using the completely unfounded assumptions that the flow was critical everywhere. The same kind of poor agreement is obtained with the present, simpler theory and the nonexistence of suitable solutions becomes obvious. A field theory solution is needed and some detailed experimental studies at a corridor open end would be most helpful.

The present work suggests that there are some fundamental effects not yet understood. In addition, the present theory must be extended to large two-dimensional ceilings, to closed or partially open corridors, to include the burning of fuels left over from the originating fire or added by pyrolysis of a flammable ceiling.



CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: The Pennsylvania State University

Grant No.: 60NANB8D0849

Grant Title: Upward Flame Spread on a Vertical Wall

Principal Investigator: Dr. Anil K. Kulkarni
Department of Mechanical Engineering
209 Mechanical Engineering Building
University Park, PA 16802

Other Professional Personnel: Choong I. Kim, Doctoral Student
Ellen Brehob, Doctoral Student
Chung H. Kuo, Graduate Student
Shailesh Manohar, Graduate Student

NIST Scientific Officer: Dr. W.J. Parker

Technical Abstract:

Introduction: Most compartment fires involve burning of vertical walls made of finite thickness combustible materials (like wood panels) or walls made of an inert substrate covered with a thin, combustible material (as in case of a metal panel covered with carpet in an aircraft cabin). Behavior of these walls under fire situation is substantially different from that of an idealized semi-infinite wall. Since the upward flame spread process often provides an important vehicle for fire growth in compartment fires, it is imperative that we are able to adequately understand and predict upward flame spread on vertical walls of thin combustible materials. The knowledge of fundamental mechanisms of upward flame spread can also help in assessing the material flammability in common fire situations. The objective of the present work was to study the upward flame spread process on vertical walls for materials actually used in practice and thereby understand the mechanisms and behavior of upward flame spread in realistic fire situations.

When compared to a semi-infinite wall of homogeneous solid fuel, flame spread over a thin, practical wall material is complicated by several processes: (a) The local burning rate ($\dot{m}''$) is a transient function which depends on the intrinsic and geometric properties of the wall material. For example, there may be an initial peak due to volatile gases in case of a wood panel followed by slow burning of char; (b) There is a substantial time-dependent heat loss to the solid interior when the panel is thin; (c) As a result of the time-dependent local mass loss rate, the flame height (which is dependent on the total heat release rate) must be carefully computed based on the cumulative burning rate of the wall, from the bottom to the top of the pyrolyzing zone, while various parts of the walls are at different stages of burning; (d) The heat flux ahead of the pyrolysis front is a function of time, distance from the pyrolysis edge, size of the flame, and the radiation characteristics of flame gases, which in turn depend on the burning rate and material characteristics. These must be properly accounted for, by defining appropriate new fire properties; (e) The temperature of the wall surface depends on the transient conduction into the wall of finite thickness; this is also not a trivial calculation. The work conducted under the

present grant attempts to address the upward flame spread problem with an integral approach, i.e., a complete predictive method is provided for practical materials (such as laminated wall materials, woods, composites, etc.) which do not necessarily burn in "analytically simple" way. In order to handle peculiar behavior of the practical materials, the model defines and accepts certain "fire properties" as input which can be obtained in well-defined small scale experiments. An extension of this work has recently been started, which includes theoretical and experimental investigation of upward flame spread on vertical walls under external radiation simulating fire surrounding the wall, and the determination of indepth radiation absorption properties for various materials.

Theoretical Approach: The physical model for upward flame spread is described in detail in publication 8. A vertical flammable wall with infinite width and height h is ignited at the bottom using a line burner of known energy output, placed at the bottom of the vertical wall. Flames from the burning of pyrolyzed fuel (in addition to the igniter) continuously cover the solid fuel above the pyrolysis front which is heated by the energy feedback from the flames. When any particular location on the unburnt fuel heats upto a certain characteristic ignition temperature, it starts pyrolyzing, the pyrolysis front is advanced to that location, the flames grow taller, and thus, the process of upward flame spread continues. The important parameters contributing to the upward flame spread, therefore, are the heat feedback from flames to unburnt wall surface, $\dot{q}''_w$, mass loss rate of the wall on the pyrolyzing surface ($\dot{m}''$), the flame tip height, x_f, and other physical and chemical material properties. Depending upon the characteristics of the material, wall thickness, and the heat loss to the atmosphere, the flame spread may accelerate, or it may cease because insufficient fuel is supplied to sustain the flames.

A mathematical model has been developed which accounts for the processes described earlier for a thin, combustible wall; details can be found in publication 8. In this model, the surface temperature as well as the inner temperature of the two-dimensional vertical slab, initially at the temperature of T_o, are obtained by solving transient two dimensional heat conduction equation with the transient boundary conditions of flame heat feedback absorbed by the yet unburnt surface and heat loss at the back surface of the wall. An examination of the heat feedback data for typical room-size fires (up to 2.5 m high) for several different materials available in literature as well as from our own experiments, reveals that the data may be collapsed in a generalized form,

$$\dot{q}''_w(x,t) = \dot{q}''_{wo}\, g\,\{x_p(t), x_f(t), x\}$$
$$= \dot{q}''_{wo} \exp\left[-0.693\left(\frac{x-x_p}{x_f-x_p}\right)\right]$$

where $\dot{q}''_{wo}$ is a "fire property" of the wall material and g is a generalized function of pyrolysis height (x_p), flame tip height (x_f), and the vertical location (x). The property $\dot{q}''_{wo}$ of the material is the heat feedback from flames to surface just above $x = x_p$. The local mass loss rate m" is assumed to be a material property independent of the location, and it can be obtained in a small scale experiment. It is expressed as a fourth-order polynomial of $(t-t_p)$, where $(t-t_p)$ is the time measured from the inception of pyrolysis at the given location. A comprehensive justification for this approach and a detailed description of the small scale apparatus in which m" $(t-t_p)$ is measured is given in publication 7. The model is solved using a finite-difference numerical scheme.

Experimental Approach: Experiments were conducted on 30 cm wide, 1.2 m high, and 3.2 mm thick samples of black PMMA (polymethylmethacrylate) and masonite, and 5.0 mm thick samples of cardboard. PMMA is a clean, ashless burning, noncharring polymer, masonite is a char-forming wood product, and cardboard is a laminated paper product. These three materials burn differently and are commonly used in practice. The samples were mounted on a 12.7 mm

thick board of marinite (an inert material) to simulate a vertical wall having a panel of combustible material mounted on an inert substrate. The samples were ignited using a 40 cm long natural gas burner set at 18 kW/m energy release rate. The flame height, heat feedback and (when possible) pyrolysis height were recorded as a function of time. Also, local mass loss rate, $\dot{m}''$ defined and discussed earlier, was measured in a specially designed small scale apparatus for each of the materials mounted on marinite plates under essentially similar conditions. The local mass loss rate function is an input property to the mathematical model and it is shown for the three samples in Figure 1. Details on these experimental setups and additional experimental data are being included in the doctoral dissertation of Choong I. Kim..

Results and Technical Accomplishments: Comparison of predictions and data for the flame height and pyrolysis height for masonite, black PMMA, and cardboard are shown in Figures 2, 3, and 4 respectively. The bars in Figure 2 for masonite indicate the range of xf due to flame fluctuations. The flame height is constant upto approximately 60 s because the material has not yet started pyrolyzing and the flames are entirely those from the gas burner. After 60 s, the masonite sample starts pyrolyzing and thus the flame height and pyrolysis height grows. The trends and magnitudes of the flame height, and therefore the upward flame spread, are clearly well-predicted by the model for masonite as well as for the other two materials.

An important point to be made here is that the prediction methodology developed here is useful for *practical* materials under *realistic* wall fire situations. The wall materials may possess special characteristics (such as early volatilization, charring, etc.) and they may burn as a thin material or as a composite. The mathematical model and the needed properties are clearly defined, the model is validated with data; and thus, the present methodology can be used in fire hazard prediction studies or in testing wall materials for their flammability characteristics in the upward flame spread configuration in real fire situations.

Publications:

[1] Kim, C.I. and A.K. Kulkarni. A Numerical Model for Upward Flame Spread. Proceedings of the Fall Technical Meeting of the Eastern Section of The Combustion Institute, Albany, New York, paper no. 47, November 1989.

[2] Kulkarni, A.K. and S. Fischer. Upward Flame Spread on Vertical Walls: An Approximate But Complete Model and Experiments. Proceedings of ASME Winter Annual Meeting, Heat Transfer in Combustion Systems, HTD-Vol. 122, pp. 53-61, (1989).

[3] Kulkarni, A.K. and C.I. Kim. Heat Loss to the Interior of a Free Burning Vertical Wall and Its Influence on Estimation of Effective Heat of Gasification. To appear in Combustion Science and Technology.

[4] Kulkarni, A.K. and S. Fischer. Upward Flame Spread on Vertical Wall: Model and Experiments. Proceedings of the III International Seminar on Fires, Alma-Ata, USSR, (1989).

[5] Kulkarni, A.K. Radiative and Total Heat Feedback from Flames to Surface in Vertical Wall Fires. To appear in Experimental Heat Transfer.

[6] Kuo, C.H. and A.K. Kulkarni. Analysis of Heat Flux Measurement by Circular Foil Gages in a Mixed Convection/Radiation Environment. Submitted for publication; under review.

[7] Kulkarni, A.K., C.I. Kim, and H.E. Mitler. Time-Dependent Local Mass Loss Rate of Burning Walls. Submitted for publication; under review.

[8] Kim, C.I. and A.K. Kulkarni. Upward Flame Spread on Vertical Walls of Finite Thickness. Submitted for publication; under review.

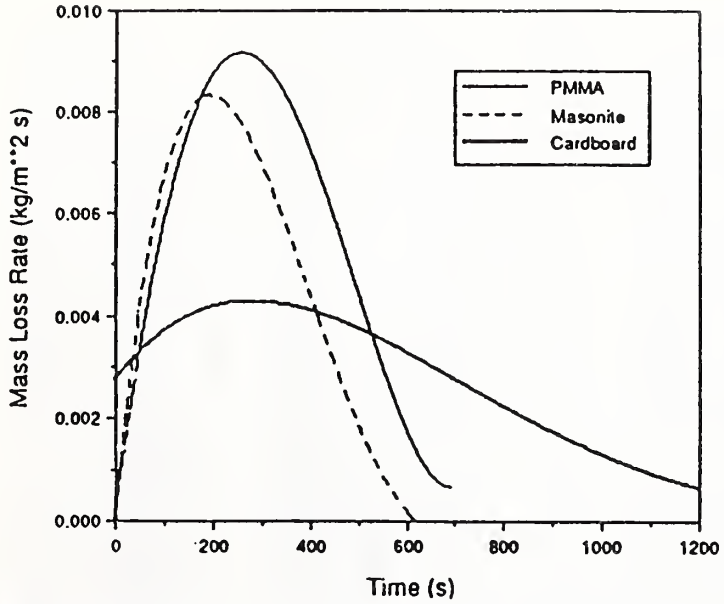


Figure 1. Mass loss rate as a function of time for PMMA, masonite, and cardboard.

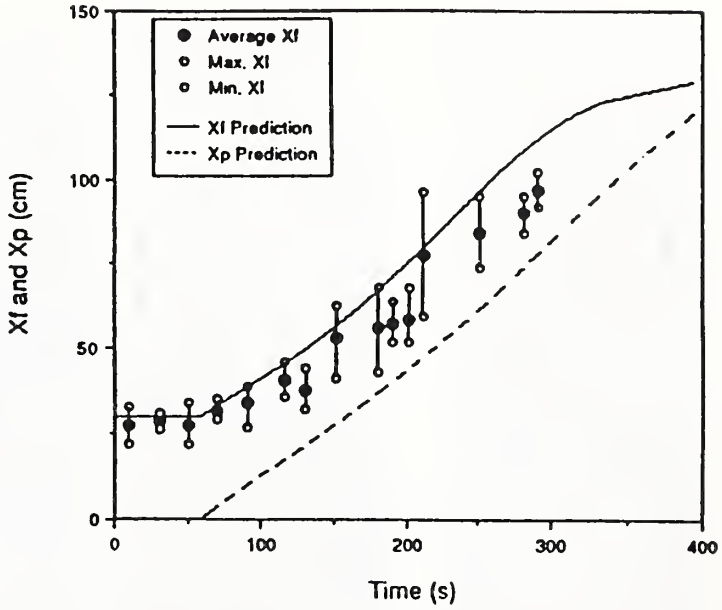


Figure 2. Prediction of Xp and Xf compared to experimental data for 3.2 mm thick masonite.

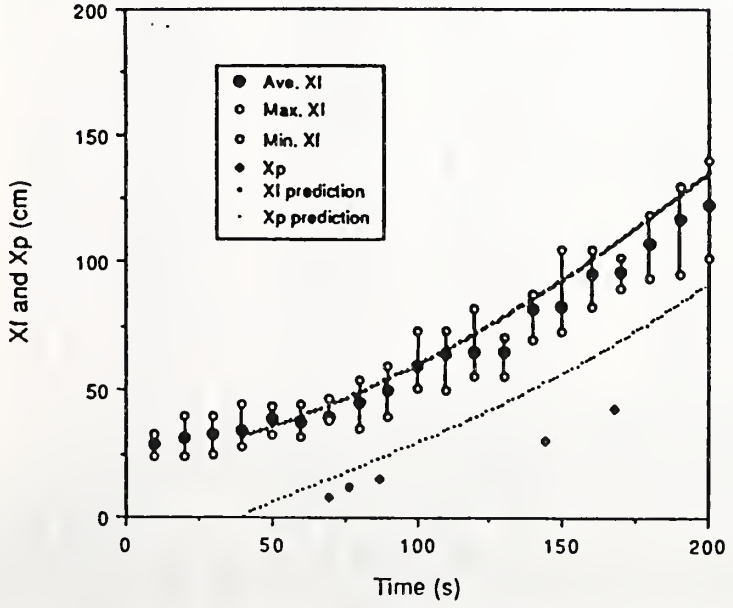


Figure 3. Prediction of Xp and Xf compared to experimental data for 3.2 mm thick PMMA slab.

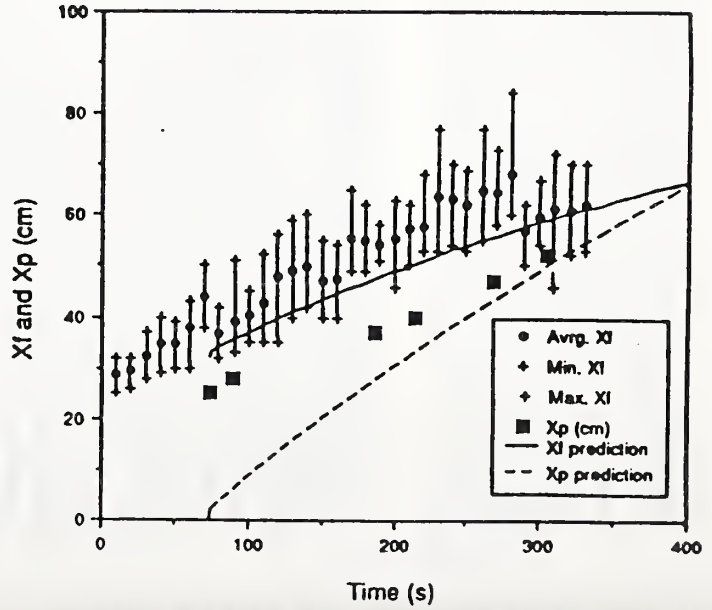


Figure 4. Prediction of Xp and Xf compared to experimental data

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	The University of Kentucky
Grant No.:	60NANB0D1031
Grant Title:	A Study of Fire Induced Flow along the Vertical Corner Wall
Principal Investigator:	Kozo Saito Associate Professor Dept. of Mechanical Engineering Lexington, KY 40506-0046
Co-Principal Investigator:	William A. Gruver Director of Center for Robotics and Manufacturing Systems Lexington, KY 40506-0108
Other Professional Personnel:	Toshi Daikoku, Visiting Scientist Wen-Xiu Lin, Master Student
NIST Scientific Officer:	Dr. Henry Mitler

Technical Abstract:

The objective of this study is to understand three dimensional character of the boundary layer which will be developed along the vertical corner wall by the heat generated from the gas burner. To visualize the fire induced flow, a 1/2-scale room corner model (a schematic is shown in Fig. 1) was designed based on the NIST prototype. The corner wall was made of two Marinite boards (non-combustible material) of 0.02 m thickness and was fixed on a steel frame. A square-shaped gas burner (0.3m long x 0.3m wide x 0.05m high) through which a methane-air premixed gas was flown was placed on the corner floor with the zero burner stand-off distance. Flow visualization apparatus is composed of a smoke generator (Japanese incense was used as smoke source) and a copper tube with narrow holes through which smoke streak lines were produced. A series of flow visualizaton experiments are planned by changing the bur ner heat release rate and the burner stand-off distance from the wall. Typical example photographs which show (a) flow along the vertical corner wall without burner on, and (b) that with the burner on (the burner heat release rate is 3.6 kW) are shown in Figs. 2 and 3, respectively. The visualized overall flow pattern was schematically illustrated and shown in Fig. 4.

As a next phase of the experiment, we are planning to use IR camera system to obtain an instantaneous temperature mappings at the vertical wall.

Fig. 2 Without the burner on.

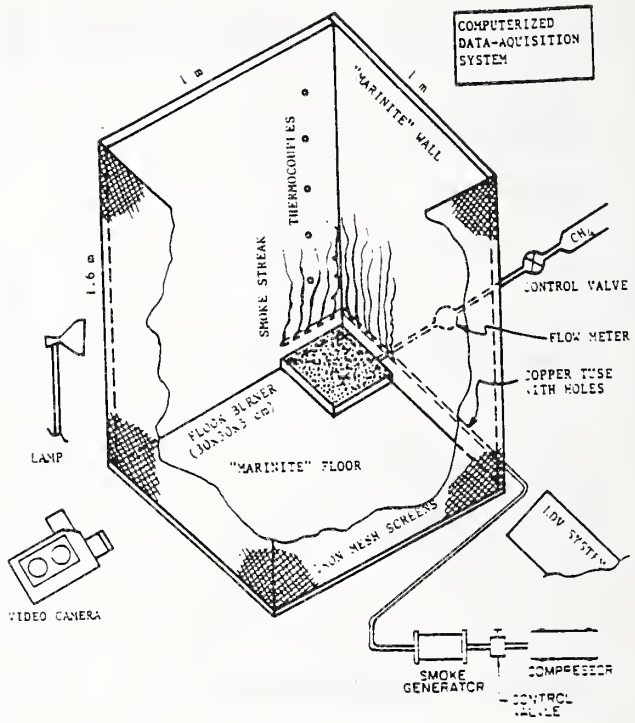
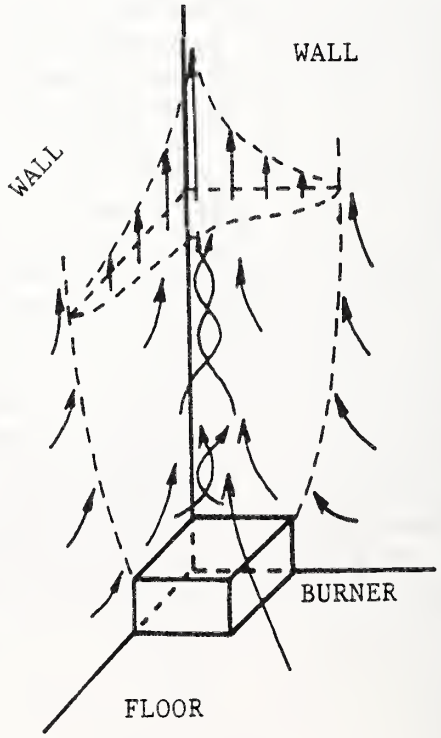


Fig. 1 Experimental Apparatus.

Fig. 3 With the burner on.

Fig. 4 A schematic illustration of the fire induced flow along the corner wall.



F. TOXIC POTENCY

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

TOXIC POTENCY MEASUREMENT

Professional Personnel

Vytenis Babrauskas, Group Leader
Barbara C. Levin, Toxicologist
Maya Paabo, Research Chemist
Emil Braun, Physicist
Richard H. Harris, Jr., Chemist
Magdalene Navarro, Biologist

Project Objective

To provide by July 1991 a rational and practical system for obtaining accurate toxic potency data for hazard models and product evaluation; to predict toxic effects of fire gases on rodents and humans.

Technical Approach

1. Various materials will continue to be explored in the SwRI radiant heat system, in an effort to discover and set right any points of weakness.

2. Prepare a protocol for use of the bench-scale data in predicting real-scale performance.

3. A writeup of the test procedure will be provided in ASTM format.

4. Experimental work needed to complete N-gas model will be finished. A final report will be prepared describing the complete model.

5. The modified CFK equation for CO prediction will be documented against NIST rat data and against literature human data.

Technical Accomplishments

During this year the most important accomplishment was the completion of the pilot validation study. In this study, real-scale fire tests were conducted on 3 different materials in a room/corridor/room arrangement. The same materials were also examined in a variety of small and medium scale methods. The focus of the investigation was to develop validation hypotheses which are appropriate and are useful in the task of predicting fire hazards from test data. The results will appear in an NIST Technical Note this Fall.

During this past year we also continued the development of the bench-scale radiant heat toxicity apparatus which was originally developed at Southwest Research Institute. In cooperation with SwRI we have been developing a test protocol which is intended to be an improvement upon existing methods, and which correctly can test composite specimens. This work is in progress and is scheduled to be completed in one year.

During the year also significant progress was made in setting up a computational model for CO production and elimination which can correctly predict both rat and human responses. This work is also scheduled for completion during the next year. To be completed at the same time is a

consolidated presentation of the N-Gas model. At present, we are studying the non-linear interaction between NO_2 and HCN effects and are also incorporating HCl into the model.

During this year, some aspects of our studies were partially funded by the following organizations: International Copper Association, The Society of the Plastics Industry, Inc., BFGoodrich, and The Industry Coalition.

Reports and Publications

Babrauskas, V., Harris, R.H., Jr., Braun, E., Levin, B.C., Paabo, M., and Gann, R.G., The Role of Bench-Scale Test Data in Assessing Full-Scale Fire Toxicity, NIST Technical Note to be issued (1990).

Babrauskas, V., Harris, R.H., Jr., Braun, E., Levin, B.C., Paabo, M., and Gann, R.G., Large-scale Validation of Bench-scale Fire Toxicity Tests, pp. 3-12 in *INTERFLAM '90: Fifth Intl. Fire Conf. Proc.*, London (1990).

Levin, B.C. and Gann, R.G., Toxic potency of fire smoke: measurement and use. *Fire and Polymers: Hazards Identification and Prevention*, Ed. by G.L. Nelson, ACS Symposium Series 425, American Chemical Society, Washington, DC, pp.3-11, 1990.

Braun, E., Gann, R.G., Levin, B.C., and Paabo, M., Combustion product toxic potency measurements: comparison of a small-scale test and "real-world" fires. J. Fire Sciences 8:63-79 (1990)

Levin, B.C., Rechani, P.R., Gurman, J.L., Landron, F., Clark, H.M., Yoklavich, M., Rodriguez, J.R., Droz, L., Mattos de Cabrera, F., and Kaye, S., Analysis of carboxyhemoglobin and cyanide in blood from victims of the Dupont Plaza Hotel fire in Puerto Rico. Journal of Forensic Sciences 35:151-168 (1990).

Levin, B.C., Paabo, M., Harris, R.H., Clark, H.M., Yoklavich, M.F., Eller, N. and Highbarger, L., The effect of copper additives on atmospheric hydrogen cyanide and acute inhalation toxicity from the combustion products of flexible polyurethane. Proceedings of The Fire Retardant Chemicals Association Fall Conference, Scottsdale, AR, October, 1989, pp. 107-112.

Levin, B.C., Progress Report on Fire Toxicity and Chemistry Research in the United States. Proceedings of the 11th UJNR meeting held in California, October 19-24, 1989. (In press).

Levin, B.C., Paabo, M., Highbarger, L., and Eller, N., Synergistic effects of nitrogen dioxide and carbon dioxide following acute inhalation exposures in rats. NISTIR 89-4105, National Institute of Standards and Technology, Gaithersburg, MD, June, 1989.

Levin, B.C., Rechani, P.R., Gurman, J.L., Landron, F., Clark, H.M., Yoklavich, M.F., Rodriguez, J.R., Droz, L., and Kaye, S., Analysis of carboxyhemoglobin and cyanide in blood from victims of the Dupont Plaza Hotel fire in Puerto Rico, *J. of Forensic Sci. 35*, 151-168 (1990).

Related Grants

1. Southwest Research Institute, PI - Arthur Grand, Laboratory Smoke Evolution STudies using the SwRI Radiant Combustion/Exposure Apparatus.
2. University of Pittsburgh, PI - Yves Alarie, Toxicity of Plastic Combustion Products.
3. Southwest Research Institute, PI - Walter G. Switzer, Analysis of Hazards to Life Safety in Fires: A Comprehensive Multi-dimensional Program, Part IV (work from FY89).

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	Southwest Research Institute
Grant No.:	60NANBOD1056
Grant Title:	Laboratory Smoke Evolution Studies Using the SwRI Radiant Combustion/Exposure Apparatus
Principal Investigator:	Dr. Arthur F. Grand
Other Professional Personnel:	Walter G. Switzer LeMoyne Boyer
NIST Scientific Officer:	Dr. Vytenis Babrauskas

Technical Abstract:

Objectives The purpose of this project is to develop a correlation between ambient oxygen concentration and the evolution of carbon monoxide and hydrogen cyanide from the burning of polymeric materials in a laboratory-scale apparatus. Specimens will be subjected to an externally-applied radiant heat flux, in the presence of an ignition source, under a variety of oxygen concentrations. It is expected that the results will provide insight into the production of toxic gases under vitiated oxygen atmospheres, as might occur in larger-scale fires.

Approach The radiant combustion/exposure apparatus developed at Southwest Research Institute (SwRI), under contract to the National Institute of Building Sciences (NIBS), will be used for this study. The apparatus consists of an enclosed 200-L exposure chamber with an attached all-quartz combustion cell. The two parts are connected by a stainless steel chimney through which the smoke is transported. Specimens are placed inside the combustion cell and are subjected to a radiant heat flux supplied by tungsten-quartz lamps, which are located external to the combustion cell. The specimen rests on a platform attached to a load cell for continuous mass loss measurements. A spark ignition source is provided for initiating flaming combustion.

This apparatus is unique for studying the effects of various O_2 atmospheres on the combustion of polymeric materials. It is an enclosed system; therefore, oxygen may be adjusted prior to starting combustion and then added in relatively small quantities during combustion in order to maintain a constant O_2 concentration during the experiment. Furthermore, it is possible to adjust the ambient oxygen concentration either up or down during combustion. This may be necessary for certain experiments conducted at lower oxygen levels, where sustained burning might not occur at the desired O_2 concentration (e.g., below 13 percent). In such cases, the oxygen level will be set somewhat higher (e.g., 16 percent) in order to develop a period of flaming combustion and then reduced at a predetermined time in order to observe the effect of the lower O_2 level on CO production.

Several different polymeric materials will be studied, including wood and polyurethane foam. The following experimental variables will be considered: 1) specimen size (surface areas from 26 to 103 cm^2), 2) external radiant heat flux (25 to 50 kW/m^2), and 3) oxygen concentration (12- to 21-percent). The rate of evolution of CO and HCN may be dependent on any of these test parameters. Although the anticipated results of this study have implications for smoke toxicology, no animal experiments are planned for this program. There is a large quantity of data on the effects of CO and HCN on rodents and on humans and it would serve no purpose at this time to expose animals to the smoke produced.

Future Plans This study has only just begun.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution: University of Pittsburgh

Grant No.: 60NANBOD1032

Grant Title: Toxicity of Plastic Combustion Products

Principal Investigator: Professor Yves Alarie, Ph.D.
Toxicology Laboratory
Graduate School of Public Health
University of Pittsburgh
Pittsburgh, PA 15261
Telephone: (412) 624-3047

Other Professional Personnel: Daniel Caldwell (Ph.D. Candidate)

NIST Scientific Officer: Dr. Barbara C. Levin

Technical Abstract:

The overall goal of this project is to develop a system to study toxicity of smoke from burning materials which can be used to predict toxic hazard.

I. Technical:

To meet the overall goal, basic requirements must be satisfied within three separate modules.

a) Combustion Module:

Combustion (flaming) must be controlled and the number of variables measured must be sufficient to permit an evaluation of combustion conditions. The lowest number of variables to satisfy the above requirement are heat flux ($\dot{Q}$) to the specimen, ventilation of the compartment where combustion occurs ($\dot{V}$) and mass loss rate of the specimen ($\dot{m}$).

b) Analytical Chemistry Module:

The minimum requirement is for continuous analysis of O_2, CO_2 and CO. These are required to assess combustion conditions in conjunction with the above variables. Also, analysis of HCN is required with nitrogen containing polymers and HCl analysis is required with chlorine containing polymers.

c) Toxicity Assessment Module:

Smoke produced from the combustion module must be captured in or directed to an exposure chamber for exposure of animals. The minimum requirement for assessing toxic potency is determination of

the LC_{50}. This requires only 4 animals/group. Since a time based hazard model is desired the minimum requirement was extended for statistical analysis. Thus, 16 mice/exposure group were used but this number will be reduced to 12 or possibly 8 after more experience is gained. The data (time to death) were then analyzed using the product limit method and the results obtained as survival distribution function, probability distribution function, hazard function and cumulative hazard function over exposure time. Also, the conventional LC_{50} was calculated.

II. Results:

A. UPITT II Flaming Combustion/Toxicity of Smoke Assessment Apparatus.

A diagram of the apparatus is presented in Figure 1 and a detailed description has been published (1). $\dot{Q}$ levels used have been between 20 and 50 kW/m^2 while $\dot{V}$ levels have been varied from the level to just maintain flaming above the specimen to levels resulting in very efficient burning, i.e., very low CO production. The air coming out of the cone hood is directly exhausted (line B) or directed toward the exposure chamber. This arrangement permits the greatest flexibility in that exposure of animals can be initiated not only from the beginning of irradiation of the specimen but for any period after this such as after ignition occurs or at any stage of combustion. The exposure chamber permits using up to 16 animals depending upon the statistical requirements for determination of LC_{50} or for cumulative hazard analysis. Analyzers for O_2, CO_2 and CO are as shown on the diagram and sampling ports are available on the exposure chamber for sampling gases such as HCN and HCl.

B. UPITT II Flaming Combustion/Toxicity of Smoke Assessment Protocol.

Using the above apparatus we undertook a series of experiments using Douglas fir. Specimens were 38 mm thick and 110 x 110 mm (0.01 m^2 exposed surface area). These specimens were irradiated at 21, 35 or 50 kW/m^2. For each $\dot{Q}$ investigated, $\dot{V}$ was varied so that the lowest $\dot{V}$ was just sufficient to maintain flaming above the specimens up to high $\dot{V}$ levels to produce vigorous flaming and efficient (i.e., low CO) combustion. A group of 16 mice was used for exposure to the smoke produced under each condition. Exposure was for 30 minutes starting with irradiation of the specimen. Under inefficient burning conditions carbon monoxide evolved slowly and was found to be the principal toxicant. Under highly efficient burning conditions deaths also occurred, <u>but not due to CO</u>. Combining all the results (all $\dot{Q}$ and $\dot{V}$ combinations used) as shown in Figure 2 permitted the calculation of an LC_{50} of 113 mg/L for a planned 30 minute exposure and 10 minute observation period following exposure. Larger specimens (0.016 and 0.028 m^2) also produced data within the range of 0.01 m^2 and combining all specimen sizes resulted in an LC_{50} of 112 mg/L. A survivable exposure concentration of 76 mg/L is suggested as shown in Figure

2. Lethality data were also analyzed for time to death to obtain median time to death, survival distribution function and cummulative hazard. These showed that although the LC_{50} was similar for the different burning conditions investigated, the time to effect was very different. The cumulative hazard was highest under the most efficient flaming conditions producing low CO; a completely unexpected result. Thus, the lethal effect of smoke from Douglas fir cannot be predicted from analysis of CO.

III. Conclusions:

The UPITT II flaming combustion/toxicity of smoke method is the most fundamentally sound method from both the combustion aspect and toxicity assessment aspect. Each aspect can be rigidly controlled and analyzed. It is also the only method which provides for controlled flaming conditions for a long period of time (30 minutes) in order to assess toxicity of smoke. The method is now completed and we have met our objective. Since CO is not the principal toxicant under highly efficient conditions the toxicant(s) involved remain to be determined. Finally, investigations using other polymers have been initiated with no major technical problem and thus the method will be applicable to investigate specimens other than wood.

This is the only method permitting a statistically correct analysis of time to death data and cumulative hazard over time. Since differentiation was easily obtained for Douglas fir between efficient and inefficient burning conditions it appears that the technique will be powerful enough to distinguish between materials. Similarly, the potency range is very narrow with Douglas fir and statistical differences between this material and other polymers should be easy to obtain.

Reports and Papers:

1. Caldwell, D. J. and Alarie, Y. A method to determine the potential toxicity of smoke from burning polymers: I. Experiments with Douglas fir. J. Fire Sciences 8, 23-62, 1990.

2. Caldwell, D. J. and Alarie, Y. A method to determine the potential toxicity of smoke from burning polymers: II. The Toxicity of Smoke from Douglas Fir. J. Fire Sciences. Submitted.

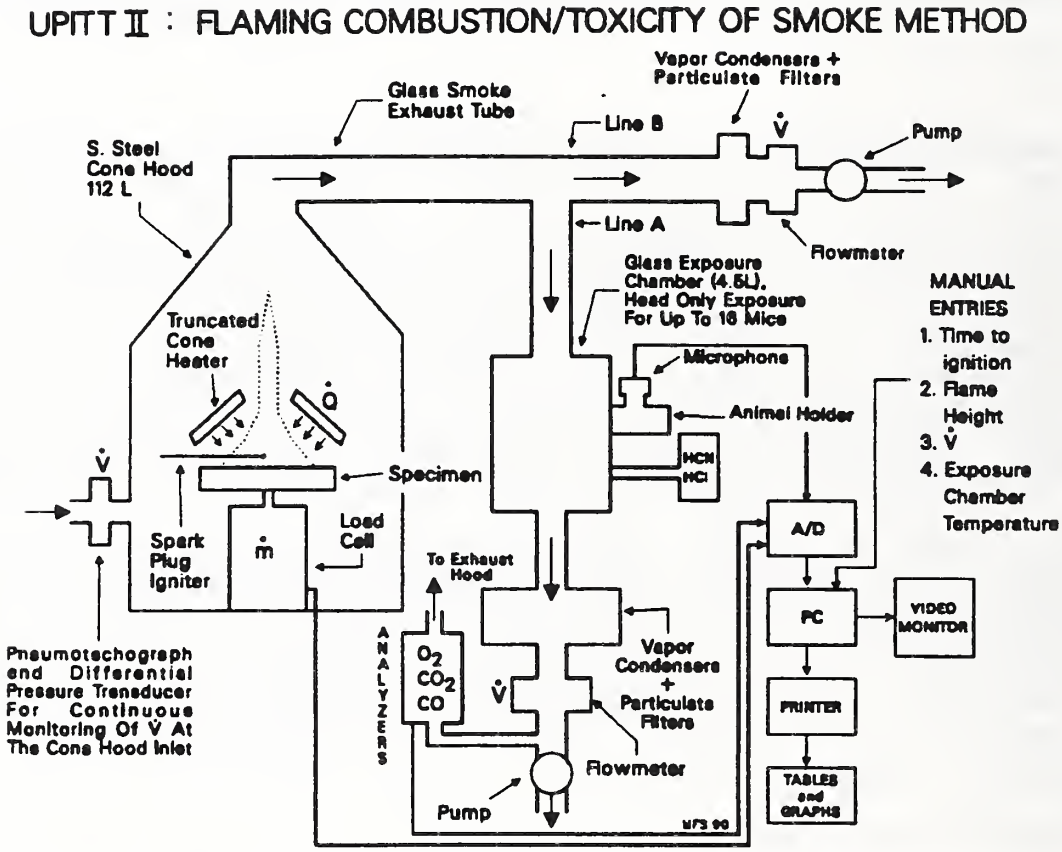


Figure 1 UPITT II Flaming Combustion/Toxicity of Smoke Assessment Apparatus. The apparatus consists of a cone hood which contains a cone heater (developed at NIST) to irradiate specimens at selected $\dot{Q}$ levels and under different airflows ($\dot{V}$) through the cone hood while measuring $\dot{m}$ of the specimens placed on a load cell.

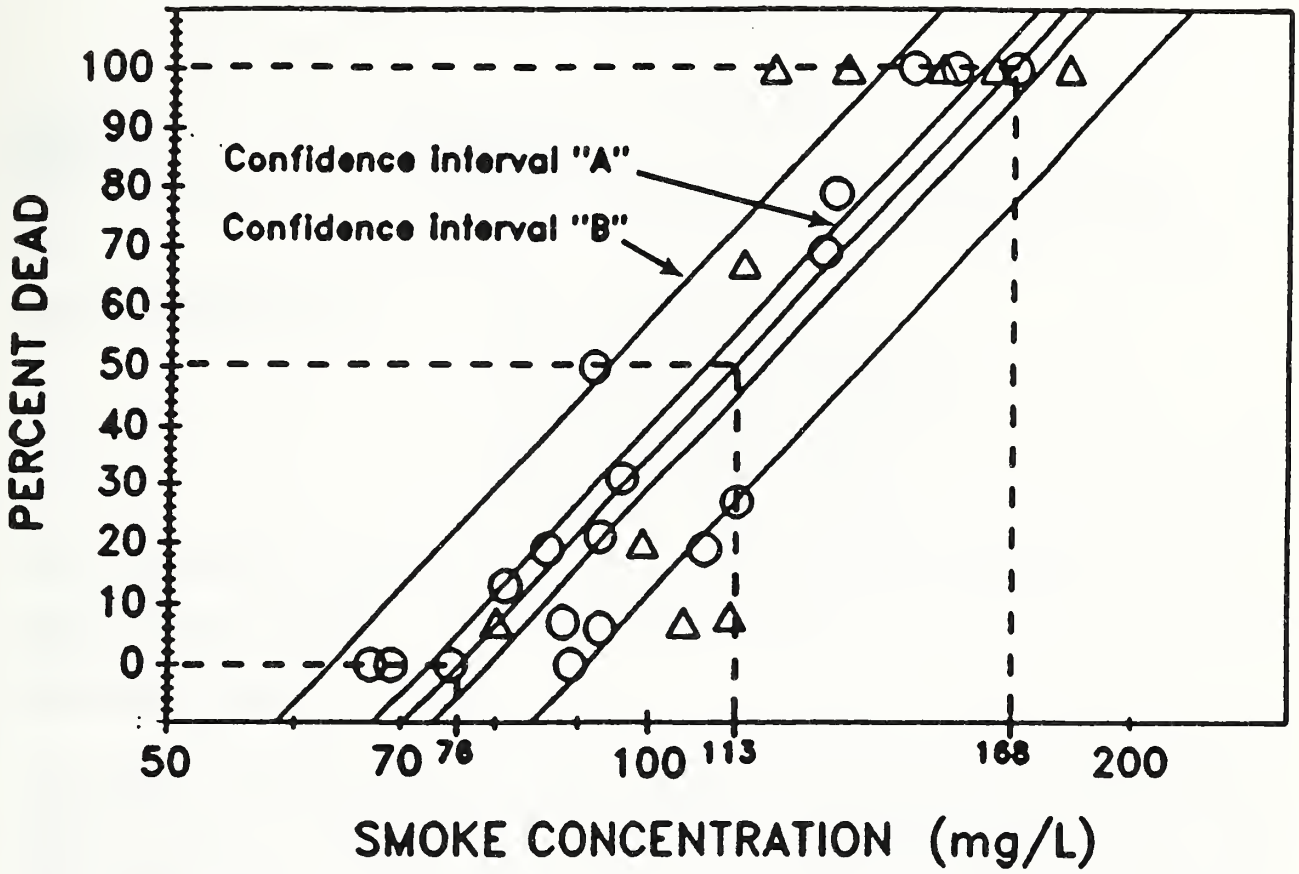


Figure 2. Potency of Douglas fir smoke obtained by combining the individual data points for percent death vs. nominal smoke concentration (calculated as $\dot{m}/\dot{V}$) at varying levels of $\dot{Q}$ and $\dot{V}$. Open circles are the data points for 0.01 m^2 specimens. These were used to develop the regression line and 95% confidence intervals. Regression equation is Y (X) = - 549 + 292 x log X. "A" is the 95% confidence interval for the estimated mean value of Y for a given X. "B" is the 95% confidence interval for the predicted individual Y value for a given X. The LC_{50} value was calculated to be 113 mg/L (95% confidence intervals: "A" is 108 to 117 mg/L, "B" is 94 to 135 mg/L) and the range from 0 to 100% death is 76 to 168 mg/L. Open triangles are additional data points for 0.016 and 0.028 m^2 specimens not used in the regression calculation. If included, the calculated LC_{50} becomes 112 mg/L.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution: Southwest Research Institute, San Antonio, TX
Grant No.: 60NANB6D0635
Grant Title: "Analysis of Hazards to Life Safety in Fires: A Comprehensive Multi-Dimensional Research Program - Part 4"

Principal Investigator: Walter G. Switzer
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Southwest Research Institute
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NBS Scientific Officer: Dr. Barbara C. Levin

Technical Abstract:

Smoke inhalation is recognized as a major cause of fire fatalities. The overall objective of this research program is to provide data and develop methodology to be used for modeling the effects from inhalation of toxic fire gases. Combustion atmospheres can consist of a variable, complex mixture of toxic gases. Even single materials can produce multiple toxicants at significant levels. Predicting the combined toxic effects of these mixtures is one of the most difficult problems in combustion toxicology. Basic toxicological data is needed to develop models to predict the degree of potential interaction and enable incorporation of laboratory toxicological data into a hazard analysis applicable to humans. A model can also function as an interim research tool to extrapolate small scale results to large scale, improve testing protocols, and reduce the number of animals required for testing. Our approach consists of exposing animals to selected toxic fire gases, both individually and in combination, in order to compare the effects observed with estimates from predictive models. The primary measure of toxicity has been lethality. Additional toxicological measures are taken to gain further insight into the mechanisms of action.

During this reporting period, we issued the final report which incorporated lethality and associated toxicological data for hydrogen bromide (HBr), binary combinations of hydrogen cyanide (HCN) and hydrogen chloride (HCl), and tertiary mixtures containing carbon monoxide (CO), HCN and HCl. The data from two additional tertiary mixture tests are summarized in this report. This data was analyzed and discussed in the final report.

Experimental Approach:

Exposure of Animals

Apparatus

The exposure apparatus used in these studies is similar in size and shape to that commonly used in the NBS smoke toxicity test. However, it was modified to create a 'flow-through' system. The air flow through the exposure chamber ranged from about 140 L/min to about 200 L/min. This high air flow rate permitted rapid equilibration of the test atmospheres in the animal exposure chamber. An animal isolation system was used to protect the animals from the test atmosphere until equilibrium was established.

Exposure Protocol

Each animal exposure test involved the exposure of six, young adult Sprague-Dawley rats positioned in tubular restrainers to provide for head-only exposure. Following insertion of the tubed animals into position through the wall of the chamber, the animal isolation system was closed and breathing air provided during the establishment of the test atmosphere. Exposures were initiated by opening the isolation system and continued for 30 minutes. The endpoint recorded was lethality. Surviving animals were observed until either postexposure death or 14 days. Animals surviving 14 days were euthanized. In experiments involving CO, animals dying during exposure or shortly post exposure were bled by cardiac puncture for percent carboxyhemoglobin analysis on an Instrumentation Laboratories IL 282 CO-Oximeter.

Generation of Test Atmospheres

Pure Gas Atmospheres

Atmospheres were generated by the metering of the appropriate gases from cylinder sources into the exposure chamber, with continuous analytical monitoring of selected gases. Supplemental O2 was provided as necessary to maintain O2 concentration at 20.5 +/- 1.0%.

Sources were:

Carbon Monoxide (99.9%): Scientific Gas Products
Hydrogen Chloride (99.5%): Scientific Gas Products
Hydrogen Cyanide (10% balance Nitrogen) Scott Specialty Gases

Analysis of Test Atmospheres

Continuous Instrumentation

Analyses of exposure atmospheres for CO, CO2, and O2 were continuously conducted using a closed loop sampling system and the following instrumentation:

Carbon Monoxide: Beckman 865
Carbon Dioxide: Beckman 865
Oxygen: Beckman OM-11

Hydrogen Chloride and Hydrogen Cyanide

The method used for continuous monitoring of hydrogen chloride (HCl) gas has been described in the literature. The method, called a continuous titration analyzer (CTA), is based on one reported in a French standard test method, with instrumentation and procedures modified in our laboratories. Good success has been obtained with this technique; however, verification, including measurement of interferences, has not been completed. Therefore, for most experiments, backup analyses of HCl and HCN were also performed by sorption tube sampling followed by extraction and titration.

A sample of an atmosphere containing HCl is drawn continuously by a pump into a gas-solution impinger containing 0.1 N HNO3 aqueous solution. Silver nitrate (AgNO3) solution is automatically metered into the cell to react with the chloride ion in order to maintain a preset electromagnetic force (emf), as measured by the silver electrode in the titration cell. The rate of addition of titrant is directly proportional to the concentration of HCl in the sample gas stream. This process is continued as needed to maintain the solution at the set point, which is near the equivalence point of a silver-chloride titration. The CTA method for measuring hydrogen cyanide (HCN) in the combination gas series was essentially the same as that used for monitoring HCl, except that a different absorbing solution was used.

The output of the automatic burette (mL of titrant) is linked directly to an Apple IIe microcomputer for computation of HCl concentration. A mass flowmeter is used to monitor and control the gas flow, its output also going to the computer. Calculations are performed every 10 seconds in order to time-average the quantity of AgNO3 being used. Due to fluctuations in the quantity of HCl introduced into the impinger during any given 10-second increment, an additional time average is performed over three successive readings.

Multiple Gas Exposures

Simultaneous real-time monitoring of both HCN and HCl was impractical as only one titration unit was available. Therefore, the flow rate of HCN was first set with the CTA and then the monitoring system was switched to HCl. When the HCl concentration reached the target level, the experiment was initiated using the predetermined flow settings for HCN. This order was used because HCl is much more difficult to control and requires more adjustments than HCN. Also, it was determined that HCN did not interfere with HCl analyses under these test conditions, whereas HCl did interfere with the HCN analysis using the CTA. Final values for HCN were done using the SLT's. Combinations of CO, HCN and HCl were done as above except that CO was monitored with the Beckman 865 analyzer.

Results:

Multiple Gas Combinations CO, HCl, HCN

Lethality Data

A total of five experiments were conducted with combinations of CO, HCl and HCN (Table 1). In the last report, three tests had been done with this

combination of gases. Since then, two more tests were done. Various ratios of the three gases, calculated to result in a total of 1.0 (LC50), were tested. Two of the initial experiments gave results in support of the estimate, resulting in 50% mortality. The pattern of lethalities is of interest in these tests. In the first test, Test 1, an HCl level of 1200 ppm would not be expected to result in 50% lethality by itself, although all deaths took place post exposure, which is indicative of irritant related lethality. This apparent interactive effect of CO and HCl toxicity has been noted before with HCl/CO combinations (1,2). The summation of values for the second test, Test 2, equalled 0.96 of an LC50 and also resulted in 50% mortality. The role of HCl in this test is unclear as the summation of HCN and CO alone was equal to 0.76 and all deaths occurred during the exposure period. The summation of the values for Test 3 equalled 0.93 but did not result in any lethalities even though the HCl level exceeded that of the first test in which all deaths took place post exposure. Replicates of Tests 1 and 3 were performed in order to gain more information. A repeat of Test 3 (Test 6), in which the same proportion of gases was attempted, resulted on one lethality. Test 5, a repeat of Test 1 in which the individual gases were targeted to be 33% of the total, did not result in any lethality.

Technical Accomplishments:

The final report included data on animal weight gain analysis and pathology results, demonstrating the importance of including additional toxicological indices in modeling studies. Directions for experimentation and statistical procedures to enhance the models were developed. These included the incorporation of statistical variation into the n-gas calculations and additional toxicological indices.

TABLE 1
DATA SUMMARY
HCl/HCN/CO COMBINATIONS
RAT, 30-MINUTE EXPOSURE

GAS	AVERAGE GAS CONC. ppm	FRACTION LC50 *	EXPOSURE NUMBER DEAD	POSTEXPOSURE NUMBER DEAD n=6			TOTAL NUMBER DEAD	Σ FED LETHALITY
				DAY 0	DAYS 1-4	DAYS 5-14		
Test 1								
HCL	1196	0.31						
HCN	76	0.36	0	0	0	3	3	1.01
CO	2138	0.33						
Test 5**								
HCL	1225	0.32						
HCN	70	0.33	0	0	0	0	0	0.98
CO	2124	0.33						
Test 3								
HCL	1867	0.49						
HCN	39	0.18	0	0	0	0	0	0.93
CO	1613	0.25						
Test 6								
HCL	2077	0.55						
HCN	40	0.19	0	0	1	0	1	0.99
CO	1612	0.25						
Test 2								
HCL	717	0.19						
HCN	79	0.37	3***	0	0	0	3	0.96
CO	2527	0.39						

* Based on the following LC50 values: CO=6410, HCl=3810, HCN=212
** TEST 4 - Aborted due to power failure
*** Mean %COHb=70.7 s.d. 1.5

G. FURNITURE FLAMMABILITY

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

FURNITURE FLAMMABILITY

Professional Personnel

W. Parker, Project Leader
T. Ohlemiller, Chemical Engineer
J. Quintiere, Division Chief
K. Villa, Textile Technologist
K. Tu, Mechanical Engineer
G. Damant, Chief, California Bureau of Home Furnishings
S. Nurbakhsh, Mechanical Engineer, CBHF

Project Objective

To provide a technical basis for evaluating the California Technical Bulletin 133 (TB133) room fire test [1] and making recommendations with regard to modifications that might improve its utility as a fire test method for upholstered furniture.

Scope

Ten sets of upholstered chairs were obtained. One chair from each set was tested in the ASTM room [2] at NIST, two chairs from each set were tested in the furniture calorimeter [3] at NIST, and four chairs from each of the six sets having the lowest flammability were tested at CBHF. The chairs in the different sets varied only in the type of fabric, type of foam, and whether or not there was a fiberglass interliner present. The foams were either melamine-treated polyurethane foam or a less fire-retarded polyurethane foam that had simply passed the California Bulletin 117 test (TB117) [4]. The four fabrics were either nylon, polyolefin, a fire retardant polyvinylchloride or wool.The size, frame and style remained constant. They were of plain rectilinear construction with side arms and wood frames.Some of the chairs were ignited with the standard TB133 newspaper ignition source. The others were ignited by a gas burner [5] designed to simulate the newspaper ignition source. Both rooms were instrumented to measure the total heat release rate of the chairs by oxygen consumption. Calculations were made of the upper layer temperature in the room, using HAZARD I [6] and the measured heat release rates.

Technical Accomplishments

RESULTS

The peak temperatures measured near the ceiling above the chair in all of the tests conducted in the TB133 and ASTM rooms are plotted against the peak heat release rate in figure 1. The depression of the temperature at 2.8 MW in figure 1 is probably real. The fire has become ventilation limited so that any increase in the rate of pyrolysis simply leads

to more burning outside the room without contributing to any increase in the interior temperature. Indeed the unburned pyrolysis products in the room actually lower the room temperature slightly due to dilution. This relationship makes it possible to predict the temperature rise in either the TB133 room or the ASTM room from the heat release rate measured in the furniture calorimeter provided that the interaction with the room does not have a significant impact on the total heat release rate of the chair. This interaction would be due to heat feed back and ventilation restrictions.

Measurements were also made in the NIST furniture calorimeter for all ten chairs using the same newspaper ignition source for comparison with the ASTM room. In order to examine the impact of the room on the burning rate of the chair, the peak heat release rates measured in the TB133 and ASTM rooms are plotted against the peak heat release rate in the furniture calorimeter in figure 2. The data on the plot is taken only from the tests using the newspaper ignition source. The lower solid line in the plot is the equality line. Except for one outlier the peak heat release rate in the room is similar to that in the furniture calorimeter for heat release rates under 600 kW. Beyond that point the heat feedback from the hot upper layer and room surfaces enhances the burning rate significantly as seen from the upper line in figure 2.

The heat release rates measured as a function of time in the ASTM room were used in HAZARD I to calculate the temperature histories of the upper layer for all ten chairs. The peak calculated values are compared with the peak measured values in figure 3. The temperatures were measured with a 5 mil thermocouple located 100 mm below the ceiling at the center of the room. Except for one chair the points fall close to the equality line. This chair had a considerably higher heat release rate than any of the other chairs but a significant fraction of the burning took place outside of the room. The calculations performed with HAZARD I assumed all of the heat was released inside of the room. The impact of the increased rate of pyrolysis was to decrease the temperature due to dilution as discussed in connection with figure 1. This figure demonstrates once again the strong relationship between the heat release rate of the chair and the temperature of the hot upper layer near the ceiling of the room.

The results of this research are covered in three technical reports [7,5,8].

CONCLUSIONS

The following conclusions apply to the burning of upholstered chairs:

(1) The TB133 test could be conducted in an ASTM room with similar results.

(2) A temperature rise of 111°C (200°C) in the TB133 room test is equivalent to a heat release rate of approximately 65 kW in the furniture calorimeter.

(3) Below a peak heat release rate of 600 kW there is no significant interaction between the chair and the room so that the heat release rates in the room would be the same as those in the furniture calorimeter. This is true for the ASTM and TB133 rooms and rooms of

larger size. However, for rooms with low thermal conductivity lining materials and smaller size rooms the interaction would be expected to occur at lower peak heat release rates.

(4) For a chair with a sufficiently low heat release rate to pass the TB133 test, the temperature measured above the chair is reasonably representative of the upper layer temperature and thus might be calculated by Hazard I.

REFERENCES

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2. Proposed Method for Room Fire Test of Wall and Ceiling Materials and Assemblies, 1982 Annual Book of ASTM Standards, Part 18, p 1618, (1982)

3. Babrauskas, V., Lawson, J.R., Walton, W.D., and Twilley, W.H., Upholstered Furniture Heat Release Rates Measured with a Furniture Calorimeter (NBSIR 82-2604). U.S. Natl. Bur. Stand. (1982).

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5. Ohlemiller, T. and Villa, K., "Furniture Flammability: An Investigation of the California Technical Bulletin 133 Test. Part II: Characterization of Ignition Source and Comparable Gas Burner," NISTIR 4348, U.S. Natl. Inst. Stands. and Tech. (1990)

6. Bukowski, R.W.; Peacock, R.D.; Jones, W.W.; and Forney, C. L.; "HAZARD I Assessment Method--Software Users Guide, and Example Cases," NIST Handbook 146, NIST, 1989

7. Parker, W.J., Tu, K., Nurbakhsh, S. and Damant, G.H., "Furniture Flammability: An Investigation of the California Technical Bulletin 133 Test. Part III: Full Scale Chair Burns", NISTIR 4375, U.S. Natl. Inst. Stands. and Tech., (1990)

8. Quintiere, J., "Furniture Flammability: An Investigation of the California Technical Bulletin 133 Test. Part I: Measuring the Hazards of Furniture Fires", NISTIR 4360, U.S. Natl. Inst. Stands. and Tech. (1990)

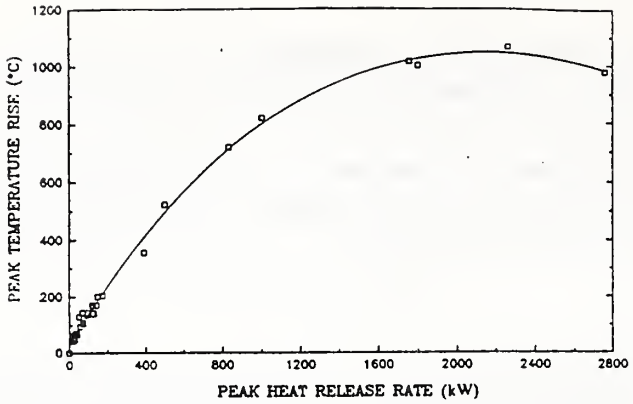

Figure 1. Temperature Rise vs. Heat Release Rate for TB133 and ASTM Rooms.

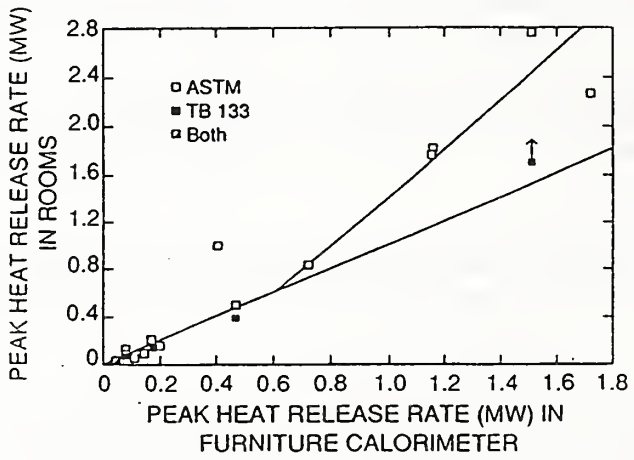

Figure 2. Heat Release Rate in Rooms vs. Heat Release Rate in Furniture Calorimeter.

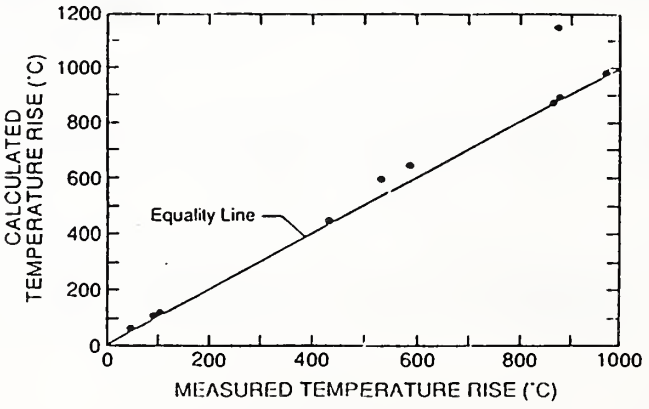

Figure 3. Calculated Temperature Rise Using Hazard I.

H. BUILDING FIRE MODELING AND SMOKE TRANSFER

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

Unified model of fire growth and smoke transport Objective

Professional Staff:

Walter W. Jones & Glenn Forney

Project Objective:

Modify the FAST model suite to incorporate the lessons learned in building the structure of the consolidated compartment fire model (CCFM).

Scope:

The CFR models of fire growth and smoke spread are becoming widely available and generally used. This project is intended to accomplish two tasks related to this fact. It is to provide developers and users of fire spread models with an open code suitable as a development platform on a range of computing platforms. In addition, the purpose is to provide the best effort possible on modeling from within the Center's resources, including robustness, and accountablility.

Technical Accomplishments:

The general result is a suite of software (models) and documentation (Programmer's Guide). It has been developed to allow for exposition, maintainability and enhancement. The Programmers Guide details the procedure for such enhancements and the method by which these modifications can be incorporated into the official CFR model for fire grwoth and smoke transport, CFAST. The interface was developed in cooperation with the Hazard Methodology Project to insure compatibility in the future. We examined and modified the FAST programs, in concert with a definition of environment as stated in the modification protocol. The appropriate portions of the CCFM code which would enhance the usability of the resulting model were included.

Publications:

Jones, W. W. and Forney, G. P., A Programmer's Reference Manual for CFAST, the Unified Model of Fire Growth and Smoke Transport, Nat. Inst. Stand. and Tech. Tech Note 1283 (1990).

Forney, G. P. and Jones, W. W., Software Development Tools, NISTIR 4363 (1990).

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

SURFACE HEAT TRANSFER ALGORITHM

Professional Personnel: Leonard Y. Cooper, Project Leader
Tokiyoshi Yamada, Guest Researcher

Program Objectives

Develop algorithms and associated subroutines that generalize the calculation of radiation and convection heat transfer exchanges between fire, layers, and ceiling/wall/floor surfaces in compartment fires.

Scope

The algorithms and associated subroutine software to be developed should be well-documented, modular in design, and generally usable in multi-room zone-type compartment fire model computer codes.

Technical Accomplishments

A strategy for defining room geometry and the radiation properties of inside surfaces and upper and lower gas layers was implemented. A data structure for dividing and identifying each of the six surfaces of an arbitrary rectangular-parallelopiped room into an arbitrary number of rectangular elements (and a "residual" element) was implemented. As depicted in Figure 1, a "net radiation-type" analysis and associated subroutine software for calculating heat transfer exchanges between all surface elements, the two gas layers, and a radiating point-source fire of arbitrary location and strength was completed. Testing of the software was carried out. In calculating radiation exchange for the generic room of a facility, a strategy was developed to take account of radiation leaving and entering vents. The radiation calculation methodology must still be documented. Algorithms/software for convective heat transfer from the fire plume and from vent flow-driven plumes to ceiling/wall surface elements must be developed and documented.

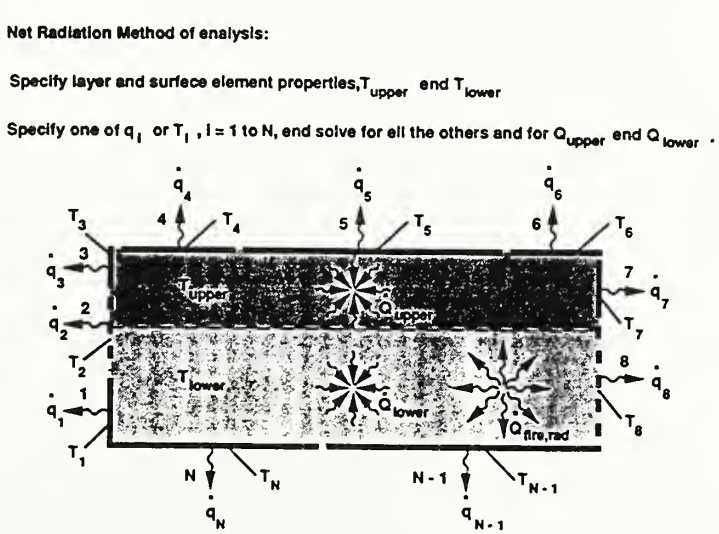

Figure 1. Depiction of the use of the Net-Radiation Method of Analysis.

I. FIRE HAZARD ASSESSMENT

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

FIRE HAZARD ASSESSMENT

Professional Personnel

Richard D. Peacock, Project Leader
Walter W. Jones, General Physical Scientist
Richard W. Bukowski, Manager, Technology Transfer
C. Lynn Forney, Mathematician
Emil Braun, Physicist
Paul A. Reneke, Computer Scientist
Phyliss M. Martin, Computer Specialist

Project Objective

To plan and implement a second generation hazard methodology (HAZARD II) by July 1994.

Scope

The project is intended to produce a fundamental capability to analyze the hazards associated with a specified fire scenario. This capability has been provided in the form of a fully-supported software package for personal computers. While initially limited to residential-style occupancies, the software design will be such that it can be used across a broad range of applications from fire safety education to fire reconstruction. It is intended that the resulting product will provide a predictive tool for use by manufacturers, purchasers, architects, FPE's, code officials, and practitioners in evaluating safety performance, code equivalency, and code change proposal issues.

Technical Accomplishments

1. Plan for HAZARD II

The next major release of the hazard methodology, HAZARD II, will include new phenomenon and features as appropriate to continue the tradition set with HAZARD I of providing a state-of-the-art tool for hazard analysis for use by fire protection professionals. This year, a plan detailed our intentions for the content of HAZARD II. These fall into four areas: fire model, egress and tenability models, databases, and user interface / documentation.

Fire Model will be enhanced with new phenomena that are (or will become) available from other projects: four wall radiation, flow through vertical (holes in floor/ceiling) openings, construction design files – (databases used for building and ship design), self consistent fire - flame spread and pyrolysis models, multiple burning objects, suppression and detection algorithms. In addition, the input and output modules will be enhanced to

facilitate input and output of data for these new phenomena. Naturally, we must support comparisons of the model with real fires to provide a degree of validation and user confidence in the predicted results.

Egress and tenability models will be combined and a pharmacokinetec model added. Minimal changes will be made as necessary to access the data from the unified fire model. If funding allows, we will expand beyond residential applications to include a non-residential traffic flow model.

Databases will look and function as the current version. Hopefully, data will be transferred directly from the databases to the models of HAZARD II.

User interface / documentation will be upgraded to support and document the new version of the unified model. One thing we learned from HAZARD I was the *enormous* amount of time needed for review and approval of such a massive document.

2. Experimental Database

BFRL has been working to develop a generic methodology for fire model evaluation. Consistent documentation of model than 125 individual room fire tests that can be used for comparison with zone-based predictive models has been developed. Five different test series were included in the discussion:

- a single room test series with furniture and varied opening sizes,
- a single room test series with furniture and wall burning,
- a three room test series including a corridor with multiple replicates of several different experimental conditions,
- a four room test series including a corridor with large growing fires, and
- a multiple-story building test series with a zoned smoke control system.

Derived outputs from individual raw data elements were developed for all the tests in a single, consistent format together with the mathematical treatment used to make the calculations. Geometry of the room(s) and the measurements taken for all the tests were reviewed and presented using the same nomenclature for all tests, simplifying comparison of data from different tests (from different laboratories).

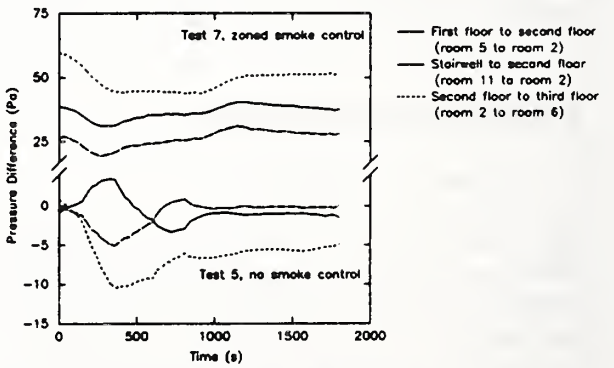

Figure 1. A sample of the data included in the experimentel database showing measured pressure differences in a set of tests in e multiple story building with zoned smoke control.

Since the tests to be included in this database were chosen to present a broad range of challenges for the current generation of fire models, the comparisons with current fire models may not always be favorable. In some cases, the tests include physical phenomena not included in some models (such as forced ventilation, flow in long corridors, or multiple stories in a building). Thus this base of data can also be viewed as providing input for model developers to extend the capabilities of the models.

Analysis of such complex and voluminous data requires the development of a series of algorithms that combine individual data elements to produce the desired output parameter. CFR has prepared a specially designed computer program for the reduction of full scale fire test data. In addition to easing the burden of repetitive and similar calculations, the program provides a standard set of algorithms for the analysis of fire test data based upon published research results and a standard form for detailing the calculations to be performed and for examining the results of the calculations. The program combines automated instrument calibrations with more complex, fire-specific calculations such as

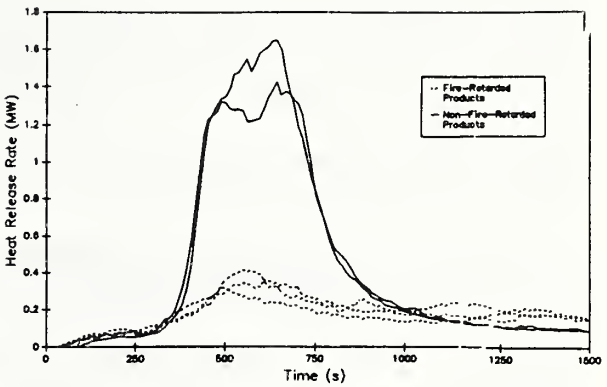

Figure 2. An example of heat release rate based upon oxygen consumption calorimetry in several large scale fire tests calculated with RAPID.

- smoke and gas analysis,
- layer temperature and interface position,
- mass loss and flows, and
- rate of heat release.

Reports and Publications

Peacock, R. D. and Bukowski, R. W., A Prototype Methodology for Fire Hazard Analysis, Fire Technology, 26:1, 15-40 (February 1990).

Peacock, R. D., and Babrauskas, V., Analysis of Large-Scale Fire Test Data, submitted to the Fire Safety Journal.

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Peacock, R. D., Davis, S., and Forney, C. L., Data for Room Fire Model Comparisons, to be published by NIST.

Forney, C. L., A Sensitivity Analysis of a Simple Fire Growth Model, to be published.

Related Grants

"Modifications to Furniture Fire Model for HAZARD System," M. A. Dietenberger, University of Dayton Research Institute.

"Mathematical Modeling of Human Egress from Fires in Residential Buildings," M. Kostreva, Clemson University.

"Incorporating Convective and Radiative Heat Transfer into the Code CCFM.VENTS," W. F. Moss, Clemson University.

"Fire Risk Analysis Methodology," G. Apostolakis, University of California at Los Angeles.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNONOLOGY
FY 90

Institution: Clemson University

Grant No.: 60NANB0D1023

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

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

Other Professional Personnel: Malgorzata Wiecek, Assistant Professor
Teodros Getachew, Doctoral Student

NIST Scientific Officer: Richard Peacock

Technical Abstract:

Research supporting mathematical modeling of egress of the individual occupants from residential buildings is being performed in this project. Techniques include multiple objective analysis and dynamic programming.

Introduction. The mathematical modeling of egress from a building on fire is an important facet of fire research. Such modeling generally falls into one of two categories. In the first the aim is to simulate egress paths of individual occupants using behavioral decision rules built into the model and an algorithm for optimizing a given quantity, usually distance or time. One example of efforts in this direction is HAZARD I [1], a simulation model which, taking as input the results of a smoke model, yields the trajectories of evacuees and the impact of toxins on the occupants.

The second category of modeling has as its focus the determination of globally optimal egress paths. Knowledge of such paths can be useful in establishing benchmarks for actual egress and can serve as a basis for assessing the impact of building design on evacuation. Actual egress from a fire involves multiple criteria decisions in a dynamically evolving environment. An evacuee may want to minimize both time and distance, while at the same time avoiding the smoke and the fire. The determination of optimal paths in this more realistic setting involves the successful integration of dynamic programming with multiple criteria optimization theory.

Theoretical Framework. The mathematical model that serves as the setting for this analysis is a network superimposed on a residential building. Nodes in the network represent locations within and around the building, while links comprise potential egress routes. Each link carries one or more attributes, to be referred to as costs. The assignments of nodes, links and costs are made to closely reflect an actual

scenario. Each occupant in the building is initially located at a unique node of the network, an origin node. The problem is to find for each such occupant a path of minimum cost leading from his origin node to a single destination node.

One of the classical approaches to solving the above problem is the Principle of Optimality: "An optimal policy has the property that whatever the initial decisions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision" [2, 3].

The appearance of a fire at a node introduces time dependence into the situation. This is modeled by costs which are step functions. When a node is impassable at say time t, the cost of entering the node becomes a large positive number M. The process of determining an optimal path proceeds in two steps:
1) Optimize the network with pre-fire costs on each link. This yields an optimal path from each origin node to the destination node. If all optimal paths pass through the given node before it is rendered impassable, STOP. The problem is solved. Otherwise go to 2).
2) For each link entering the impassable node, substitute M for the cost and for links leaving the node, leave the costs unmodified. Optimize again. All resulting paths with costs which do not include terms in M are optimal and avoid the impassable node.

The treatment of the multiple criteria case is similar to the single criterion case. One looks then for non-dominated paths; i.e. paths which are optimal in the sense that all their criteria values cannot be improved simultaneously. The determination of non-dominated paths in the dynamic setting involves the integration of time-dependent analysis described above and the search for non-dominated paths [1a].

Technical Accomplishments. As was noted in the introduction the thrust of research in the modeling of egress from a building on fire has been on simulation, the tracing of individual paths of evacuation. The determination of the best egress paths is a relatively recent undertaking. Notable in this direction is the computer program EVACNET+ [6] which determines shortest-time evacuation plans for a given building. However, not only does it not trace the movements of individuals, but it also does not consider people-fire interactions. The research we are undertaking employs optimization to show occupants' movements and people-fire interactions. Initial calculations suggest that the methods of dynamic programming and multiple objective optimization can be successfully used to solve the following problems:
1) Finding best egress paths from all given origin nodes to a destination node, for single and multiple criteria models.
2) Finding the optimal paths when a node is rendered impassable by fire or smoke.

Figure 1 depicts the floor plan of a simple ranch house with nodes that have been assigned to rooms or secondary locations within rooms. An egress path could be any path leading from node 1,2,...,6 to the destination node 7 located outside the house. Figure 2 shows an egress network associated with the house. Two attributes (time and distance) are assigned to each link of the network and node 5 is rendered impassable due to the fire. All the non-dominated paths (darkened) found in the network with constant costs and time dependent costs and their origin node numbers are shown in Figure 3. Each point represents a non-dominated path from a given

origin node and the point coordinates give the total time and distance of the path. The points relative position on the graph before and after a node becomes impassable can determine regions of high-risk and low-risk within a building. Assuming one node at a time becomes impassable, a set of such multi-attribute graphs can be used to gain insight into building design and occupant decisions during evacuation. This research has shown that plots of non-dominated paths can yield a novel tool for the analysis of the impact of building-design on egress.

Two directions of further research suggest themselves. (a) The dynamic models have been developed so far under the simplifying assumption of a single impassable node. This needs to be generalized to the more realistic time-dependency of multiple impassable nodes with possibly different times. (b) In its present form the model allows one to have snapshots of the system at discrete node-arrival times. In actuality, the system evolves in a continuous fashion with respect to time. Further work needs to be done in the refinement of the time-dependency.

References:

1. Bukowski, R.B., Peacock, R. D., Jones, W. W. and Forney, C. L., "Technical Reference Guide for HAZARD I, Fire Hazard Assessment Method", Handbook 146, Volume II, U.S. National Institute of Standards and Technology, Gaithersburg, Maryland, 1989.
2. Bellman, R. and Kalaba, R., Dynamic Programming and Modern Control Theory, Academic Press, New York, 1965.
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4. Daellenbach, H. G. and de Kluyver, C. A., "Note on Multiple Objective Dynamic Programming", Journal of the Operational Research Society 31, pp. 591-594, 1980.
5. Kisko, T. M. and Francis, R. L., "EVACNET+: A Computer Program to Determine Optimal Building Evacuation Plans", Fire Safety Journal 9, pp. 211-220, 1985.

Papers and Presentations:

1a. Kostreva, M. M. , Wiecek, M. M. and Getachew, T., "Optimization Models in Fire Egress Analysis for Residential Buildings", submitted for publication, 1990.

2a. Kostreva, M.M., "Path-Following Techniques for Nonlinear Multi-Criteria Decision Problems", presented at the 9th International Conference on Multiple Criteria Decision Making, Washington, D.C., August 5-8, 1990.

3a. Wiecek, M. M., "Modeling Preference Trade-Offs in Multiple Objective Linear Programming", presented at the 9th International Conference on Multiple Criteria Decision Making, Washington, D.C., August 5-8, 1990.

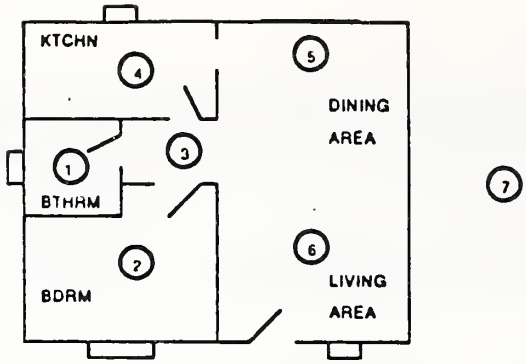


Figure 1. Floor plan of a ranch house with arbitrary assignment of nodes.

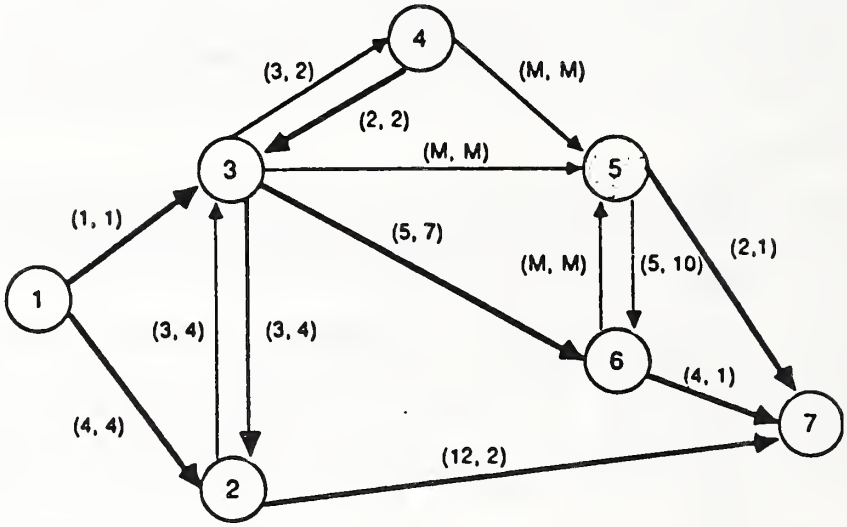


Figure 2. Two-attribute network with time dependent costs and non-dominated paths.

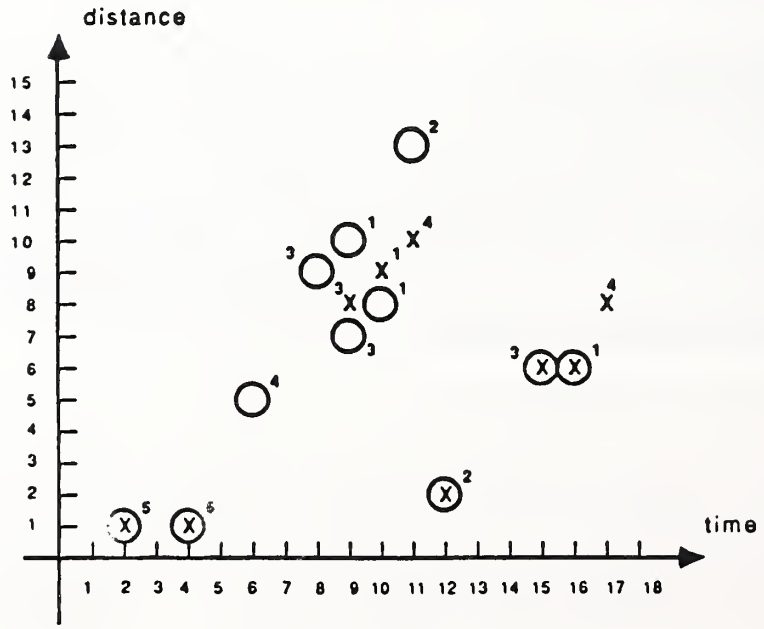


Figure 3. Non-dominated paths for the two-attribute network with constant costs (◯) and time dependent costs (X) with origin node numbers.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution:	University of Dayton Research Institute
Grant No.:	60NANB0D1051
Grant Title:	Modifications to Furniture Fire Model for HAZARD System
Principal Investigator:	Mark A. Dietenberger Research Physicist University of Dayton Research Institute 300 College Park - JPC/232 Dayton, Ohio 45469-0120 (513) 229-3037
Other Professional Personnel:	Joyce Smith, Research Programmer
NIST Scientific Officer:	Dr. Walter W. Jones

Technical Abstract:

This contract, which began in August 1990, supports the modifications to the furniture fire model (FFM) for eventual inclusion to the HAZARD system. The FAST/FFM model simulates growth and burnout of furniture fires in a room as well as to simulate the spread of nontoxic and toxic gases and smoke to other rooms. The unique features of the model are the following. The dynamic quasi-three-dimensional features include the flame spreading in any direction on the mockup, the burn histories of facets on the mockup panels that result in dynamic mass and heat release rates in multiple flames, the temperature rises of the mockup facets, walls, and gas layers, and the growth of the upper gas layer. The reliance of the model on effective scaling of the cone calorimeter data and of the flame spreading data, and its validation with the full scale fire tests is another unique feature. The modular construction of the model and of its computer code permits application to new fire scenarios or to upgrades of FAST model. The goals of this new project are (1) to use the current FFM model to compare with more selections of full-scale fire tests, (2) to develop and code an algorithm for the automatic calculation of the ignition and flame spread parameters, (3) and to assist in the simplication and conversion of the FFM to the HAZARD system.

Model Validation The plan in this project is to compare the current FAST/FFM predictions with an approved set of full scale fire tests. Ideally, the full scale burns database should contain (1) the furniture calorimeter measurements of heat and mass release rates and the soot extinction areas versus time, (2) and the recordings of burn fraction of each cushion panel versus time. A more common, but indirect, full scale database would have measurements of temperature, soot extinction areas, gaseous concentrations, and interface position for the upper gas layer versus time. These indirect measurements should produce valid comparisons providing the FAST model has been validated in connecting the furniture calorimeter measurements with the various measurements of the upper gas layer. For the validation efforts, it

is essential to have corresponding bench-scale database from the cone calorimeter and the flame spread apparatus at various irradiance levels. The existing bench-scale and full-scale fire database at NIST are currently being reveiwed in conjunction with the FHA group at NIST-CFR.

Ignition and flame spread parameters The automated determination of the ignition and flame spread parameters involves three phases: 1) a scheme to determine thermal constants, such as ignition temperature, thermal inertia, and thermal thickness, from the piloted ignition measurements, 2) a scheme to obtain the flame spread constants, which are the convective flame surface heat flux and the convective flame foot length, from the LIFT apparatus, and 3) the application of the corresponding formulae to a furniture fire spread. The new formulae include explicitly a thermally thin layer on a substrate thick layer and a prediction of the minimum surface temperature for flame spreading. The objective is to construct appropriate curve-fitting algorithms that fit with the Hazard protocol.

FFM Conversion to Hazard Protocol The current furniture fire model needs to be simplified and made more user friendly for a better fit into the Hazard system. The objective is to assist the FHA group in this conversion process. Depending on circumstances, we would reprogram FFM subroutines to reduce computer memory requirements, to change algorithms that read the FFM database, and to implement changes in FFM considered necessary by the FHA group. We also will assist in the efforts to ensure the interface between FFM and FAST (and thus the HAZARD code) are functioning correctly.

Conclusion The FFM model has been documented and the code has been installed on CFR computers. The model is now being developed to rely less on the user's judgement in using the bench-scale data and to fit more directly into the Hazard protocol. Concurrently, model validations are underway as a basis for future developments of new model features.

References

r1. M. A. Dietenberger,"Technical Reference and User's Guide For FAST/FFM Version 3," UDR-TR-89-83, October 1989.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution: Clemson University

Grant No.: 60NANB8D0857

Grant Title: Incorporating Convective and Radiative Heat Transfer into the Code CCFM.VENTS

Principal Investigator: Professor William F. Moss

NBS Scientific Officer: Dr. Glenn P. Forney

Technical Abstract:

Introduction The title of this grant renewal should have been "Incorporating Conductive and Radiative Heat Transfer into Zone Fire Models." This research focuses on the following tasks. Task 1: Modification of the research code CCFM.MOSS to produce a one room test code for modeling heat conduction through the ceiling and radiative heat transfer from the fire to the lower ceiling surface, from the lower ceiling surface to the floor, and from the upper ceiling surface to a fictitious outside surface. This test code is designed to solve the one dimensional heat equation to high accuracy in a homogeneous ceiling and in a ceiling containing three layers with different heat conduction coefficients. The purpose of this test code is to produce high accuracy solutions of the equations that can be used in benchmarking approximate solutions. Task 2: Study the efficiency and accuracy of two methods for approximating conductive and radiative heat transfer. Task 3: Extend the conductive heat transfer to walls and floors and the radiative heat transfer to layers and other surfaces.

One Room Test Code The heat equation is solved simultaneously with the ordinary differential equations which track the zone model variables. These equations are coupled by a heat flux boundary condition.

The equations solved are

$$\frac{d(\Delta P)}{dt} = \left(\frac{R}{C_V\, VOL}\right)(q_U + q_L) \qquad (1)$$

$$\frac{dY}{dt} = \left(\frac{R}{C_p\, VOL}\right)\left[\frac{(YH - Y)\, q_L - Y\, q_U}{P}\right] \qquad (2)$$

$$\frac{dM_U}{dt} = m_U \qquad (3)$$

$$\frac{dM_L}{dt} = m_L \qquad (4)$$

$$T_U = \frac{P}{\rho_U R}\ , \quad \rho_U = \frac{M_U}{(YH - Y)} \qquad (5)$$

$$\frac{\partial u}{\partial t}(x, t) = \left[\frac{H}{C_{CP}\,\rho} \right] \frac{\partial^2 u}{\partial x^2}(x, t) \ , \ 0 < x < W, \ t > 0 \tag{6}$$

$$u(x, 0) = T_{amb} \ , 0 < x < W \tag{7}$$

$$\frac{\partial u}{\partial x}(0, t) = - \frac{F_{CL}(t)}{H} \qquad \frac{\partial u}{\partial x}(W, t) = \frac{F_{CU}(t)}{H} \tag{8}$$

$$F_{CL} = F_{fire}(t) + H_{CL} \left[T_U(t) - u(0, t) \right] - \frac{\sigma \left[\{u(0, t)\}^4 - T_{amb}^4 \right]}{\frac{1}{\varepsilon_L} + \frac{1}{\varepsilon_{floor}} - 1} \tag{9}$$

$$F_{CU} = - H_{CU} \left[u(W, t) - T_{amb} \right] - \frac{\sigma \left[\{u(W, t)\}^4 - T_{amb}^4 \right]}{\frac{1}{\varepsilon_U} + \frac{1}{\varepsilon_{cav}} - 1} \tag{10}$$

where $P = P_0 + \Delta P$ is the pressure at the floor, P_0 is the ambient pressure at the floor, Y is the layer height, M_U is the mass of the upper layer, and M_L is the mass of the lower layer, q_U and m_U are the rates at which enthalpy and mass are added to the upper layer, and q_L and m_L are the rates at which enthalpy and mass are added to the lower layer. The constants R, VOL, C_V, and C_P are, respectively, the ideal gas constant, the room volume, the specific heat capacity of air at constant volume, and the specific heat capacity of air at constant pressure. The rates q_U, q_L, m_U, and m_L are computed using fire plume and a vent models. At each fixed time $t > 0$, $u(x, t)$ denotes the temperature profile through the ceiling, T_U denotes the temperature in the upper layer, and T_{amb} denotes the ambient temperature. For the ceiling H, C_{CP}, and ρ denote the thermal conductivity, the specific heat capacity at constant pressure, and the density. F_{CL} and F_{CU} denote the heat fluxes into the lower and upper surfaces of the ceiling. Now, H_{CL} and H_{CU} denote the convective heat transfer coefficients at the lower and upper ceiling surfaces, σ denotes the Stefan-Boltzmann constant, ε_L and ε_U denote the effective emittances of the lower and upper ceiling surfaces, and ε_{floor} and ε_{cav} denote the effective absorptances of the floor surface and the fictitious outside surface. Finally, the enthalpy rate q_U appearing in equations (1) and (2) must be adjusted to account for the convective heat transfer from the hot upper layer to the lower ceiling surface. The quantity $A\, H_{CL} \left[T_U(t) - u(0, t) \right]$ must be subtracted from the q_U computed using the fire plume model and the vent model, where A denotes the area of the ceiling.

The method of lines has been used to convert the heat equation (6) and the boundary conditions (8) - (10) into an approximating set of ordinary differential equations which are solved simultaneously with equations (1) - (4). The method of lines has been implemented using the collocation approach found in the IMSL Library routine MOLCH. Piecewise cubic Hermite polynomials are used in the spatial approximation. The error due to the time discretization is controlled by the ordinary differential equation solver and a user specified tolerance, while the error due to the spatial discretization is proportional to h^4 where h denotes the average length of the subintervals in the spatial discretization. The spatial discretization is not required to be uniform; consequently, it can be advantageous, in certain circumstances,to let the knots cluster near $x = 0$ or $x = W$. Spatial discretizations suitable for a wide range of upper layer temperature gradients are being investigated.

Results and Technical Accomplishments The present research emphasizes the use of a benchmark code to develop robust and efficient numerical approximations to the equations of conductive and radiative heat transfer. Computations are being performed on a Apple Macintosh II, a Sun-4/65 SparcStation 1+, a DEC 5000, and an IBM320.

Presentations The work of the previous year was presented at the Center for Fire Research Annual Conference, November 1989.

Reports and Papers

1. Glenn P. Forney, Leonard Y. Cooper, and William F. Moss, "The Consolidated Compartment Fire Model (CCFM) Computer Code Application CCFM. Vents - Part IV: User Reference Guide, NISTIR 4345.
2. W. F. Moss, G. P. Forney, and L. Y. Cooper, "Incorporating Conductive and Radiative Heat Transfer in Zone Fire Models," in preparation.
3. W. F. Moss, G. P. Forney, and L. Y. Cooper, "Numerical Characteristics of Zone Fire Modeling," in preparation.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution: University of California, Los Angeles

Grant No: 60NANB9D0947

Principal Investigator: Professor George Apostolakis
38-137 Engineering IV
University of California
Los Angeles, CA 90024-1597

Other Professional Personnel: S. Thompson, M.S. Student

NIST Scientific Officer: Dr. Walter Jones

Technical Abstract:

Introduction The objective of this work is to develop probabilistic models to characterize a room fire involving upholstered furniture, including secondary ignition, detection and suppression, for the purpose of performing risk analysis. This research will build upon and enhance current methods, and will be based upon many of the physical models which have been developed to describe the physical processes that occur during a fire. The most important parameters of a fire for the purpose of risk analysis are the times to ignition, full involvement, detection and suppression. Current research will build upon the predictive model for the ignition time developed in the first phase of this project and develop models for the time to full involvement of an item (including secondary ignitions) and the times to detection and suppression. The growth time of an item will be calculated from models of the heat release rate. However, it is first necessary to develop a model for the initial growth (start-up) time of the fire from ignition to a stage of fire development characterized by a minimum value of the heat release rate.

The results of this research are expected to include probabilistic models of the burning of upholstered items in a room fire, including the ignition of secondary items. By utilizing available heat transfer and heat release rate models, quantifying their uncertainties and coupling them with room fire models, which include detection and suppression, the effects of material changes on fire risk may be assessed from changes in fire growth, detection and suppression times.

Approach The peak heat release rate is important in the modeling of upholstered furniture fires, especially as pertaining to risk calculations. Typical heat release rate curves for upholstered furniture may often be approximated by a simple triangular representation of the curve shape. The important features of this model are the peak release height, the base width, and the time from ignition to the start of the triangular burning region. This start-up time has been found not only to be a function of the property of the furniture but also depends strongly on the ignition sequence. The model for the start-up time that is being developed will, therefore, only apply to radiant ignition.

Predictive models are available for the triangular portion of the curve. Two correlations exist for the peak heat release rate, one based on bench-scale testing and the other based solely on materials identification, intended for use when destructive testing is not feasible. The method based on bench-scale testing is preferred, since the effects of fire retardants or other fabric treatments can be assessed through experimentation. A correlation also exists for the width of the base which involves the peak heat release rate and the heat of combustion and mass of the item.

A predictive model for the start-up time of an upholstered furniture fire is being developed using response surface methodology. Flame spread over upholstered furniture is dominated by radiation, and to some extent by natural convection. Numerical solutions of the boundary layer equations for a free-convective boundary layer flow will be used to represent variations in the mass burning rate with external radiant flux and will also account for various fabric/padding combinations. The method of response surface analysis will then be used to approximate the solution to the combustion equations. A response surface is a mathematical function which is fitted to the numerical solution of the problem. This mathematical function is good for a range of independent parameters in the problem, and uncertainties in these parameters may be propagated through the response surface to obtain the uncertainty in the final solution. Uncertainties in the model being developed may also be quantified by comparison to available experimental data on furniture flame spread rates and start-up times.

Future Plans Once the initial growth model is developed, the times to detection and suppression will be studied to determine the overall hazard time. This analysis may be aided by a computer fire code, such as FAST. The ignition of secondary items will then be explored, and the subsequent effect on the hazard time will be studied.

Reports and Papers:

1. M.D. Brandyberry and G.E. Apostolakis, Fire Risk Analysis Methodology: Initiating Events, NIST-GCR-89-562, Feb. 1989.

2. M.D. Brandyberry and G.E. Apostolakis, Fire Risk in Buildings: Frequency of Exposure and Physical Model, submitted to the Fire Safety Journal.

3. M.D. Brandyberry and G.E. Apostolakis, Fire Risk in Buildings: Scenario Definition and Ignition Frequency Calculations, submitted to the Fire Safety Journal.

J. ENGINEERING ANALYSIS SYSTEM AND FIRE RECONSTRUCTION

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

ENGINEERING ANALYSIS SYSTEM & FIRE RECONSTRUCTION

Professional Personnel

Harold E. Nelson, Project Leader
Scott Deal, Fire Protection 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 Engineered Fire Protection Assessment System project.)

2. Demonstrate procedures for fire reconstruction investigations. Prepare a kit of needed materials. 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, fire hazard assessment tools for hazard estimation has been completed, the report published, and distribution of the software has been initiated. Updates and improvements continue. The current version is 2.01. FPETOOL is a computerized package of relatively simple engineering equations and model presented in the language in terms of the design profession. The tools are useful in estimating potential fire hazards and the response of space and fire protection systems to the developing hazard. During the development, the results produced by FPETOOL were compared to the results produced by other available zone models when considering a simple one-room problem. Attached figures show some of the results.

2. Fire Reconstruction

The number of major fires were investigated and preliminary analysis has been completed. Reports, however, have been issued only on the analysis and subsequent full-scale test and comparison of the

fire in Sharon, Pennsylvania. Two other analyses have been completed but not released due to criminal proceedings related to the fires. Three other analyses are underway. The investigations do continue to emphasize the potential impact of high rates of generation of carbon monoxide and carbon dioxide and rapid depletion of oxygen in spaces exposed to the flow of gases emitted from a flashed-over room into building corridors and spaces adjacent to these corridors.

Funding from Other Agencies/Institutions

In addition to CFR Priority Project funding, the above activities were carried out with support from the General Services Administration, Department of Health and Human Services, and Department of Education.

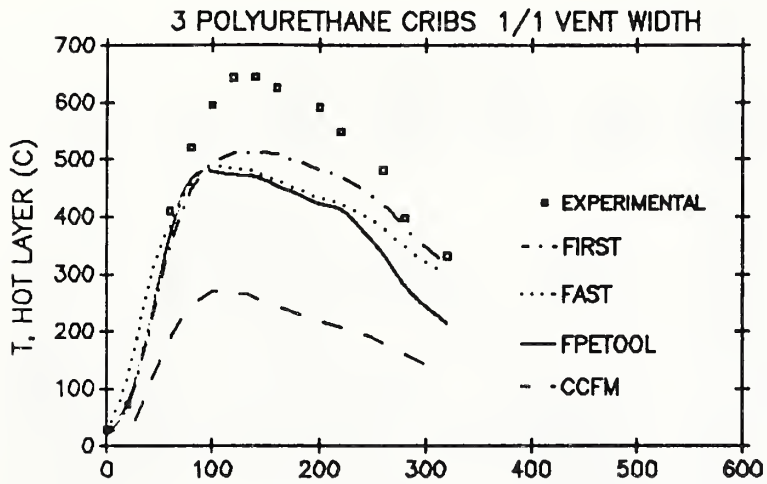
Reports and Publications

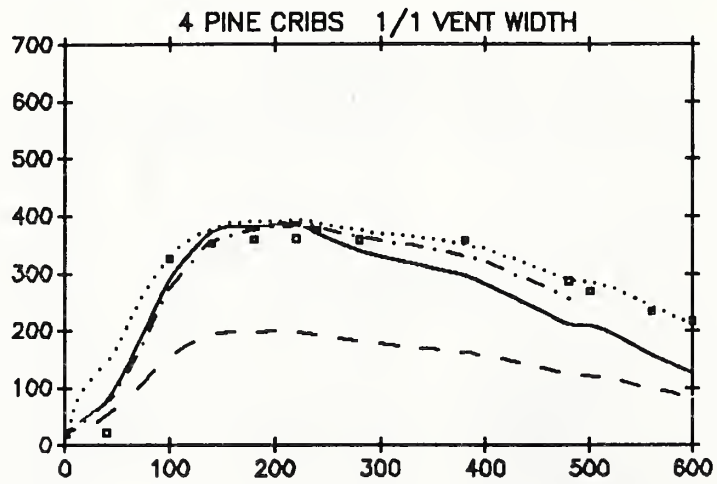
Nelson, Harold E., NISTIR 4380 FPETOOL: Fire Protection Tools for Hazard Estimation, August 1990.

Levine, Robert S. and Nelson, Harold E., NISTIR 90-4268, Full Scale Simulation of a Fatal Fire and Comparison of the Results with Two Multi-Room Models, August 1990.

Related Grants

Fire Safety in Board and Care Homes, Carl M. Harris, George Mason University.


3 POLYURETHANE CRIBS 1/1 VENT WIDTH
T, HOT LAYER (C)
EXPERIMENTAL
FIRST
FAST
FPETOOL
CCFM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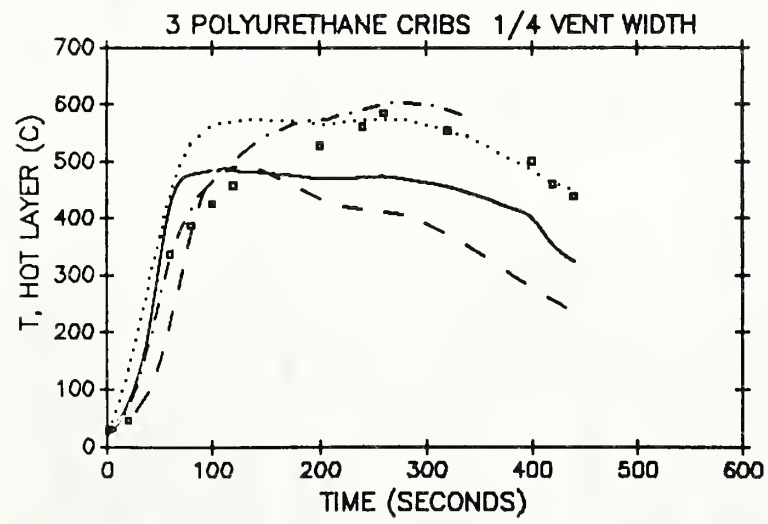
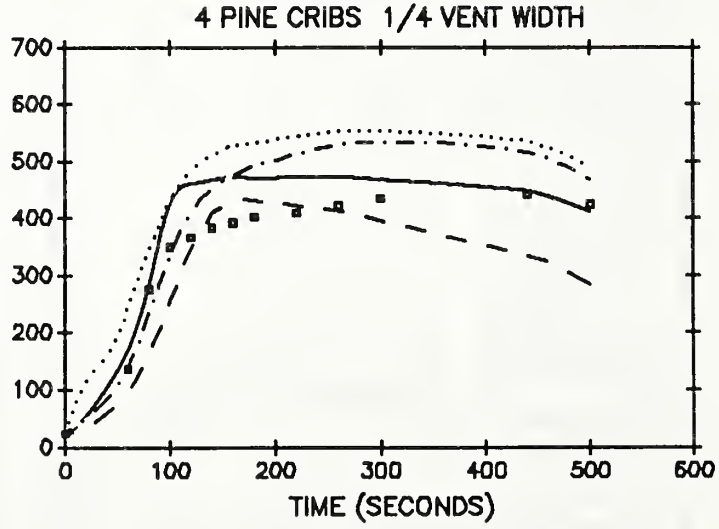
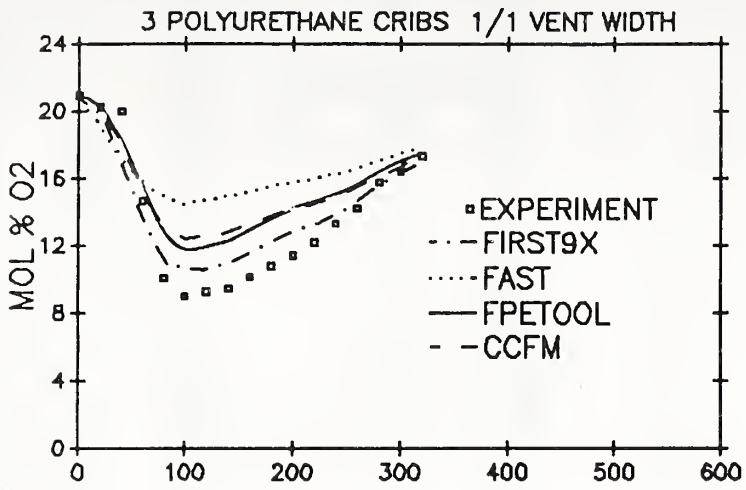
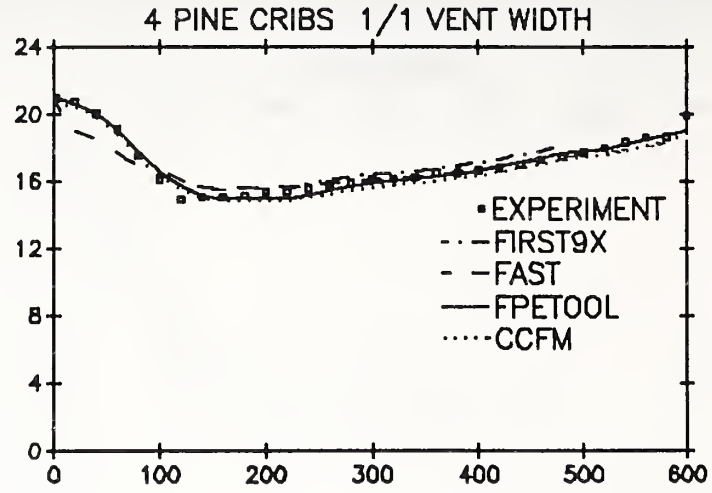

3 POLYURETHANE CRIBS 1/4 VENT WIDTH
T, HOT LAYER (C)
TIME (SECONDS)


4 PINE CRIBS 1/4 VENT WIDTH
TIME (SECONDS)


3 POLYURETHANE CRIBS 1/1 VENT WIDTH
MOL % O2
EXPERIMENT
FIRST9X
FAST
FPETOOL
CCFM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EXPERIMENT
FIRST9X
FAST
FPETOOL
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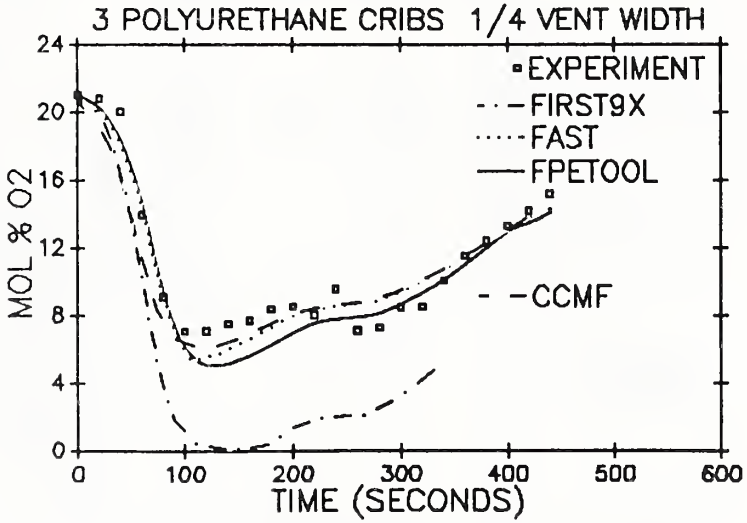
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MOL % O2
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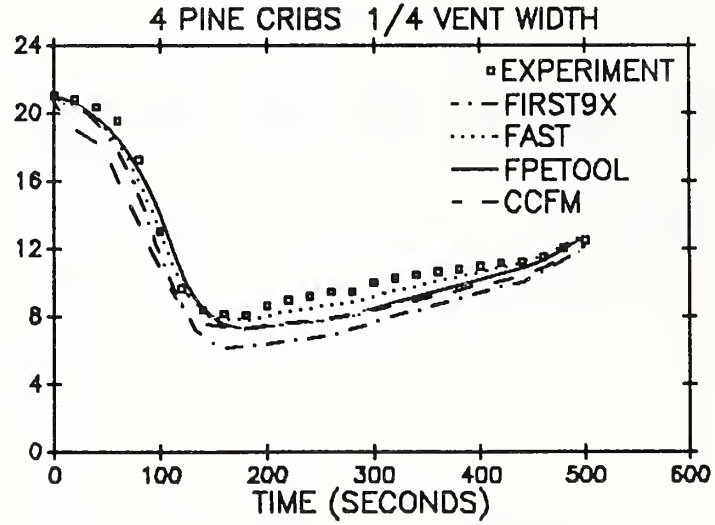
TIME (SECONDS)


4 PINE CRIBS 1/4 VENT WIDTH
EXPERIMENT
FIRST9X
FAST
FPETOOL
CCFM
TIME (SECONDS)

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: George Mason University

Grant No.: 60NANB9D0974

Grant Title: Fire Safety in Board and Care Homes

Principal Investigator: Prof. Carl M. Harris, Chairman
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Dr. Norman E. Groner
Roseanne Paulsen

NIST Scientific Officer: Harold E. Nelson

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 Life Safety Code.

Technical Summary and Accomplishments

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

I. 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 Chapter 21, Board and Care Occupancies, of the Life Safety Code has been adopted; the experiences adopting agencies have had after adopting it; and reasons agencies have had for not adopting it. When the Board and Care Chapter was first being adopted as part of the Life Safety Code, there was concern that some of the novel features of the Chapter might not be acceptable to knowledgeable regulators or might not work when actually applied.

The Board and Care Chapter of the Life Safety Code is used in most states to determine if ICF/MR facilities meet the requirements for Federal funding. This means that there are state officials in most states that are experienced with the Life Safety Code requirements. Based on our preliminary data, it appears that at least some of the facilities housing mentally ill clients must meet the Life Safety Code's Board and Care requirements in over half the states. Similarly, it appears that at least some of the facilities housing frail elderly clients must

meet the Life Safety Code's Board and Care requirements in over half the states. (Some states require the Board and Care Chapter for elderly clients but not for mentally ill clients and vice-versa.) Therefore, most states are in a position to make decisions regarding expanded use of the Board and Care requirements in the Life Safety Code based on first hand experience.

State officials, mostly from social service agencies, with knowledge of how the Chapter is being applied in their state, have indicated their opinion of the Board and Care Chapter in general. Twenty nine of 31 said that they had a positive opinion. Only one said he had a negative opinion. The other respondent was neutral. Twenty of 25 felt that the strictness of the requirements were okay as is. One thought they were too strict and four wanted substantially more fire safety. Some who thought the strictness of the requirements were o'kay did suggest specific changes. We have found only one official who wanted to stop using the Chapter and replace it with another set of requirements: the requirements were thought to be too severe (i.e. too expensive to meet) for Homes in residential settings. We do not know if this trend will continue when we expand our sample to include more fire marshals and fire service personnel.

A major concern to officials in adopting the Board and Care requirements in the Life Safety Code is the need to classify the evacuation capability of the home. This is a novel feature in the code. Homes are classified as Prompt, Slow, or Impractical. The Life Safety Code provides for several different procedures that may be used to determine the evacuation capability. In the past, officials have expressed concern about the feasibility and validity of the procedures. However, the officials we have interviewed expressed general satisfaction with the procedures they have adopted. The preliminary results of the study lead to the conclusion that this novel feature will become less of an obstacle to adoption as time passes.

The information and data will be stored and retrieved in a computer database. Considerable effort was directed at designing this database early in the project. We are using the computer database called PARADOX. Data entry procedures and formats have been developed and are being refined. Detailed data are being entered. We plan to use this database in the analysis phase of this project.

II. EXITT Simulation Model

EXITT is a computer program that simulates the decisions and actions of occupants of a residence in a fire emergency. It can be used in estimating the level of fire safety provided by various combinations of fire safety features for given fires. It was programmed in the BASIC programming language. Because of program size limitations of the BASIC language, it had been difficult to add new features to the simulation model. The program has been modified so that it can be run using the QUICKBASIC programming language. Now, new features can be added.

The current version of the model being distributed permits occupants (i.e., staff if a board and care home is being simulated) to rescue one or more occupants but does not permit reentry into the building. The program has been modified to permit residents to reenter the building and perform a second (or third) rescue. This modification greatly increases the value of the model for simulating fires in small Board and Care Homes. (Additional debugging checks are needed before this version is distributed.)

K. SUPPRESSION

FIRE SUPPRESSION

Funding Agency: STRS
NIH, Health and Human Services

Professional Staff: David Evans, Project Leader
William Walton, Fire Protection Engineer
Daniel Madrzykowski, Mechanical Engineer
Kathy Notarianni, Fire Protection Engineer
J. Randall Lawson, Physical Scientist

Project Objective:

Develop an understanding of fire extinguishment processes and derive techniques to measure and predict the performance of fire protection and fire fighting systems.

Technical Accomplishments:

1. First Generation Fire Suppression Model

The major accomplishment for the year was the formulation of the First Generation Fire Suppression Model which is intended for inclusion in future versions of the HAZARD code. The current HAZARD version 1.0 model contains limited means to assess the performance of fire sprinkler systems. Suppression analysis is limited in HAZARD to the sub-program DETACT which provides a method to calculate the time of sprinkler actuation. To extend the prediction of sprinkler effects in HAZARD past the time of sprinkler actuation the effects of water spray on the enclosure fire must be assessed. The three physical state phenomena of fire suppression with water including water spray interacting with fire gases and fuel elements is an extremely complex physical, thermal and chemical problem well beyond current engineering abilities to predict. However, progress has been made to advance hazard analysis by formulation of a first generation fire sprinkler suppression prediction method which expands capabilities to predict sprinkler response and adds an assessment of the effect of the water spray from a sprinkler on the heat release rate of the fire. The First Generation Fire Suppression Model deals with the three major areas of sprinkler performance prediction -- actuation, spray distribution, and fire suppression.

Sprinklers are actuated by reaction of a heat sensitive element to the fire gas flow. The actuation point is determined by selected operating temperature of the hardware. A calculation method for sprinkler actuation time that improves substantially on the limited capabilities of the present DETACT method by including the effects of a two layer environment with accommodations for ceiling standoff distance for pendent sprinklers has been chosen for the fire suppression model. The temperature rise of the sprinkler thermal element is calculate from correlations of fire driven gas flow

temperature and velocities and an assumed lumped mass heating using measured response time index (RTI) values to characterize the thermal lag of the sprinkler hardware.
Capabilities to make in-house measurements of RTI have been established this year with the installation of Plunge Test hardware.

The lack of accurate engineering predictions of spray dynamics in fire environments, suggests that for the purpose of this first generation fire suppression model for hazard analysis the user will specify the spray flux per unit area (spray density) reaching the fuel. User specified spray densities allow for the prediction method to take into account the consequences of water flow rates above and below the nominal design values. Thus very complicated interactions such as partial shielding of burning fuel from the spray that cannot be accommodated within the HAZARD model until a method for user specified orientation for three dimensional objects is developed, may be accommodated in an approximate and knowledgeable way by user adjustment of spray density.

The only generalized fuel source for which there is a known relationship for both the prediction of peak burning rate and time to extinction is a fully involved wood crib. This model utilizes the suppression dynamics of fully involves wood crib fires and provides a means to simulate suppression of other fuels as if they were wood cribs in order to predict the heat release rate during suppression. Wood cribs contain fully exposed, partially shielded, and fully shielded burning areas. In general wood cribs are fuels that are neither easily extinguished nor are they impossible to extinguish. The heat release rate of the fuel package at the time of sprinkler actuation and the water spray density are used to characterize the extinguishment of any fuel as if it were a fully involved wood crib.

For other than the shielded case, in which burning is assumed to be constant during suppression, the heat release rate of the fire is diminished exponentially according to:

$$Q/Q_{be} = \exp (- A \dot{m}_w''^{1.7} \Delta t_{be})$$

where:

A = Constant dependent on crib geometry

Q = Time dependent fire heat release rate after sprinkler actuation

Q_{be} = Calculated fire heat release rate at the time of sprinkler actuation

m_w'' = Spray density at the fuel location (specified by user, units: GPM/ft^2)

Δt_{be} = Time interval from time of sprinkler actuation (units: seconds)

Figure 1 shows the agreement between model predictions and measured heat release rates during suppression for 0.6m cubic wood cribs subject to different water spray densities.

2. Sprinkler System Performance Measurement

Several opportunities were presented during the year to measure the performance of both actual and experimental sprinkler systems. The performance of various sprinkler installations for protecting NIH research laboratories was assessed in a field tests in the laboratory. Systems were tested in ability to respond to a liquid spill fire. In other studies for NIH the ability of new quick response sprinkler technology to provide life safety for patient room protection was assess using a specially constructed hospital room matching NIH facility dimensions at NIST.

CFR provided technical support to the National Fire Protection Association to resolve difficulties with the use of model prediction for sprinkler actuation in large buildings. Field measurements of temperature conditions produced by an alcohol test fire in an aircraft hanger were used to test two different sprinkler response models developed by CFR -- DETACT and LAVENT. Figure 2 shows typical measured and predicted gas temperatures and control thermal lag disks used to represent sprinkler devices. Both of the model tend to over predict temperatures largely due to the effects of the assumed quasi-steady fire conditions in the large space. Even so this level of agreement was sufficient to clear up the original difficulties with the system analysis. For ordinary sprinkler installations CFR has developed thermal actuation prediction capabilities that rival the accuracy of large scale tests to assess response performance.

3. Plunge Test Apparatus

The measurement of thermal lag for sprinkler hardware is a current area if intense debate in both national and international standards organizations. At this time differing hardware, operating conditions and data analysis methods exist all of which are claimed to measure appropriate characteristics for the prediction of performance in actual fires. In the U.S. a heated air recirculating tunnel known as the Plunge Test is the preferred apparatus for measurement of thermal lag. This year CFR completed installation of a Plunge Test apparatus. This apparatus provides capabilities to make in-house measurements of thermal lag following usual testing methods. The apparatus also provides an experimental facility to obtain data to compare with field modeling predictions of sprinkler response to be started next year.

4. Droplet Surface Cooling

Cooperation with the University of Maryland continues in measure and predict of the cooling effects of water droplet evaporation of solid surfaces. This work is generating the fundamental understanding of spray heat transfer that is fundamental to the quenching action of sprinklers during fire suppression. For rapid response sprinkler technology of the type used in residences thermal quenching of the burning fuel is thought to be the dominate mechanism of fire extinction. Construction of a new apparatus to study the evaporation of droplets from a solid surface subjected to radiant heating from above. This apparatus will also be used in future measurements of water droplet suppression of burning fuels. Theoretical work was completed to predict droplet evaporation for low thermal conductivity surfaces in which there is a strong coupling of droplet evaporation and local surface temperatures.

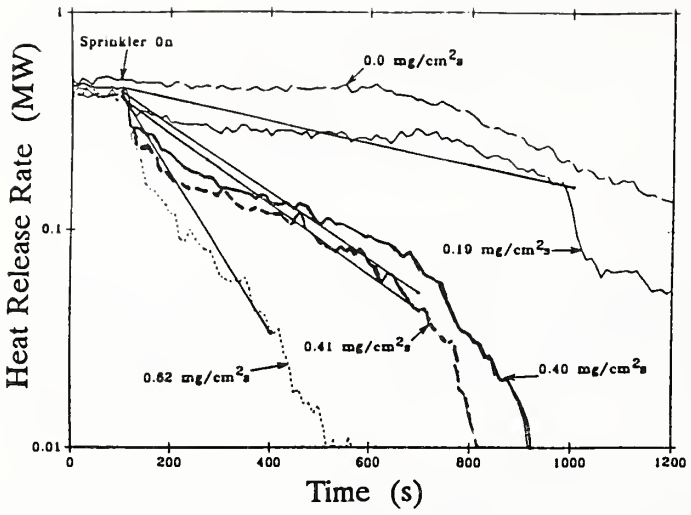

Figure 1. Predicted and measured heat release rates during suppression.

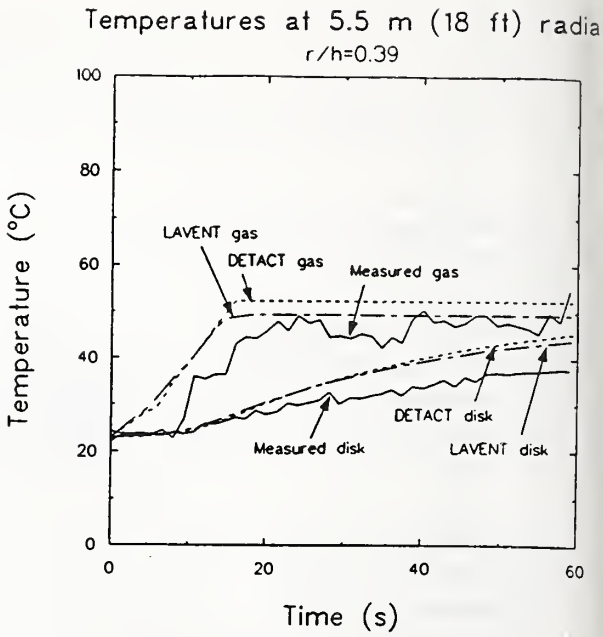

Figure 2. Calculated and measured gas and simulated sprinkler link temperatures.

Reports and Publications:

Quick Response Sprinklers in Chemical Laboratories: Fire Test Results, W. D. Walton, NISTIR 89-4200, November, 1989

Evaporation of a Water Droplet Deposited Over a Hot High Conductivity Solid Surface, M. diMarzo, D.D. Evans, J. Heat Transfer, Vol III, No. 1, 210, 1990

Infrared Thermography of Dropwise Evaporative Cooling, M. Klassen, M. diMarzo, J. Sirkis, Proc. Thermophys. Heat Transfer Conf., HTD Vol. 141, 117, 1990

Related Grants:

Extinguishment of Combustible Porous Solids by Water Droplets, Arvind Atreya, Michigan State University.

Transient Cooling of a Hot Surface by Droplet Evaporation, Marino diMarzo, University of Maryland.

Transient Behavior of a Fire-Induced Ceiling Jet in Presence of an Upper Layer: Comparison of Unconfined and Confined Ceiling Jets, Vahid Motevalli, Worcester Polytechnic Institute.

Port the Fire Demand Model to a PC Computer, Larry Pietrzak, Mission Research Corporation, Santa Barbara, California.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: Michigan State University

Grant Number: 60NANB8D0861

Title: Extinguishment of Combustible Porous Solids by Water Droplets

Principal Investigators: Arvind Atreya &
Indrek S. Wichman

Other Professional Personnel: Lin-Shyang Tzang (Ph.D candidate)
Peter Caffrey (Ph.D candidate)

NBS Scientific Officer: Dr. David D. Evans

TECHNICAL ABSTRACT:

The objective of this work is to extend the previous research on piloted ignition and cooling of inert isothermal porous ceramic solids by water droplet evaporation to real combustible materials. This new phase of the project was started and the previous work on piloted ignition was completed during FY 90. A novel apparatus has been developed to study the extinguishment of combustible solids. This apparatus along with the cone heater is being used to quantify the fire suppression rate as measured by the decrease in the energy release rate due to water droplet application and to determine the fire suppression boundary and the eventual time to extinguishment.

On the theoretical side, a simplified model for piloted ignition obtained from first principles has been developed and tested (This was a part of the previous phase of this study which has recently been completed). Also, the existing heat release rate models for porous charring materials are beeing extended to incorporate the effect of droplet evaporative cooling. A model for moisture evaporation from a porous material like wood is currently being developed. This work will be useful for the development of fire suppression models.

Extinguishment Experiments:

The cone heater was used to investigate the effect of 30 ul water droplets applied at the center of burning PMMA and wood samples of different diameters. Experiments were conducted at different incident heat fluxes and the water droplets were applied roughly once every 3 seconds. A small natural gas pilot flame was used to ensure piloted ignition of the sample.

A 2" diameter wood sample at 2.5 W/cm2 bursts into flames within 100 seconds. The water droplet application is started at this time. Upon subsequent water application the flames become weaker but they are not extinguished. However, for a similar experiment conducted at 1.5 W/cm2 the flames are eventually extinguished and are then re-ignited by the pilot flame 30 seconds after the water application is stopped. Experiments conducted on larger samples show that extinguishment does not occur even at 1.5 W/cm2 when a single droplet is used.

These experiments suggest the qualitative suppression diagram presented in figure 1. Here, the non-dimensional droplet distribution is plotted against the non-dimensional external heat flux. Flaming combustion does not occur at heat fluxes below the minimum heat flux required for piloted ignition. This minimum heat flux for various moisture contents and environmental conditions was determined in our previous study. Under conditions of no water application, the entire zone beyond the minimum heat flux represents flaming combustion. If the droplet distribution is such that the entire sample surface is affected by water application (herein called the completely soaked condition), then the zone below the non-dimensional drop distribution of unity becomes non-combustible. When the sample is too large compared with the droplet affected zone and the external heat flux is larger than the minimum heat flux then burning zone conditions exist. Likewise, for a large non-dimensional external heat flux, burning zone conditions may exist even if the droplets are closely distributed on the sample. The boundary between the burning zone and the extinguished zone is termed as the fire suppression boundary. Figure 2 shows the measured suppression boundary for PMMA. Note that while there is a considerable scatter in the data, a clear zone beyond which the fire is not extinguished is identified. A similar curve for wood is currently being determined.

From these experiments, it is clear that the important parameters are the droplet size, droplet influence area, drop frequency, minimum heat flux for piloted ignition and the external heat flux. All these parameters were measured in our previous study on porous ceramic solids. The present work is an attempt to extend the previous study to actual burning solids. Here, in addition to determining the fire suppression boundary, we are also trying to quantify the reduction in the heat release rate due to water application for regions that fall in the un-extinguished zone of figures 1 and 2.

Theoretical Investigation of Piloted Ignition:

A Ph.D thesis on theoretical investigation of piloted ignition has recently been completed by Tzeng [1]. This work develops a combined gas and solid phase theoretical model of piloted ignition for vaporizing and charring solids. The predictions of this model are largely in agreement with the experimental results of M. Abu-Zaid [2]. This model shows the history of development of a diffusion flame during piloted ignition and clarifies the the effect of various variables (such as: external radiation, wind velocity, oxygen concentration, sample moisture content and charring) on the piloted ignition process. A paper [3] regarding this work has been published in Combustion and Flame and a second paper is currently beeing written.

Reports and Papers:

1. Tzeng, L. S.,"Theoretical Investigation of Piloted Ignition of Wood," Ph.D Thesis, Michigan State University, 1990.

2. Abu-Zaid, M. , "Effect of Water on Ignition of Cellulosic Materials," Ph.D Thesis, Michigan State University, 1988. Also published as NIST-GCR-89-561, 1989.

3. Tzeng, L. S., Atreya, A., and Wichman, I. S., "A One-Dimensional Model of Piloted Ignition," Accepted for Publication in Combustion and Flame, 1989.

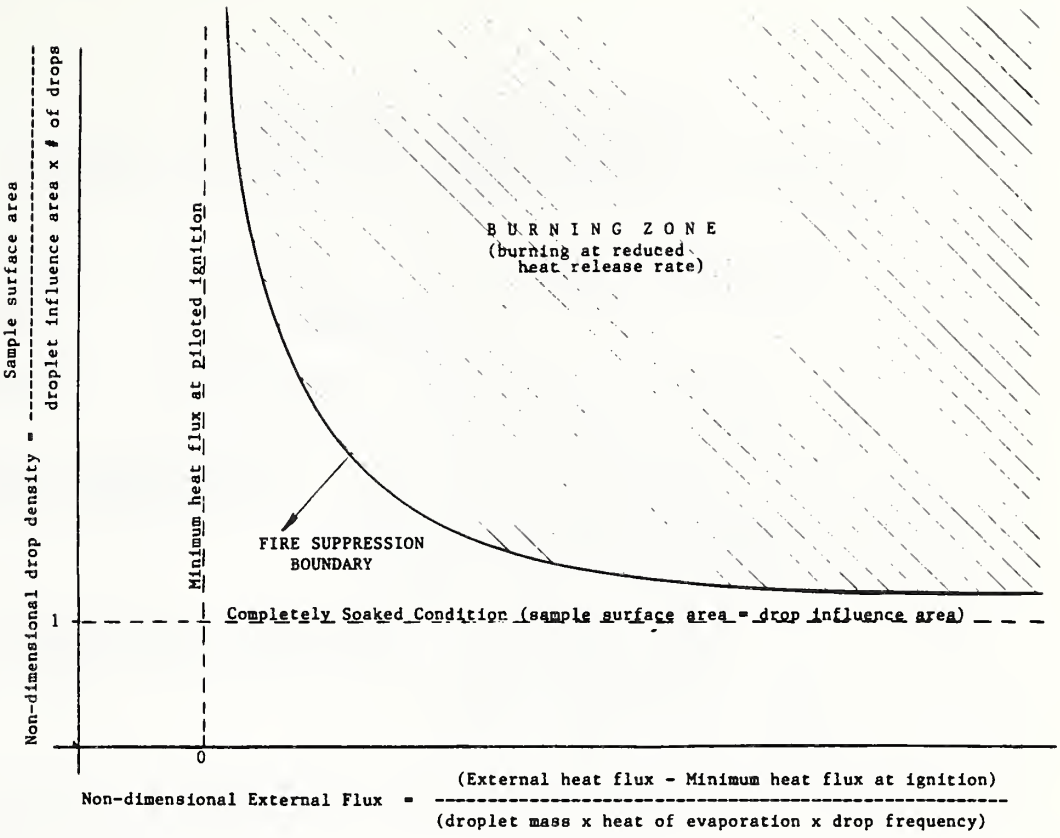

Figure 1. Qualitative Fire Supression Diagram.

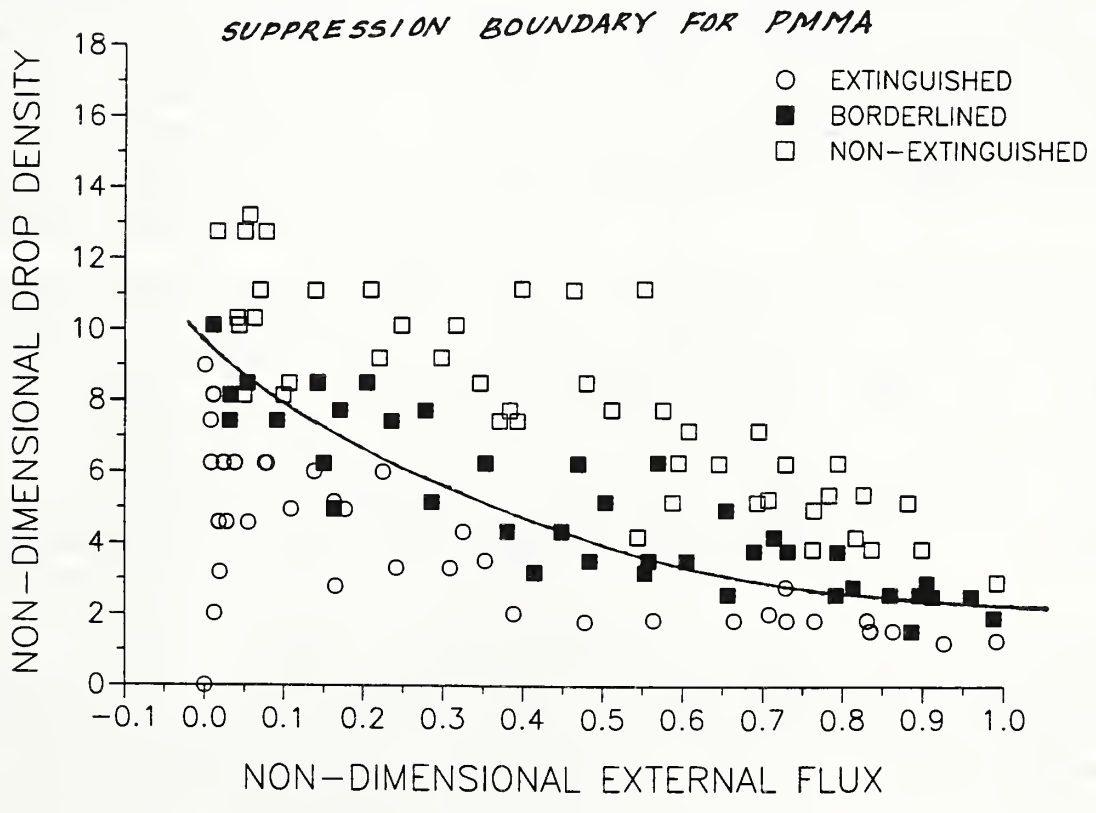

FIGURE -2

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: University of Maryland, College Park

Grant No.: COMM 70NANB8H0850,2

Grant Title: Transient Cooling of a Hot Surface by Droplets Evaporation

Principal Investigator: Dr. Marino di Marzo
Mechanical Engineering Department
University of Maryland
College Park, MD 20742

Other Professional Personnel: John Hamm, GRA
Charles Kidder, GRA
Yan Liao, GRA
Paolo Tartarini, GRA

NIST Scientific Officer: Dr. David D. Evans

Technical Abstract:

Introduction The phenomena associated with solid fuel fire extinguishment processes are related to the evaporation of water droplets deposited on hot solids. Results of the model describing the coupled thermal behavior of an evaporating droplet deposited on a semi-infinite solid surface are validated with experimental data. The hypothesis leading to a simplified model for the liquid droplet evaporation are tested against these more comprehensive computations. Insight into the evaporative cooling behavior of high and low thermal conductivity solids is obtained.

Coupled Solid-Liquid Model The integration of the governing equations describing the thermal behavior of the liquid droplet deposited on a semi-infinite solid surface is constituted of a Boundary Element Method (BEM) for the transient conduction equation written for the solid and of a Control Volume Method (CVM) for the integration of the liquid droplet transient conduction equation. The temperature and flux boundary conditions at the solid-liquid interface are enclosed and a matricial form is obtained for the whole coupled solid and liquid regions.

The details of the BEM are outlined in previous documents [1,2]. The idea of extending this treatment to the liquid droplet has been abandoned due to its analytical complexity and to the future need of including radiant heat absorption in the liquid layer. Since the BEM reduces the three dimensional transient conduction problem to a surface

integration, it is not suitable to the accounting of heat sources in the liquid layer representing the radiant heat absorption. The BEM applied to the solid reduces to the integration of the heat fluxes at the solid surface (times an appropriate Green's function) over the whole solid surface and over the time. Note that, due to the definition of the adjoint governing equation, the integration time originates at the present instant and stretches into the past as far as there is a non-negligible contribution.

The liquid region is treated with a CVM which discretizes the governing equation and its boundary conditions. The droplet shape is described as a segment of a sphere [3]. Consider a cylindrical coordinate system (r,z) with origin on the solid surface at the center of the wetted region with the z axis normal to the solid surface. The nodalization scheme consists of two sets of curves: a) arcs of circumference passing through the outer edge of the droplet (at z = 0) and centered on the z axis; b) arcs of circumference centered on z = 0 with radii inversely proportional to the distance between the origin and the intercept of the arcs with the r axis.

The governing equation integrated over each elementary control volume reduces to a transient energy balance where each incoming flux is evaluated with respect to its component normal to the surface bounding the elementary volume. The nodalization of the outer edge of the droplet is carried out by locating the nodes at half the step size from the droplet edge. Particular care is taken in the integration of the heat and mass transfer fluxes at the droplet edge to account for the sharp changes in temperature in that region.

A matrix form is used where the top portion of the matrix holds the coefficients resulting from the CVM for the liquid region, and the bottom portion consists of the corresponding weight coefficients for the solid BEM. The interfacial temperature and flux values are the communication links between the two domains. The unknown vector comprises temperatures in the liquid domain and the solid surface temperatures. The right hand side contains the known quantities vector.

Figure 1 demonstrates the model capability of predicting the evaporation time for both aluminum (k = 180 W/m ^{o}C) and Macor (k = 1.29 W/m ^{o}C). The difference of two orders of magnitude in the thermal conductivity induces a major change in temperatures for the Macor surface while the aluminum surface temperature change is limited to less than a degree centigrade.

The simplified model for droplets evaporating on high conductivity solids is based on the assumption of uniform and constant temperature under the droplet. This is the case as

demonstrated in Fig. 2. The contact temperature calculated in accordance with Seki [4] is quite close to the actual interfacial temperature. The results for Macor show that the assumptions of the simplified model fail since the solid-liquid interfacial temperature is neither constant nor uniform throughout the evaporation process.

Figure 3 validates the assumption of one dimensional heat flux in the droplet axial direction (normal to the solid surface): all the values show that the axial heat flux constitutes more than 90 per cent of the total heat flux. The few points below the 90 per cent line are for locations at the edge of a droplet deposited on Macor. This is to be expected if one considers the non-uniformity of the interfacial temperature distribution (see Fig. 2). Note that the heat fluxes at the edge of the droplet are in the range of pool boiling although nucleation is fully suppressed.

A new experimental set-up for the study of dropwise evaporative cooling with radiant heat transfer simulating flames above the solid surface has been designed and tested. An extensive series of experiments is currently under way to obtain a data base of transient surface temperature distributions using infrared thermography.

Acknowledgements The authors are indebted to Dr. H. Baum of CFR-NIST for his guidance on the development of the BEM for the modeling of the droplet-solid thermal interactions. The Computer Science Center of the University of Maryland provided partial funding for the computational expenditures.

References:

1. M. diMarzo, F. Kavoosi, M. Klassen, "Transient Cooling of a Hot Surface by Droplets Evaporation", NIST-GCR-89-559 (1989)
2. F. Kavoosi, M. diMarzo, H.R. Baum, D.D. Evans, "An Application of Boundary Element Methods to a Transient Axisymmetric Heat Conduction Problem", Proc. 26th Nat. Heat Transfer Conf., HTD Vol. 110, 79 (1989)
3. M. diMarzo, D.D. Evans, "Evaporation of a Water Droplet Deposited Over a Hot High Conductivity Solid Surface", J. Heat Transfer, Vol. 111, No.1, 210 (1990)
4. M. Seki, H. Kawamura, K. Sanokawa, "Transient Temperature profile of a Hot Wall Due to an Impinging Liquid droplet", J. Heat Transfer, Vol.100, 167 (1978)

Reports and Papers

M. Klassen, M. diMarzo, "Transient Cooling of a Hot Surface by Droplets Evaporation", NIST-GCR-90-575 (1990)

M. Klassen, M. diMarzo, J. Sirkis, "Infrared Thermography of Dropwise Evaporative Cooling", Proc. Thermophys. Heat Transfer Conf., HTD Vol. 141, 117 (1990)

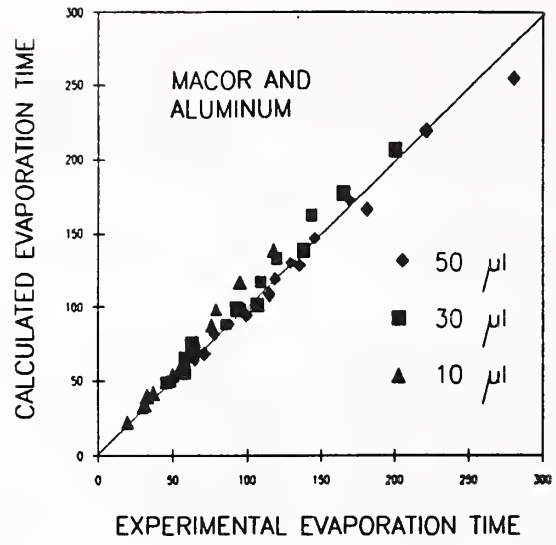

FIGURE ONE - Model validation: evaporation times for Macor and aluminum at various initial solid surface temperatures and for various drop sizes

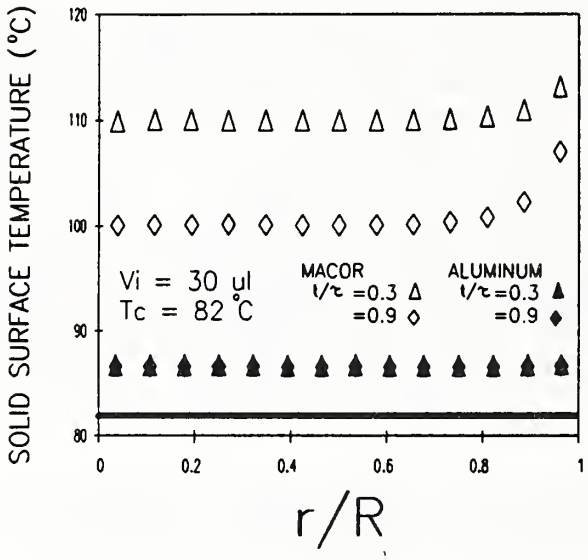

FIGURE TWO - Hypothesis of uniform and constant temperature at the liquid-solid interface: temperature distribution for Macor and aluminum at different times with respect to the calculated contact temperature

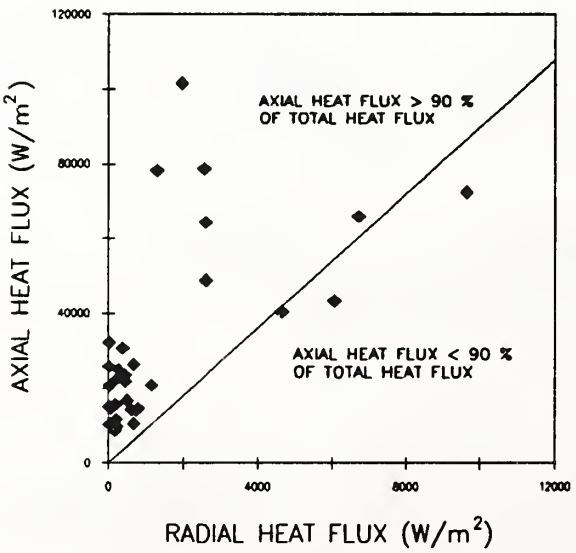

FIGURE THREE - Hypothesis of one dimensional heat flux field in the liquid droplet: Axial and radial heat flux comparison for aluminum and Macor at various locations and times

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution:	Worcester Polytechnic Institute
Grant No.	60NANB0D1049
Grant Title:	Transient Behavior of a Fire Induced Ceiling Jet in the Presence of an Upper Layer: Comparison of Unconfined and Confined Ceiling Jets
Principal Investigator:	Dr. Vahid Motevalli Center for Fire Safety Worcester Polytechnic Institute Worcester, MA 01609
Other Professional Personnel:	Christina Ricciuti, M.S. Student
NIST Scientific Officer:	Dr. Morehart

Technical Abstract:

Introduction The development of an upper layer in an enclosure during a fire has notable effects on the ceiling jet and the activation of detection and suppression systems. The presence of this hot gas layer increases temperature in the ceiling jet and heat transfer to the ceiling. This transient ceiling jet behavior is important because a great deal of emphasis is placed on prediction of fire behavior and compartment fire modeling for the early detection and suppression of fires.

Experimental correlations of ceiling jet flow temperatures and velocities for steady-state fires have been obtained by many investigators such as: Heskested and Delichatsios [1], Alpert [2], Alpert and Ward [3], and Motevalli and Marks [4]. In these studies, the ceiling jet is unconfined, no upper layer is accounted for. Evans [5], Cooper [6], and Zukoski and Kubota [7], among others, have addressed the ceiling jet flow in the upper layer for confined ceilings. In the confined ceiling jet investigations, the focus is on the plume interaction with the upper layer and heat transfer to the ceiling. The confined ceiling jet, is assumed to be retarded, when the upper layer is fully developed. When the upper layer is not fully formed, however, the ceiling jet is assumed to behave in the same manner as the unconfined conditions. Presently empirical relations for calculating unconfined ceiling jet characteristics are being used to model ceiling jets in the upper layer. These results can be extremely conservative due to differences in the ceiling jet in the presence of an upper layer. More accurate calculations of the ceiling jet characteristics in enclosures is desirable. It is anticipated that analysis of data from the confined case will yield information to quantify the relation between ceiling jet behavior in confined and unconfined situations, transience of the upper layer, its development and its effect on the ceiling jet characteristics.

Experimental Approach Data for ceiling jets under confined and unconfined ceilings was obtained from a study conducted at the Center for Fire Research, NIST by Motevalli and Marks [8]. This data was gathered from small scale experiments using steady fires. The experiment apparatus in this study is described in a previous report [4]. A confined ceiling jet was modeled by adding a 0.5 meter insulated (not shown in figure) curtain wall to a ceiling which was located 1.0 meter above a burner. Fig. 1. The ceiling, 2.13 meters in diameter was constructed of a 1.27 cm thick fiberboard material, painted with ultra-flat black paint. The ceiling was insulated with an 8.26 cm layer of fiberglass insulation. The fire source was a pre-mixed methane-air burner. Data was collected for the ceiling jet transience until steady-state conditions were reached, about 40 minutes into the test. The data collected represents a unique set of transient measurements of a confined ceiling jet and the developing upper layer. Velocity and temperature measurements were collected for 0.75 and 2.0 kilowatt fires for r/H locations of 0.26 and 0.75.

Technical Accomplishments Work on this grant is in its very initial stages. (Start date: August 1,1990) Raw data from the confined case have been reduced and further processing is in progress. The data show distinct temperature and velocity profiles exist in the upper layer of the confined ceiling. In general the following observations can be made:

- Figures 2 and 3 show that a ceiling layer develops quickly. The upper layer still contains a strong ceiling jet temperature profile for r/H of 0.26 for fires of 0.75 and 2.0 kW. In the layer below the ceiling jet a fairly constant gas temperature exists for both r/H locations once the layer is formed, as shown in figure 4. Figures 2-4 show that large temperature gradients exist near the ceiling and these gradients are quite significant during the first five minutes.
- The velocity profile close to the ceiling remains essentially constant throughout the span of the fire, figure 5. At 4.0 cm. below the ceiling scatter becomes more evident in the velocity profile as the ceiling layer develops. This result agrees quite well with the unconfined ceiling jet study where the velocity was determined to be unaffected by the ceiling heating. There is also a distinct decrease in the maximum ceiling jet velocity and velocity gradient, compared to the unconfined case.

Through dimensional analysis it may be possible to normalize these profiles and develop correlations between the confined and unconfined conditions. The objectives of the work include; quantification of the time-scale formation of the upper layer for two different fire strengths at varying radial locations, evaluation of the transient temperature field and quantification of the effect of the upper layer formation on the ceiling jet characteristics.

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[1] Heskestad, G. and Delichatsios, M.A., *Proc. 17th International Symposium on Combustion*, The Combustion Institute, Pittsburg, 1978.

[2] Alpert, R.L., *Fire Technology*, Vol. 8, 1972, p. 181.

[3] Alpert, R.L. and Ward, E. J., FMRC J.I. 01836.20, Factory Mutual Research Corporation, 1982.

[4] Motevalli, V. and Marks, H., "Transient and Steady State Study of Small-Scale, Fire-Induced Unconfined Ceiling Jets", Heat and Mass Transfer in Fire, Ed. J.G. Quintere and L.Y Cooper, HTD- Vol 14, ASME, 1990.

[5] Evans, D.D., *Comb, Sci, and Tech*, Vol. 40, p. 79, 1984.

[6] Cooper, L.Y., "A Bouyant Source in the Lower of Two Statified Layers-A Problem of Fire in an Enclosure" NBSIR83-2789, 1983.

[7] Zukoski, E.E. and Kubota, NBS/GCR 77/98, 1977.

[8] Motevalli, V. and Marks, H., "Transient Characteristics of Unconfined Fire Plume-Driven Ceiling Jets", NIST/GCR-90/574, (1990)

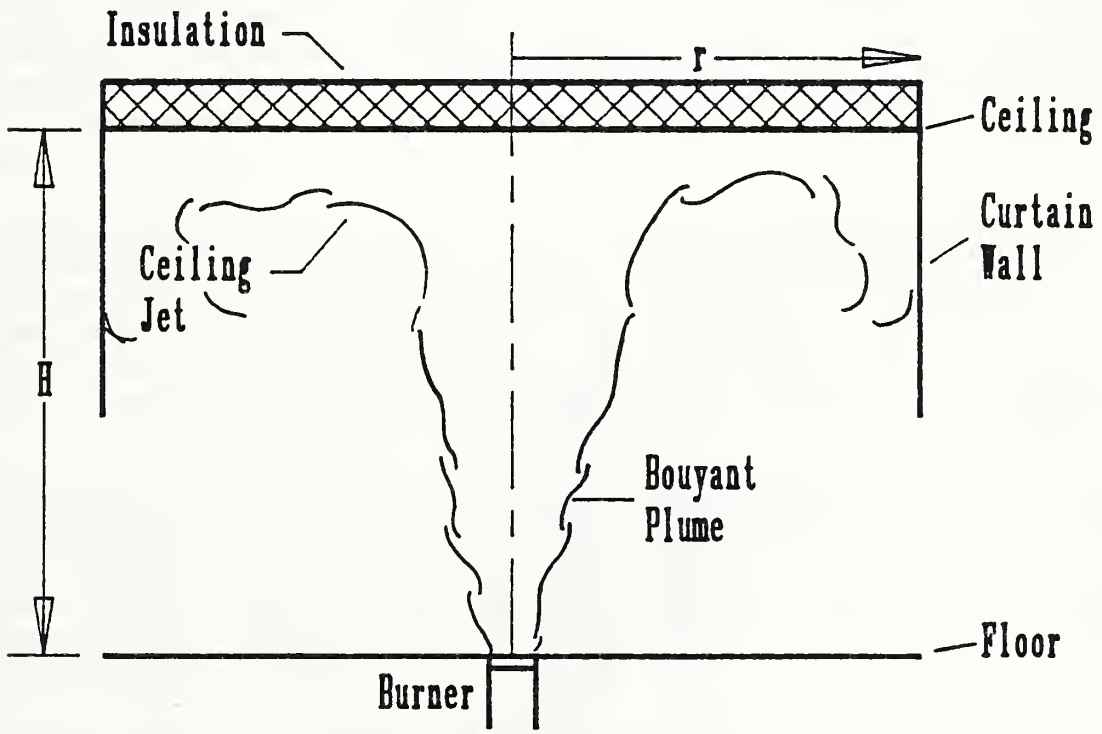


Figure 1- Schematic of Experiment Apparatus

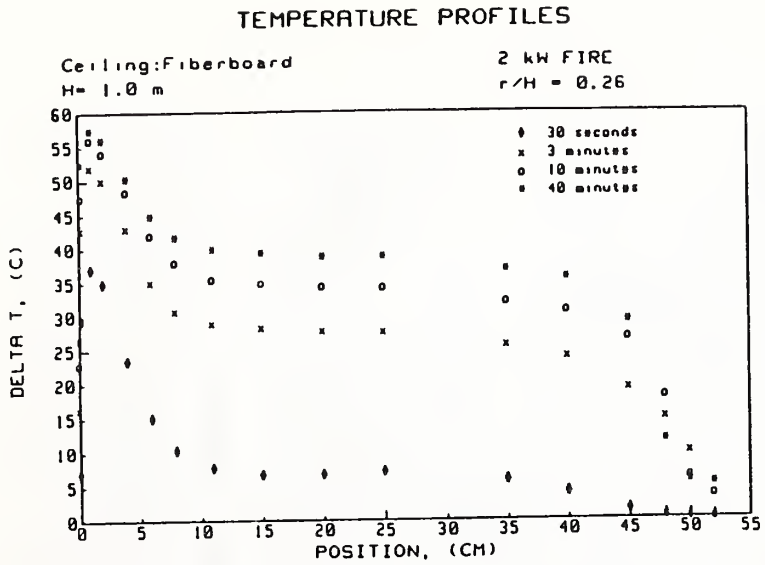


Figure 2- Variation of Temperature Profile with Time- 2.0 kW fire

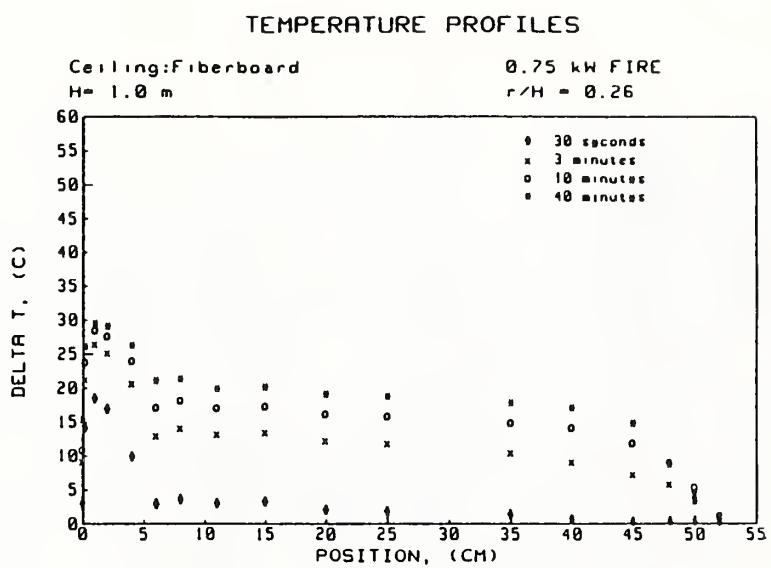


Figure 3- Variation of Temperature Profile with Time- 0.75 kW Fire

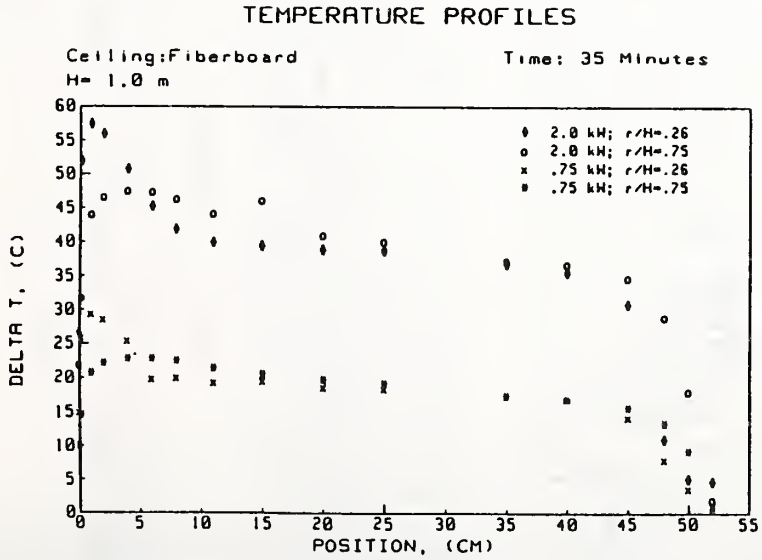


Figure 4- Steady State Upper Layer Temperature Profile

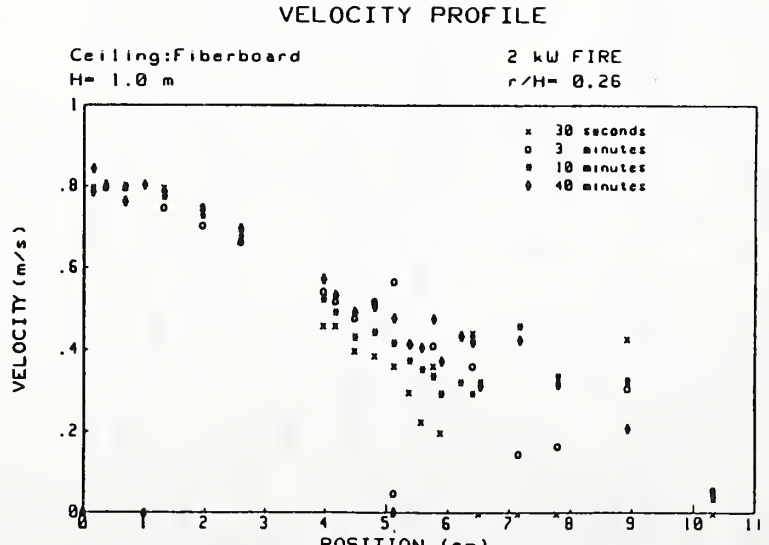


Figure 5- Variation of Velocity Profile with Time- 2.0 kW fire

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: Mission Research Corporation

Grant No.: 60NANBOD1050

Project title: Porting the Fire Demand Model to a PC Computer

Principal Investigator: Lawrence M. Pietrzak
P.O. Drawer 719
Santa Barbara, CA 93102

Other Professional Personnel: Jamie J. Dale, Computer Programmer

NIST Scientific Officer: W. Douglas Walton

Technical Abstract:

Introduction As part of a Swedish Fire Research Board (Brandforsk) research program, Mission Research Corporation (MRC) has been actively pursuing the development of a deterministic model of fire suppression to examine the effectiveness of manual fire fighting hose nozzles and water flow rate on post-flashover compartment fires. Results of this study showed that the development of a quantitative fire suppression simulation model is feasible. The product of this research, the Fire Demand Model (FDM), has been shown to be effective in predicting necessary water flow rates and spray characteristics form manual hose lines needed to suppress and extinguish post-flashover fires in simple compartments.

The FDM simulates the suppression of post-flashover of charring and non-charring solid fuel fires in compartments using water sprays from portable hose-nozzle equipment used by fire departments. The output of the FDM shows the extinguishing effects of hose-nozzle systems emitting water spry at various flow rates and droplet sizes. The calculations are based on a heat and mass balance accounting for gas and surface cooling, steam-induced smothering, direct extinguishment of the fuel, and water spray induced air inflow and venting of heat and products of combustion.

Recent controlled post-flashover suppression tests, as a joint effort between NIST and MRC, were utilized to evaluate and improve the FDM. These tests showed that in cases where the FDM predicted fire extinguishment, extinguishment was observed in the tests. Further, in cases where the FDM predicted the fire would continue burn because of insufficient water, the same was observed in the tests. Detailed comparisons of temperatures have not been completed. The FDM has shown that predictions of fire suppression events can be made and the technical insight developed can be helpful to fire fighting professionals.

Technical Approach Although the FDM was developed on a minicomputer, the use of a minicomputer for the FDM is neither convenient nor necessary. The model is small enough to fit on a personal computer and thus would be much more accessible to a variety of end users including researchers at NIST, fire training facilities, fire suppression equipment manufactures and other organizations. This project which, begun in September 1990, will involve porting the FDM to a DOS based PC.

It is essential that the porting effort retain and facilitate the FDM user friendly input and graphical output capability. Considerable effort was focused during the development of the FDM to allow the user to easily change input parameters, and to observe the effect in graphical displays where the trends and sensitivities can be easily observed. Finally the development of a user guide for the PC version of the FDM will facilitate the use of the program across the wide range of expected users.

L. CONE CALORIMETER

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1990

CONE CALORIMETER DEVELOPMENT

Professional Personnel

Vytenis Babrauskas, Project Leader
Marc Janssens, Research Associate, National Forest Products Association
Shyuitsu Yusa, Guest Worker, Building Research Institute, Japan

Project Objective

To have available, for both research and standard testing purposes, a state-of-the-art tool for measuring heat, smoke, soot, mass, and combustion gas release rates and related quantities (ignition time, heat of combustion).

Scope

The areas of work for FY90 included: (a) Cone Calorimeter round robins for both ASTM and ISO; (b) assistance to users; (c) organizing Cone Calorimeter Workshops.

Technical Accomplishments

The Cone Calorimeter standard was issued by three standards organizations during the year:

Standard Test Method for Heat and Visible Smoke Release Rates for Materials and Products using an Oxygen Consumption Calorimeter (ASTM E 1354), American Society for Testing and Materials, Philadelphia (1990).

Fire Tests – Reaction to Fire – Rate of Heat Release from Building Products. ISO DIS 5660, International Organization for Standardization, Geneva (1990).

Standard Method of Test for Heat Release Rates for Upholstered Furniture Components or Composites and Mattresses Using an Oxygen Consumption Calorimeter (ANSI/NFPA 264A). National Fire Protection Assn., Quincy, MA (1990).

The standards are similar, but not identical. The ASTM standard is the most general and complete. The ISO standard is essentially identical but excludes, for jurisdictional reasons, the sections dealing with the measurement of smoke (this is now a 'new work item' with ISO). The NFPA standard is oriented specifically towards the testing of furniture composites.

For each of the three standards organizations a separate roundrobin was completed. Two of these were organized from NIST: the ASTM one by V. Babrauskas and the ISO one by M. Janssens. We have compared the data from previous round robins for other reaction-to-fire test methods and find that our round robins produced better results than comparable data from previous methods. This is very pleasant and rewarding.

Three Cone Calorimeter Workshops were organized under the auspices of the International Heat Release Association: two in the UK and one in US. Also, the Second International Conference on Heat Release is being organized, to take place next year (Feb. 27-28, 1991) in Brussels, Belgium. A large number of contributions to this Conference will be papers focused on Cone Calorimeter work. The world population of Cone Calorimeters is now close to 50 and interest has been increasing dramatically. The Workshops are informal meetings with no formal publication, but intended for users and interested parties to exchange the latest information about operating issues, about new research projects, testing difficulties, new techniques for data analysis, etc. The Conferences are broader–they include not just Cone Calorimeters but medium and large-scale heat release studies. Their proceedings are issued in a special volume of the *Fire Safety Journal*. In the case of the upcoming Brussels conference, about half the program will consist of chapter authors from an upcoming textbook (*Heat Release in Fires*) to be published by Elsevier; the remaining half will be contributed papers.

Reports and Publications

Mulholland, G., Janssens, M., Yusa, S., and Babrauskas, V., The Effect of Oxygen Concentration on CO and Smoke Produced by Flames, submitted to *Fire Safety Science — Proc. of the Third International Symposium* (1991).

Babrauskas, V., Peacock, R.D., Janssens, M., and Batho, N.E., Standardizing the Exchange of Fire Data – The FDMS, submitted to *Fire Safety Science — Proc. of the Third International Symposium* (1991).

Babrauskas, V., and Peacock, R.D., Heat Release Rate: The Single Most Important Variable in Fire Hazard, to appear in FRCA Fall Meeting Proc., 1990.

Babrauskas, V., Modern Test Methods for Flammability, *Recent Advances in Flame Retardancy of Polymeric Materials*, Business Communications Co., Norwalk, CT (1990). Also issued as [U.S.] Natl. Inst. Stand. and Technology report NISTIR 4326 (1990).

Ryan, J.D., Babrauskas, V., O'Neill, T.J., and Hirschler, M.M., Performance Testing for the Corrosivity of Smoke, pp. 75-88 in *Characterization and Toxicity of Smoke* (STP 1082), American Society for Testing and Materials, Philadelphia (1990).

Babrauskas, V., The Cone Calorimeter — A new Tool for Fire Safety Engineering, *ASTM Standardization News. 18*, 32-5 (January 1990).

Babrauskas, V., New Test Methods for Assessing Smoke, Toxic Products, Corrosive Products, and Heat Release in Fires, pp. 20-33 in *Flame Retardants '90*, The British Plastics Federation, ed. Elsevier Applied Science, London (1990).

Babrauskas, V., Flammability of Upholstered Furniture with Flaming Sources, *Cellular Polymers. 8*, 198-224 (1989).

PART II. Timely Response to current Fire Problems
(mostly projects funded by other agencies and private sector organizations)

A. FIRE/MODELING INTERACTIONS

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

FLAME RETARDANT STUDY

Funding Agency: General Electric

Professional Staff: Takashi Kashiwagi, Project Leader

Project Objective:

To establish the effects of polymer structure and certain additives on flammability characteristics of GE's engineering thermoplastics.

Technical Accomplishments:

Various flammability properties, ignition, flame spread rate, heat release rate, CO and soot yields, and smoke extinction, are measured for various polycarbonates, polyimides and polyphenylene-oxides with and without additives. 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, a course wire screen was initially used to retain the sample surface at the original location. However, it is not clear that flammability properties obtained under such configuration represent material property characteristics which can be used for fire growth models, although the measured properties are highly reproducible. In order to examine the effects of the sample mounting method on flammability properties, additional three different sample mountings, without the wire screen, without a metal sample container, and modified sample holder frame, were used. The results indicate that heat release rate can be varied as high as factor of two to three depending on the sample mounting. Generally, heat release rate is the lowest with the wire screen and the metal container. The height of intumesced char was also affected by the presence of the metal container. Similarly flame spread behavior is significantly different with and without the use of an open wire mesh retainer depending on the type of the sample. These results indicate that some caution and further study are needed to characterize flammability properties of intumescent materials using a bench scale test method.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

RADIATIVE IGNITION AND SUBSEQUENT FLAME SPREADING IN MICROGRAVITY ENVIRONMENT

Funding Agency: NASA Microgravity Science Program

Professional Staff: Takashi Kashiwagi, Co-Project Leader
Howard Baum, Co-Project Leader
Genichiro Kushida, Guest Researcher
Hidesaburo Nambu, 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 one G environment.

Technical Accomplishment:

A two-dimensional axisymmetric time-dependent ignition model in a quiescent microgravity condition has been developed. Its gas phase model is based on irrotational flow mainly controlled by gas expansion and mass addition from degrading condensed fuel with one-step oxidative reaction with energy and species equations. Its condensed phase model is based on the thermally thin cellulosic sheet with three global degradation reactions, pyrosis reaction and oxidative degradation of the sheet to generate char and gaseous products, and oxidative char degradation. The calculated results show that the event of ignition occurs roughly 1 cm above the surface depending on kinetic constants of the gas phase oxidative reaction. An umbrella shape flame appears but this flame can not be sustained to flame spread with typical values of kinetic constants of gas phase and condensed phase reactions due to lack of enough supply of oxygen and fuel species. Effects of gas phase oxygen concentration and the fuel fraction in the degradation products on ignition are presently being studied. Determination of kinetic constants of the three degradation reactions are nearly completed using TGA analysis with multiple heating rates and oxygen concentrations and by continuous evolved gas analysis of CO, CO_2, H_2O and O_2.

Reports and Publication:

"Heat and Mass Transport From Thermally Degrading Thin Cellulosic Material in a Microgravity Environment", Kushida, G., Baum, H.R., and Kashiwagi, T., submitted to 1990 JEME/ASME Meeting, March 1991.

"Ignition of Thin Cellulosic Material in a Quiescent Microgravity Environment", Kushida, K., Baum, H.R., and Kashiwagi, T., to be presented at 1990 Fall Technical Meeting, Eastern Section of the Combustion Institute, Dec. 1990.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

MATERIAL FLAMMABILITY TEST ASSESSMENT

Funding Agency: NASA

Professional Staff: T. Ohlemiller, Project Leader
K. Villa, Textile Technologist
H. Mitler, Research Physicist

Project Objective:

Assess the current NASA flammability test method against the set of tests currently in use at NIST for measuring the elements of material flammability. Assess the feasibility of estimating micro-gravity flammability from normal gravity testing.

Technical Accomplishments:

A set of five materials of current interest to NASA for spacecraft interior usage was tested using the standard NASA flammability assessment method (NHB 8060.1B) in ambient air and using the ignition, rate of heat release and lateral flame spread tests developed at NIST. The NASA test looks at the tendency for upward flame spread on a small sample of a material when subjected to a small flaming ignition source for a fixed duration (approx. 25 sec). Only one of the tested materials exhibited substantial upward flame spread in this test; the four others exhibited flaming only under the direct influence of the igniter flame. The NIST tests all subject a material to a range of incident radiant heat fluxes comparable to those expected from the burning of other objects near the object of interest. Under these circumstances, given a sufficient external flux (which varies with the nature of the material), all of the materials ignite, exhibit a significant rate of heat release and lateral flame spread rate. Since the NASA tests did not provide a measure of flame spread which could be compared with the NIST test results, the desired comparison of test methods could not be made. The NASA test has now been modified to permit pre-heating of the sample and sample holder to facilitate flame spread. The minimum pre-heat temperature needed for full upward spread is one measure of flammability; the rate of upward spread is another. A modified set of five materials is now being tested in this manner.

The second objective above is being addressed via a study of available models of the elements of flammability and an examination of the role that gravity plays in these processes. The study is still underway.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

HEAT RELEASE FROM AIRCRAFT COMPOSITES

Funding Agency FAA

Professional Staff: W.J. Parker, Project Leader
A. Perez, Computer Scientist

Project Objective

Develop a theoretical and/or empirical or estimating technology for predicting an aircraft cabin panel's heat release rate in the OSU calorimeter. Such a methodology could provide a basis for more efficient panel design and testing.

Technical Accomplishments

A computer model was developed which calculates the temperature profile through the panel, the mass loss rate and the heat release rate based on the thermophysical and thermochemical properties of the individual components. The re-radiation from the front and rear surfaces and the internal radiation and heat conduction were taken into account. The temperature profiles were compared with experimentally measured ones when the panels were exposed to the thermal radiation from a gas fired radiant panel. The surface emissivities and the convective heat transfer coefficients were adjusted to bring the temperature profiles into closer agreement. Then the mass loss rate measured in the burning rate apparatus was brought into agreement by adjusting the kinetic parameters determined by TGA. Next, the heat release rate in the Cone calorimeter was matched by adjusting the effective heat of combustion of each component in the composite. Finally the calculated heat release rate was multiplied by a factor to account for the heat that was not recovered in the OSU calorimeter. Then the sensitivity of the peak heat release rate to changes in the core thickness, cell size and incident radiation were explored with the model. The sensitivity to changes in the material properties can also be examined with the model.

The increase in heat release rate of a particular panel with the incident radiant flux was consistent with that obtained in the Cone calorimeter. The model predicts a small decrease in the peak heat release rate with increasing cell thickness. This variation is within the scatter of data from the calorimeter.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

LOW FLAMMABILITY COMPOSITES

Funding Agency: U.S. Dept. of the Navy

Project Leaders: James E. Brown, Research Chemist
T. Ohlemiller, Research Engineer

Project Objective:

To develop a bench-scale methodology for evaluating the fire performance properties of fiber-reinforced composites in order to assist the Navy in selecting composite materials for use on ships.

Technical Accomplishments:

1. Flame Energy Feedback

The first phase of a study to quantify the heat feedback from the flame to the burning surface was completed. Based on a energy balance concept for mass loss rate, the flame heat flux to the surface is ascertained from the difference in the inferred mass loss rates where the external flux approaches zero. Figure 1 shows examples of the mass loss rates of a composite in a flaming mode and nonflaming modes in nitrogen and in 10% oxygen. Moreover, the inferred energy loss from such plots approximates the critical external energy flux for lateral flame spread.

2. Edge Effect on Composite Flammability

Composite materials have the potential for a form of non-ideal behavior which is termed an "edge effect". Pyrolysis gases generated between the fiber plies during surface heating of a composite will seek the path of least resistance in escaping from the composite. This path may lead to the edge of the sample rather than the face if the plies have some tendency to delaminate and if the outer plies are clogged by char from the binder resin. This effect is more likely to affect the small samples used in Cone Calorimeter and LIFT tests than it is to affect full scale wall panels; the path to an edge is likely to be much longer in the latter case.

A modified sample holder was designed to allow a study of the effect of edges. To prevent the leakage path to sample edges, the sample size is increased by 2½ cm. around the periphery; this added edge material is kept cool and tightly clamped during exposure of the normal area of sample face to a radiant heat flux. Such a holder was utilized to examine rate of heat release, burning rates and thermal sensitivity indices of composites in the Cone Calorimeter. Figure 2 demonstrates the observed effect on a FR vinylester/woven glass composite with respect to ignition and time dependent heat release rates. Preliminary analyses of the results indicate that the conventional Cone results represent the worst case scenario.

An analogous holder was also built for the LIFT apparatus to allow assessment of the impact of edge effects on lateral flame spread behavior. This study is ongoing; preliminary results indicate that the magnitude of such effects is strongly dependent on the nature of the binder resin and, most likely, the nature of the fiber weave in the composite.

Figure 1. Peak (smoothed) Mass Loss Rate of 4.5 mm Vinyl Ester in Flaming and Nonflaming (nitrogen) Modes

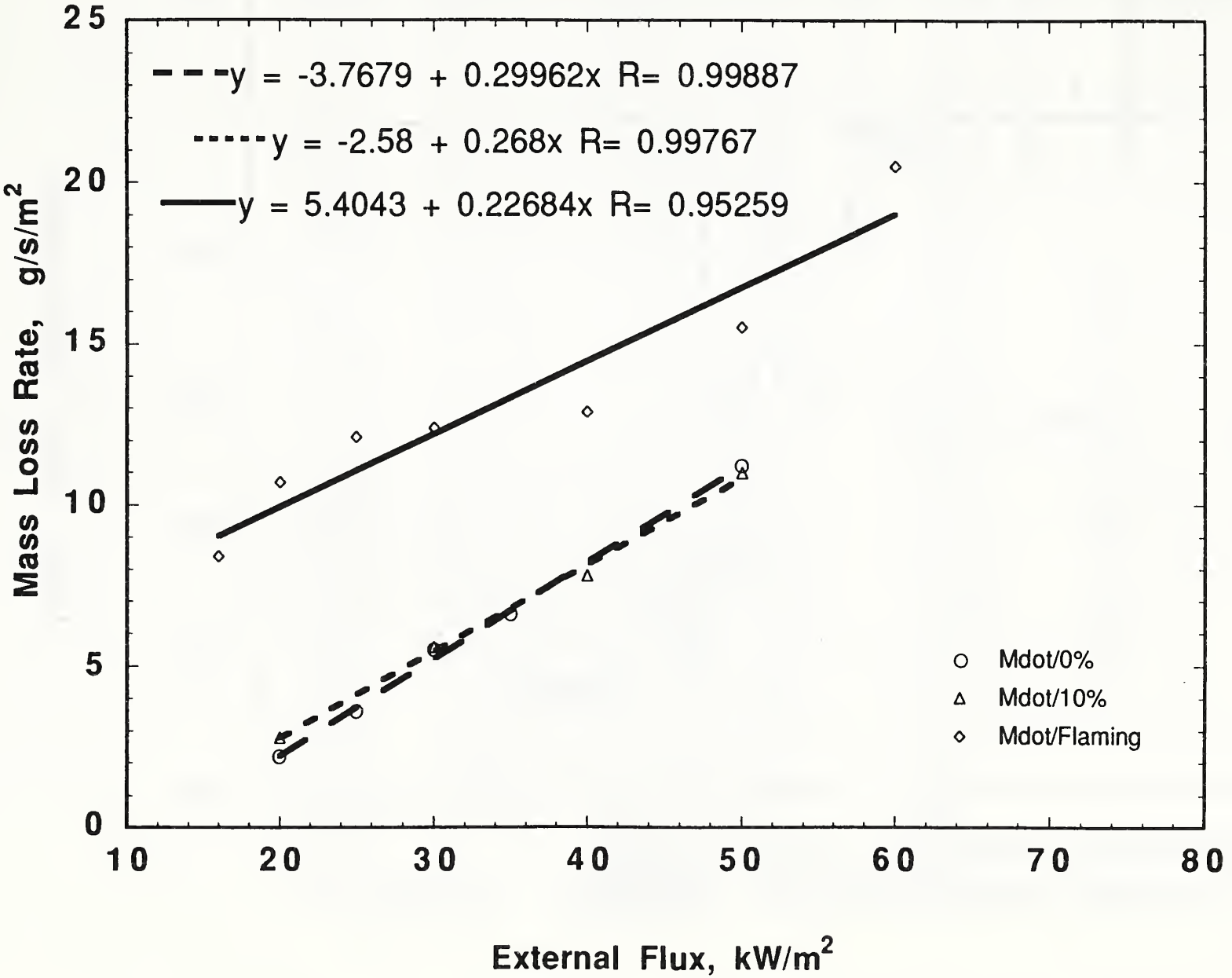
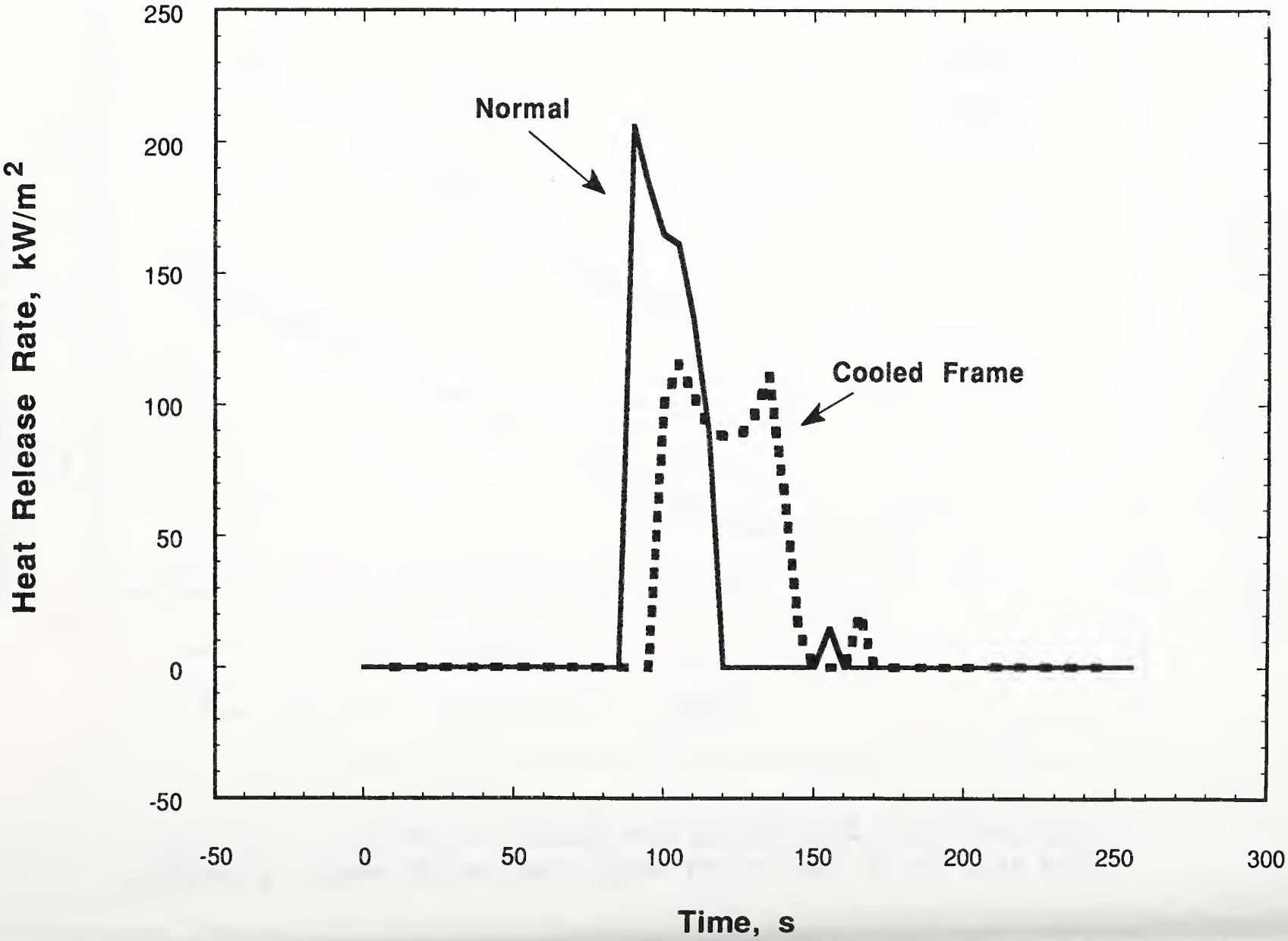


Figure 2. Influence of Cooled Edge Frame on HRR of 13 mm Vinyl Ester Composite



CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

AUTOIGNITION OF HYDROCARBON FUELS

Funding Agency: Air Force

Professional Staff: Kermit C. Smyth, Project Leader
Nelson P. Bryner, Chemical Engineer

Project Objectives

Devise a reliable method for measuring the autoignition behavior of hydrocarbon fuels for short duration exposures to heated metal surfaces in order to formulate appropriate strategies to reduce autoignition tendencies.

Technical Accomplishments

A new apparatus has been designed, built, and extensively tested for making 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. Over 1100 individual autoignition temperature determinations have been made for the ignition of 15 hydrocarbon fuels on heated nickel, stainless steel, and titanium surfaces for three different fuel/air mixtures (stoichiometry ϕ = 0.7, 1.0, and 1.3). Excellent reproducibility has been achieved with the new apparatus.

The measured autoignition temperatures generally decrease for the larger hydrocarbons and for richer mixtures, with the C_2 hydrocarbons (ethane, ethylene, and acetylene) having particularly low values. The highest autoignition temperatures are observed for nickel surfaces and the lowest for stainless steel, with titanium being an intermediate case.

A review of the autoignition literature suggests that the branched alkanes should be more resistant to autoignition than the linear isomers, and thus present a reduced hazard. Limited data obtained in this study are consistent with this prediction. Promising areas of future research have been outlined.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

COPPER INTERACTIONS WITH FIRE GASES

Funding Agencies: International Copper Association, Ltd.
The Society of the Plastics Industry, Inc.

Professional Staff: Barbara C. Levin, Project Leader
Maya Paabo, Research Chemist
Emil Braun, Physicist
Richard H. Harris, Jr., Chemist
Magdalena Navarro, Biologist

Project objectives:

1. To determine if the reduced levels of HCN generation and resultant toxicity from copper-impregnated flexible polyurethane foams observed under small-scale laboratory conditions still occurs when such copper-treated materials are combusted under medium- and large-scale conditions.

2. To examine the flammability characteristics of copper-impregnated flexible polyurethane foams. i.e., ignitability, rate of heat release, rate of flame spread, and smoke obscuration.

Technical Accomplishments:

Previous reports from this laboratory have shown that flexible polyurethane foams (FPU) treated with copper dust, cupric oxide, cuprous oxide or copper sulfate produced significantly less hydrogen cyanide (HCN) when thermally decomposed than the identical but untreated control foams. The decreased atmospheric concentrations of HCN resulted in the reduction of the acute inhalation toxicity (as measured by lethality in Fischer 344 rats) produced from exposure to this smoke. This reduction of HCN and toxicity occurred regardless of whether the copper or copper compound was added to the foam during its formulation (prior to the foaming process) or added as a post-treatment (after formulation). In all these reported experiments, the foams were thermally decomposed in the NBS Toxicity Test Method apparatus via a two phase procedure previously shown to produce high concentrations of HCN.

This year the following flammability properties were examined in foams with and without 0.1% cuprous oxide: 1. ignitability in three systems [the NBS Toxicity Test Method, the Cone Calorimeter, and Lateral Ignition and Flame Spread Test (LIFT)], 2. rate of heat release, 3. smoke obscuration, and 4. rate of flame spread. In all cases, no differences in flammability characteristics between the treated and untreated foam were observed.

Medium (furniture calorimeter) and full-scale (room burns) tests of copper-impregnated foam cushions were conducted to examine the effect of different combustion conditions. The results of this work are now being analyzed. However, it appears that under the large-scale conditions examined the HCN levels were not reduced by the presence of 0.1% cuprous-oxide. More work is necessary to understand the mechanism of copper-induced HCN reduction and to explain the different results obtained under the large-scale combustion conditions.

Reports and Publications:

Levin, B.C., Paabo, M., Harris, R.H., Clark, H.M., Yoklavich, M.F., Eller, N. and Highbarger, L., The effect of copper additives on atmospheric hydrogen cyanide and acute inhalation toxicity from the combustion products of flexible polyurethane. Proceedings of The Fire Retardant Chemicals Association Fall Conference, Scottsdale, AR, October, 1989, pp. 107-112.

Levin, B.C., Paabo, M., Harris, R.H., Eller, N., and Highbarger, L., Copper additives decrease the acute inhalation toxicity of the combustion products of flexible polyurethane by inhibiting hydrogen cyanide generation. Annual Report, Year 2, Submitted to the International Copper Association, Ltd., June, 1989.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

Fire and Smoke Spread in Ships

Funding Agency:

Naval Research Laboratory

Professional Staff:

Walter W. Jones, Paul Reneke

Objective:

To support the full scale fire testing on the Ex USS Shadwell by providing data analysis, predictive capability, display and data acquisition.

Scope:

To implement version the most recent version of CFAST on the Navy minicomputer based on the Ex Shadwell. This will include mechanical ventilation, hydrogen chloride deposition and display of the results in real time. Included in the model will be the capability for calculating vitiated combustion, hypergolic and rocket fuels as well as class a materials.

Technical Accomplishments:

There were 3 tasks associated with this project: (1) Install version 1.0 of CFAST on the Masscomp (Concurrent) Computer on the Ex Shadwell. Version 1.0 includes mechanical ventilation, ventilation controlled as well as unconstrained fires, and hydrogen chloride deposition. (2) Perform a series of calculations will be done which will show the some of the effects of ventilation, structural damage (breaking bulkheads) and various fuels in the context of shipboard fires. The data sets to do these calculations will be installed on the shipboard computer. (3) As a series of experiments are performed on the Ex Shadwell, NIST will assist NRL in setting up the data files to run the model for these configurations (ongoing).

The result of this project is that the model and associated support programs running on the Shadwell. The data reduction and model validation projects have just been started. In FY91, vertical flow (through horizontal hatches in the floor/ceiling) will be incorporated. Also, the smoke ejection concept will be studied, and the associated SES experiments will be analyzed.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

Fire Performance of School Bus Interiors

Funding Agency:

National Highway and Transportation Safety Adminstration

Professional Staff:

Sanford Davis and Emil Braun

Objective:

Assess the fire performance of school bus seat assemblies when exposed to internal and external fires and to develop a laboratory scale protocol for evaluating the fire performance of materials used in school bus seats which will predict the results of large scale tests.

Scope:

The National Highway and Transportation Safety Administration is considering requirements for safety of school bus seats. This was prompted by a recent accident in which several children died in a fire inside a bus. This work is to ascertain what sort of a screening or testing procedure would be suitable for materials in such a configuration. The procedure amy encompass small scale testing, large scale testing, full scale testing (actual busses) or computer models.

Technical Accomplishments:

A screening procedure was developed which indicate the suitability of material combinations in seats used in busses. It disallows materials which are clearly unsuitable, and provides guidance for further testing of combinations which meet general criteria.

Publications:

Braun, E., Klote, J., Davis, S., Paabo, M., and Gann, R., An Assessment Methodology for the Fire Performance of School Bus Interior Compartments, NISTIR (1990).

Braun, E., Klote, J., and Davis, S., School Bus Seats: A Fire Hazard Assessment, Fall 1990 Fire Retardant Chemicals Association Conference.

B. FIRE PROTECTION TECHNOLOGY

SAFETY IN OFFSHORE DRILLING

Funding Agency: Minerals Management Service, U.S. Department of Interior
U.S. Coast Guard, Department of Transportation

Professional Staff: David Evans, Project Leader
William Walton, Fire Protection Engineer
Howard Baum, NIST Fellow
George Mulholland, Chemist
J. Randall Lawson, Physical Scientist
Richard Harris, Chemist
Ronald Rehm, NIST Fellow

Project Objective:

Examine technologies that can mitigate the effects of oil spills and fires from offshore platform accidents.

Technical Accomplishments:

The Center for Fire Research has conducted research to examine phenomena associated with crude oil combustion and the impact of using burning as a spill response method. These studies have been conducted for several years using laboratory measurements and testing in CFR's Large Scale Test Facility. This year a major effort was begun to develop means to perform measurements of the oil spill burning process in field tests of 15 m diameter pool fires. Field test measurements of burning rate, fire radiation, smoke emission, smoke composition and smoke dispersion in the atmosphere are being attempted to increase understanding of the impact of burning on the local environment. This information is expected to be critical to gaining acceptance for the use of burning as an option in oil spill response.

Specialized instrumentation for measurement of soot yield by carbon balance and sampling for Polycyclic Aromatic Hydrocarbons (PAH) has been developed in a way that sensing and data acquisition systems can be flown through the smoke plume during large fires. Mini-blimps (6 m in length) capable of lifting 5 kg. have been used to transport and station instrument packages in the near field fire plume.

Calculation of plume dynamics has progress by incorporating vortex element calculations method to simulate the dispersion of the smoke plume in the local atmosphere and the deposition of soot particles from the plume. Classical methods of plume dispersion analysis routinely used in industry have also been performed for the large fires.

Safety relative to both drill string blowouts and diverter fires on offshore platforms is being examined though a cooperative grant to Professor Jay Gore at the University of Maryland. Both the effect of

water spray on vertical methane jet flames and the radiation and structure of horizontal jet flames are being examined through experiments and analysis.

Reports and Publications:

Burning, Smoke Production, and Smoke Dispersion from Oil Spill Combustion, D. Evans, G. Mulholland, D. Gross, H. Baum, W. Walton, and K Saito,
NISTIR 89-4091, November, 1989

Measurement of Large Scale Oil Spill Burns, D. Evans, W. Walton, H. Baum, R. Lawson, R. Rehm, R. Harris, A. Ghoniem, and J. Holland, Proceedings of the Thirteenth Arctic and Marine Oil Spill Program Technical Seminar, Edmonton, Alberta, Canada, June 6-8, 1990.

Boilover Phenomenon in Pool Fires of Liquid Fuels Supported on Water, K. Saito, A. Ito, T. Inamura, and A. Goto, 27th National Heat Transfer Symposium of Japan, Vol II, P.718, Nagoya, 1990

Polycyclic Aromatic Hydrocarbon Emissions from the Combustion of Crude Oil on Water, B. Benner, N. Bryner, S. Wise, G. Mulholland, R. Lee, and M. Fingas, Environmental Science and Technology, Vol. 24, 1990.

Structure and Radiation Properties of Large Two Phase Flames, J. Gore, S. Skinner, D. Stroup, D. Madrzykowski and D. Evans, Heat Transfer in Combustion Systems, (N. Ashgriz, J. Quintiere, H. Semerjian, and S. Slezak, eds.) HTD-Vol 122, ASME, New York, 1989.

Radiation Properties of Laminar and Turbulent Nonpremixed Methane and Acetylene/Air Flames, J. Gore and S. Skinner, Heat and Mass Transfer in Fires, (J.G. Quintiere and L.Y. Cooper, eds.) HTD-Vol.141, ASME, New York, 1990.

Related Grants:

Numerical Modeling of Plume Dispersal and Smoke Deposition from Large Scale Fires, A Ghoniem, Massachusetts Institute of Technology.

A Study of Pool Combustion of Crude Oil Supported on Water, K. Saito, University of Kentucky.

An Investigation of Simulated Oil Well Blowout Fires, J. P. Gore, University of Maryland.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARD AND TECHNOLOGY
FY 90

Institution:	Massachusetts Institute of Technology
Grant No.:	60NANB0D1036
Grant Title:	Numerical Modeling of Plume Dispersal and Smoke Deposition from Large Scale Fires
Principal Investigator:	Prof. Ahmed F. Ghoniem Department of Mechanical Engineering #3-339, M.I.T. Cambridge, MA 02139
Other Professional Personnel:	One Ph.D. Student
NIST Scientific Officer:	Dr. Howard R. Baum

Technical Abstract:

The objectives of this work are to develop and apply a numerical methodology for the prediction of the rise, dispersal, fall and downwind settlement of smoke plumes generated from large, open fires. Model predictions will determine the effects of fire and atmospheric conditions, and ground terrain topology, on smoke distribution within the plume as it is transported by the combined action of buoyancy and wind. Simulations will be utilized to construct improved models of fire smoke plume dispersal and deposition. The computed smoke plume trajectory and smoke concentration distribution on the ground will be used in the planning of small and intermediate scale field tests which will be conducted by NIST/CFR scientists to investigate the cleanup of oil spills using combustion. The numerical model will utilize the transport element method to obtain solutions of the equations governing this buoyancy-driven, wind-transported, smoke-laden hot plume into a stratified atmosphere.

Background: Combustion has been suggested and partially utilized in the emergency response to accidents which result in massive oil spill on water surfaces. A primary concern in this regard is smoke generation by incomplete combustion, its transport down wind to regions far from the spill site, and the resulting environmental damage and health hazards. To assess the damage potential, smoke plume trajectory and smoke deposits distribution should be carefully estimated under different atmospheric conditions, wind patterns and earth terrains. An extensive experimental and theoretical investigation of this problem has been undertaken by NIST/CFR. During this investigation, a number of laboratory and field experiments, in which oil will be spilled and burned over the surface of artificial and natural bodies of water, are

planned to study smoke production in pool fires. Complementary theoretical and numerical analyses of smoke generation and plume motion are underway.

The success of the planned tests depends to a large extent on a prior knowledge of: (1) where does the smoke plume go as it rises in the turbulent, stratified atmosphere; (2) where and what is the maximum deposition of smoke on the ground; (3) what is the horizontal extent of smoke deposition and what is the concentration expected over this region; (4) how much time it takes the smoke to travel from the fire to the area of deposition; (5) how do all these processes depend on fire physics and atmospheric conditions; (6) what are the most important atmospheric variables which affect the smoke dispersal that should be determined during and after the test ; and (7) how and in what form should one compile the measurements in a way that is most informative and illustrative. Some of these tests may be conducted in hostile environment in which collecting data may not be easy. After the measurements, one has to be able to interpret the results and represent them in a model which can be used in future studies of similar problems.

Models which quantitatively describe the transport and deposition of smoke plumes in an open environment and under the influence of gravity, wind shear and stratified atmosphere are far from satisfactory (see, e.g., Atmospheric Chemistry and Physics of Air Pollution by J.H. Seinfeld, Wiley Interscience, 1985, and Turbulent Buoyant Jets and Plumes ed by W. Rodi, Pergamon Press, 1982). Phenomenological models rely on an overall description of the problem using simplifying assumptions to reduce the governing equations, and a set of empirical constants to fit available experimental data collected at specific conditions. In all cases, atmospheric turbulence is assumed to be homogeneous, with Gaussian fluctuations, and the plume dispersion is shown to be Gaussian in the plane normal to the plume axis. The effect of the plume dynamics on its motion is vastly simplified in these analyses, and a number of empirical correlations are used to describe the trajectory of the plume as simple functions of atmospheric conditions. Some solutions of the Reynolds equations with simple closure have been obtained for vertical plumes. An accurate determination of the plume trajectory as a function of the smoke and atmospheric conditions, including the wind state and the stratification, is needed to determine the dispersion of smoke from the fire location.

Numerical methods for the simulation of flows of the type encountered in fire and smoke plume dynamics have become available, and can be used to (1) improve our understanding of the dynamics of plumes in cross flows and the effect of different environmental and fire conditions on there dispersion; (2) provide predictions of specific cases of interest; and (3) contribute, along with accurate experimental data, to the development of working models of these flows. Lagrangian vortex methods are particularly suited for the study of the dynamics of turbulent shear layers, jets and wakes; fields which are dominated by high concentration and continuous redistribution of vorticity including gravity-driven flows. Results of the numerical simulations have been compared with theoretical and experimental results showing the accuracy and high

temporal and spatial resolution of the methods. An attractive feature of these methods is their efficiency in dealing with unbounded flows. The adaptive form of the calculations allows one to simulate high Reynolds number flows in an infinite domain while concentrating all the effort around zones of strong gradients for long flow development time.

Research Plan. The mathematical model describing the problem of transport, dispersal and deposition of smoke plumes generated from large scale fires consists of the multi-dimensional unsteady Navier-Stokes and species transport equations at high Reynolds number. The proper normalization of these equations reduces the independent parameters of the problem: the mass flow rate, initial plume size, smoke flow/ atmospheric density ratio and the gravitational acceleration, into one parameter in the case of a uniform atmosphere. For a stratified atmosphere, one must introduce an extra length scale to characterize the variation of the density in which the smoke plume is flowing. We will start by computing the fall of a smoke plume from a specified height. Along the plume trajectory, this problem can be reduced to the integration of the unsteady, two-dimensional, inviscid Navier-Stokes equations describing the conservation of mass, momentum and energy of an incompressible fluid flowing in a gravitational field and under the influence of wind. In collaboration with NIST/CFR scientists, we will relax these assumption and extend the model to include more complex physics.

The transport element method, a vortex method for variable density flow, is a Lagrangian, grid-free field algorithm in which the gradients of the flow are discretized among elements of finite size. These elements are transported be (1) convection along material particle trajectories with the proper change in shape associated with the prevailing strain field; (2) local diffusion; and (3) change in strength according to the source terms in the governing equation. The values of the gas dynamic variables are obtained by direct summation over the individual fields of these elements. The method optimizes the computational effort by concentrating the numerical elements around zones of strong gradients. It maintains high resolution well into the late stages of flow development after very strong strains, high concentration of vorticity and sharp gradients have been generated in the flow, without introducing unacceptable values of numerical diffusion.

Numerical solutions will be obtained for models with progressively increasing degrees of complexity, i.e. with more interactions between the plume motion and the atmosphere retained in the model. Computations will be carried out in three phases:
In the first phase, attention will be focused on the problem of the settling of a wind-blown smoke plume flowing in a uniform atmosphere and falling on a flat terrain. Initial conditions regarding the distribution of smoke within the plume will be estimated from available models or experimental data, and solutions will be obtained for different values of the characteristic ratio between the buoyancy forces and the inertia of the plume fluid.

In the second phase, we will start the simulation from the fire and compute the rise of the smoke plume, its stabilization at a finite height above the ground and its fall onto the ground. In this case, atmospheric stratification is important and will be included in the model. Other effects, such as wind shear near the ground and particle aging within the smoke plume by coagulation will also be modeled.
In the third phase, we will include the effect of atmospheric fluctuations, non-flat ground terrain, particle settling with respect to the carrying fluid, vortex line curvature within the plume, the interactions between multiple plumes, finite-rate chemical interactions with the atmosphere, local effect of the plume on the atmosphere, etc.

In each phase, parametric analysis will be used to study the effect of fire conditions in terms of smoke flow rate, initial temperature, dimensions of the fire, initial smoke distribution, and atmospheric conditions in terms of the density and pressure and their variation with elevation, on the smoke plume trajectory and the smoke distribution on the ground. The reduction and presentation of the numerical results will be directed to serve the planning of the field tests of oil spill cleanup. Preliminary results, obtained at the end the p.i.'s stay at CFR/NIST during October-November 1989 and shown in Figure 1, reveal important consequences of the plume dynamics on the distribution of smoke on the ground. The distribution is far from Gaussian and is clearly influenced by the interaction between the vortex pair formed during the fall of the plume and the ground.

Reports and Papers:
(1)Ghoniem, A.F., Baum, H.R., and Rehm, R.G., "Vortex Simulation of Particulate Plume Dispersal and Settling," presented at the Int. Conf. Numer. Meth. in Fluid Dynamics, Oxford, England, July 1990.

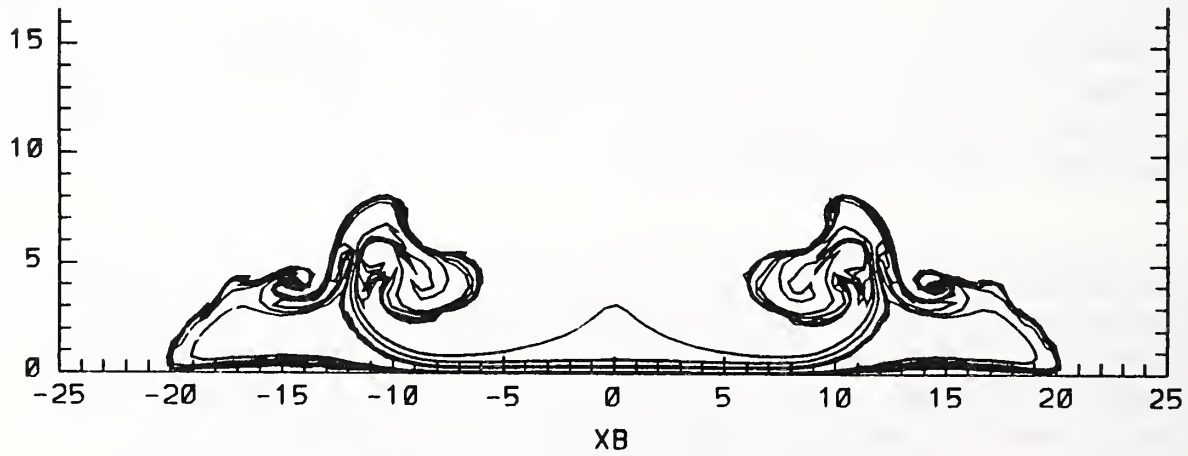


Figure 1. The ground distribution of smoke due to the fall of a negatively buoyant plume. The initial source is located one plume diameter above ground. The contours are constant density line and the highest density is at the centre of the plume.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution:	The University of Kentucky
Grant No.:	60NANB9D0960
Grant Title:	A Study of Crude Oil Combustion Supported on Water
Principal Investigator:	Kozo Saito Associate Professor Dept. of Mechanical Engineering
Other Professional Personnel:	Takao Inamura, Visiting Scientist Akihiko Ito, Visiting Scientist
NIST Scientific Officer:	Dr. Dave Evans

Technical Abstract:

This is a continuation of the project carried out as part of the NIST project on in-situ burning of crude oil (Project officer: D. Evans) [1,2]. In the 1989 project, the following two tasks were completed and summarized here [3-7]

One-dimensional model: A one-dimensional model to predict the time for water sublayer to start to boil was developed. The model includes heat transfer by conduction, evaporation, and in-depth radiation absorption. The governing equation is as follows:

$$\rho c(\partial T/\partial t) = \kappa(\partial^2 T/\partial x^2) + q_r \mu e^{-\mu x} \qquad (1)$$

Here ρ: density, c: specific heat, T: temperature, t: time, κ: thermal conductivity, x: vertical coordinate into fuel, q_r: average heat flux at the fuel surface, and μ: absorption coefficient. Equation (1) was solved using finite differences with the Crank-Nicolson scheme and Gauss-Seidel iteration. To predict the time for the water sublayer to start to boil, an accurate assessment of in-depth radiation absorption and heat feedback rate to the fuel surface is essential [6,9]. Thus, the heat flux was measured at the center of the pan by a Gardon-Gauge type heat flux meter with water cooling. The fuel surface level relative to the edge of the free board rim was controlled by operating a fuel level controller during combustion. To protect the heat flux meter from fuel splashes during the test, it was sheathed in a stainless steel cylinder whose exit height was kept above the fuel surface. Several different liquid fuels were tested in this system and the data obtained was used in the theoretical model.

HI Studies: In 1989 we were awarded a new Thermal Sensing Laboratory equipped with an optical bench, an HI system, an IR camera system and a Phase Doppler Particle Analyzer. A holographic interferometer connected to

a holography recording system can detect a sudden and sensitive temperature change occurring in a distributed area (see Fig. 1 for schematic illustration of the HI system used for the present studies). Contrary, the conventional thermocouple point-by-point measurement technique is incapable of satisfying these requirements, because of the effects of the wire disturbances on the flow and the limited spatial resolution of the thermocouple bead. We successfully obtained a series of interferograms from which a detailed temperature structure of the liquid layer (interferograms taken at three different times after ignition are shown in Fig. 2) can be resolved. Interestingly, these interferograms revealed Rayleigh convection near the fuel surface. This effect will be quantified and can be implemented in the theoretical model (Eq. 1). However, to understand large scale pool fires based on the results of the HI mesurements (which were carried out for small pool fires), the dependency of radiant heat on pool diameter and the dependency of the heat loss effects to the burner free board on pool diameter should be estimated correctly. This effect will be studied in the future.

To prevent boilover which is hazardous in large pool fires, a new method has been proposed by NIST. This method requires circulation of water under the burning oil layer, thus increasing the heat loss rate to the water sublayer. Boilover occurs when the water sublayer is superheated, therefore the circulating water restricts any large increase of temperature in the sublayer. Some researchers believe that boilover only occurs in small-scale pool fires but not in large-scale pool fires [12]. To verify this, the basic mechanism of boilover must be understood clearly, and this can be studied best in small-scale apparatus as they can be well controlled [13].

References

[1] D. Evans, G. Mulholand, D. Gross, H. Baum and K. Saito (1987). Environment Effects of Oil Spill Combustion, Proceedings of the 10th Arctic Marine Oil Spill Program Technical Seminar, Edmonton, Alberta, Canada, June 9-12.

[2] D. Evans, G. Mulholand, D. Gross, H. Baum and K. Saito (1988). Burning, Smoke Production, and Smoke Dispersion from Oil SpillCombustion, Proceedings of 11th Arctic Marine Oil Spill Program Technical Seminar, Vancouver, British Columbia, Canada, June 7-9.

[3] K. Saito (1988). A Study of Oil Slick Combustion, Final Report for Grant (#60NANB7D0739) submitted to National Institute of Standards and Technology.

[4] S.K. Elam, M. Arai, K. Saito and R.A. Altenkirch (1990). Cone Heater Test of Liquid Fuels, Fire Safety Journal, (in press).

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Supported on Water, Combustion Science and Technology, 71, 1-3, p.25.

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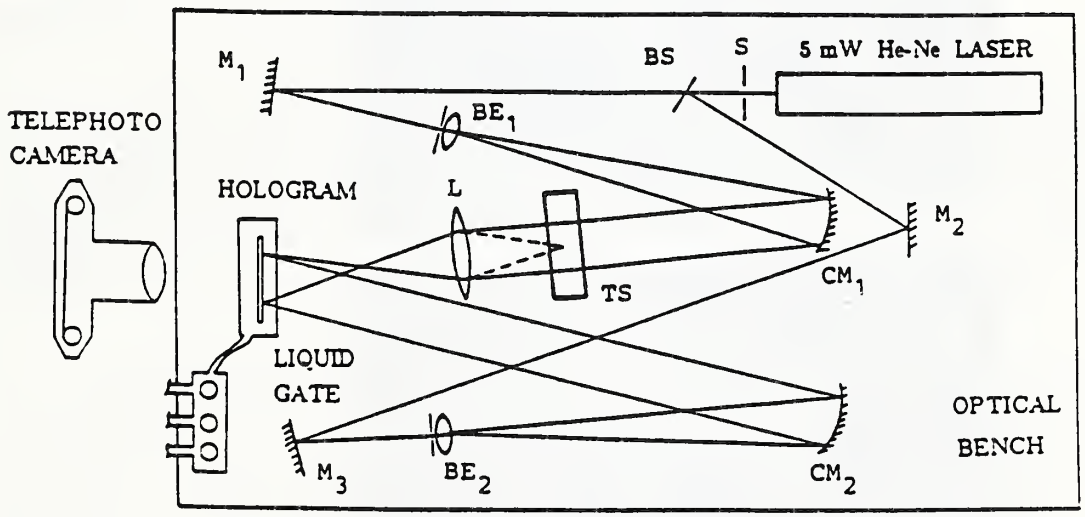
[7] S.K. Elam, R.A. Altenkirch and K. Saito (1990). Design of a Radiant Strip Heater for Use of Flame Spread Tests on Liquid Fuels, Fire

Technology, 26, p. 156.
[8] A. Ito, D. Masuda and K. Saito (1989). Holographic Interferometry Temperature Measurement of Liquid Phase under Spreading Flame Conditions, the 26th National Heat Transfer Conference, Philadelphia, PA, August.
[9] A. Ito, D. Masuda and K. Saito (1990). A Study of Flame Spread Over Alcohols Using Holographic Interferometry, Combustion and Flame, (in press).
[10] A. Ito, T. Inamura, K. Saito and D. Evans (1990). Temperature Structure of Liquid Phase in Pool Fires Supported on Water: Implication to Boilover Phenomenon, Poster Session of the 23rd Symposium (International) on Combustion, Orleans, France, July 22-27, 1990.
[11] K. Saito, Final Report for NIST Grant # NANB9D0960 (to be submitted).
[12] H. Koseki, G. Mulholland and T. Jin, The Joint Study Between NIST/CFR, the 11th UJNR Meeting on Fire Safety, San Francisco, CA, 1989.
[13] F.A. Williams, Combustion Theory, 2nd ed., Benjamin/Cummings, 1985.



S: Shutter BS: Beam splitter BE: Beam expander

CM: Concave mirror M: Mirror L: Lens

Fig. 1 Optical system used for holographic interferometry.

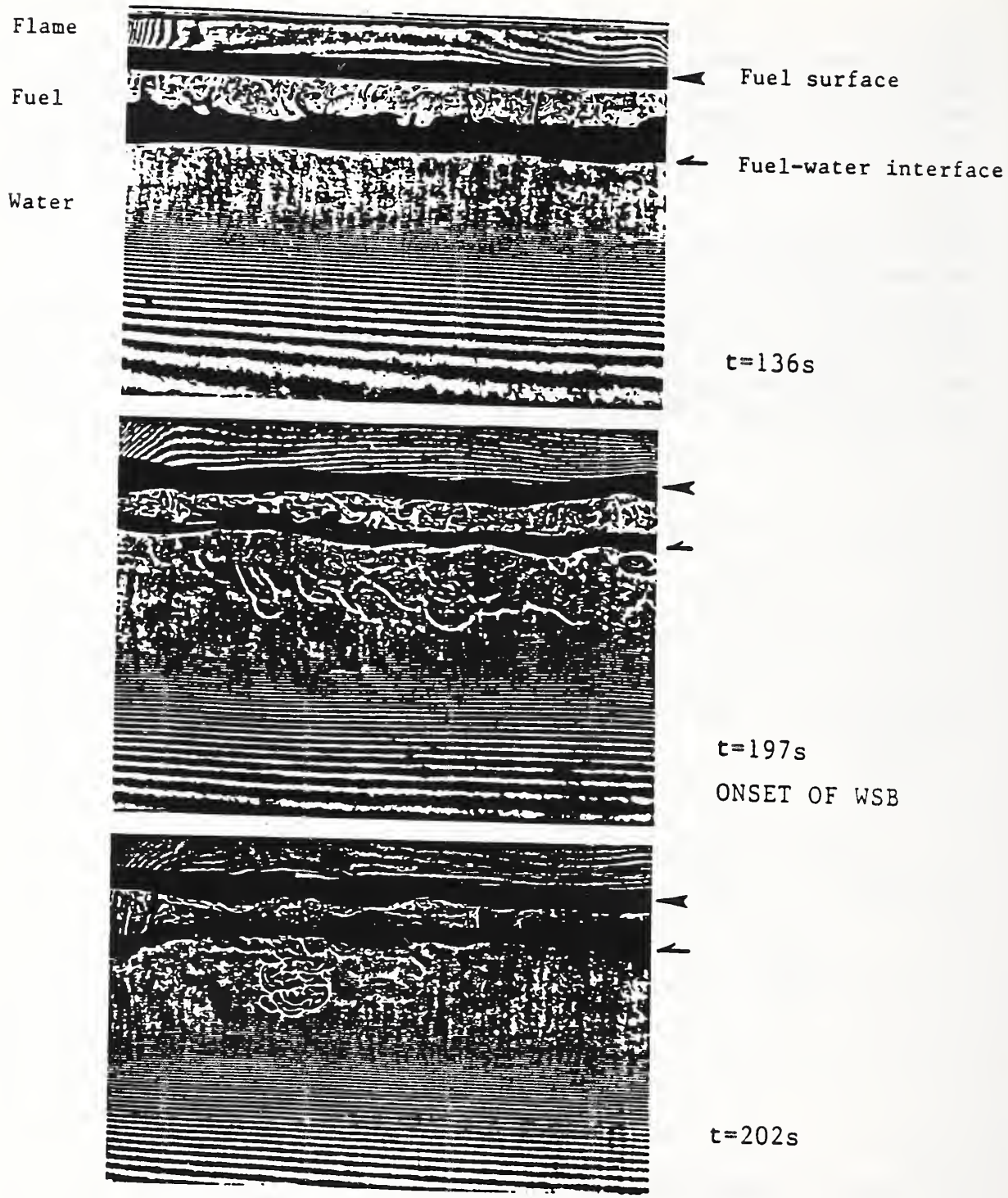


Fig. 2 Three different interferograms obtained at time, t=136s, 197s (onset of boiling of water sublayer:WSB) and 202s after ignition using a rectangular tray of 0.5cm wide and 5cm long. Initial fuel temperature:297K and fuel:n-decane.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

Institution: University of Maryland, College Park

Grant No.: 60NANB8D0834

Grant Title: An Investigation of Simulated Oil Well Blowout Fires

Principal Investigator: Professor J. P. Gore
Mechanical Engineering Department
University of Maryland
College Park, MD 20742
Telephone: (301) 405-5288

Other Professional Personnel: S. M. Skinner (M. S. Candidate)
C. Q. Jian (Ph. D. Candidate)
Dr. Y. R. Sivathanu (Research Associate)

N. I. S. T. Scientific Officers: Dr. D. D. Evans

Technical Abstract:

The overall objective of this project is to develop capabilities for predicting radiative heat flux surrounding oil well blowout and diverter fires and effects of water suppressant. Two aspects of this project were addressed during the past year: (1) direct evaluation of rules for obtaining state relationships for fuel mixtures using those for pure fuels; and (2) numerical prediction of trajectories of buoyant horizontal turbulent jet flames and evaluation using new experimental data.

State Relationships for Fuel Mixtures: Typical oil well blowout and diverter fires involve simultaneous non-premixed combustion of two or more gaseous and liquid fuels. In order to construct state relationships for a variety of possible fuel mixtures using those for pure fuels, a simple mixing rule was devised. This rule involves the assumption that the two or more fuels react with air independent of each other and the products of their individual reactions mix to produce the products of the reaction of the fuel mixture. In order to evaluate this mixing rule, measurements of gas species concentrations in four coflow laminar jet diffusion flames burning mixtures of methane and acetylene were conducted. Two gaseous fuels were selected for simplicity. Methane to represent the natural gas in oil well fires and acetylene to represent a second fuel component which may have high sooting tendency.

Due to the high sooting tendency of acetylene, a sampling probe/scheme capable of obtaining gas samples in spite of clogging by soot particle was designed. Figure 1 shows a

schematic of this sampling system. The design relies on the simple principle that the flow that clogs the probe also carries the gas sample. The sampling system consists of a quartz microprobe (250 μm and 350 μm orifice sizes were used) connected to an evacuated (typically to 0.3 atm.) and purged (with the carrier gas helium) sampling bulb with an isolation valve. A purge line carrying a small flow of helium is also connected to the probe. The sampling bulb is equipped with an evacuation port, a carrier gas pressurizing line, an absolute pressure gauge and a sampling septum. During operation, the probe is inserted to a desired location within the flame while carrying a small (just to maintain the overpressure) purge flow of helium. The bulb is isolated during this process. Once the probe is at the desired location, the purge flow is shut off and the bulb isolation valve is opened. The pressure inside the bulb is monitored. If the probe does not clog, then the sampling ends when the pressure in the bulb reaches 1 atm and a gas sample is removed for routine chromatography. If the probe clogs, the bulb reaches a constant subatmospheric pressure. At this time, the isolation valve is shut off and a flow of helium is started through the pressurizing valve to bring the bulb pressure to 1 atm. The amount of sample collected is known from the pressure reading at the time of clogging. A sample from the bulb is now removed for analysis. The bulb is then evacuated and purged with helium for the next measurement. This probe has been successfully operated in the highest soot concentration regions of acetylene/air diffusion flames. To our knowledge, gas sampling within this region has never been possible before.

Fig. 2 shows measurements of gas species concentrations in a flame burning 27 % methane in acetylene with air plotted as a function of local mixture fraction. The concentrations of N_2, O_2, CH_4, C_2H_2, CO_2 and CO are seen to correlate very well. Several measurements were conducted at three different heights from the burner exit and observed to correlate similar to those shown in Fig. 2 supporting the laminar flamelet concept for fuel mixtures. The lines shown in Fig. 2 represent the mixing rule based on past measurements of species concentrations for the pure fuels. If the present measurements for the pure fuels are used, then good agreement between the mixing rule and the data for CO and CO_2 is also observed. These findings have established a convenient method for estimating the major gas species concentrations in flames burning fuel mixtures.

Buoyant Horizontal Turbulent Diffusion Flames Diverter fires near oil well platforms pose hazards to structures and personnel surrounding them. The flame structure is complicated by the effects of buoyancy turbulence interactions. This flame configuration has received very little attention in the literature. We have developed a parabolic finite difference scheme using a grid that adapts to the jet trajectory as it turns under the action of buoyancy. Fig. 3 shows the predictions of the flame centerline trajectory using the present method compared with measurements (based on visible flame trajectory) for flames

with initial Reynolds numbers varying by a factor of 3. The agreement between measurements and predictions is very encouraging.

Measurements of flame surface intermittency using 30 (out of 9000) randomly selected digitized images show that buoyancy increases the intermittency significantly for all three Reynolds numbers. Thus buoyancy-turbulence interactions are expected to be important in this flow and are being addressed.

Reports and Papers:

1. J. P. Gore, D. D. Evans and B. J. McCaffrey, 1990, "Temperature and Radiation of Diffusion Flames with Suppression," Comb. Sci. Tech., in press.
2. J. P. Gore, S. M. Skinner, D. W. Stroup, D. Madrzykowski, and D. D. Evans, 1990, "Radiation Properties of Large Two Phase Flames," Comb. Sci. Tech., submitted.
3. J. P. Gore and S. M. Skinner, 1990, "Mixing Rules for State Relationships of Methane and Acetylene/Air Flames," Comb. Flame, submitted.
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5. J. P. Gore and C. Q. Jian, 1990, "Flame Trajectories of Buoyant Horizontal Jet Flames," ASME/JSME Joint Thermal Engineering Conference, Reno, NV, submitted.
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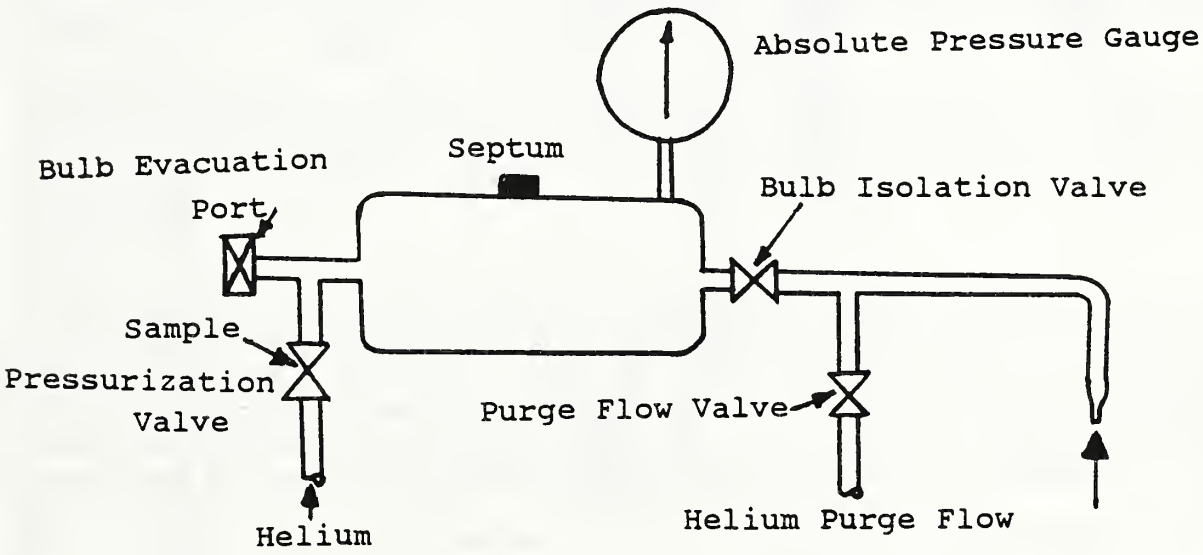

Figure 1: Gas Sampling System for Heavily Sooting Flames.

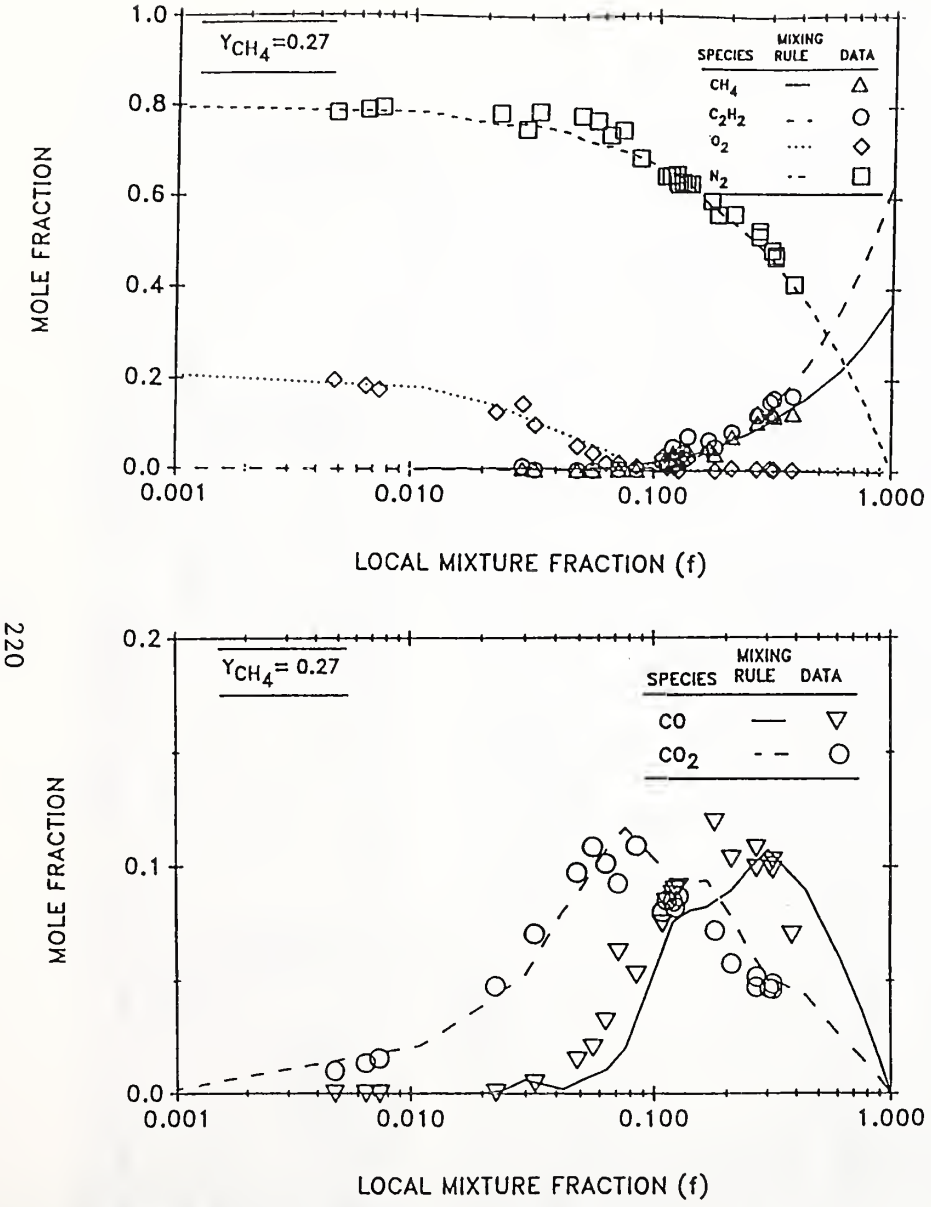

Figure 2: State Relationships for C_2H_2/CH_4 Mixture Flames.

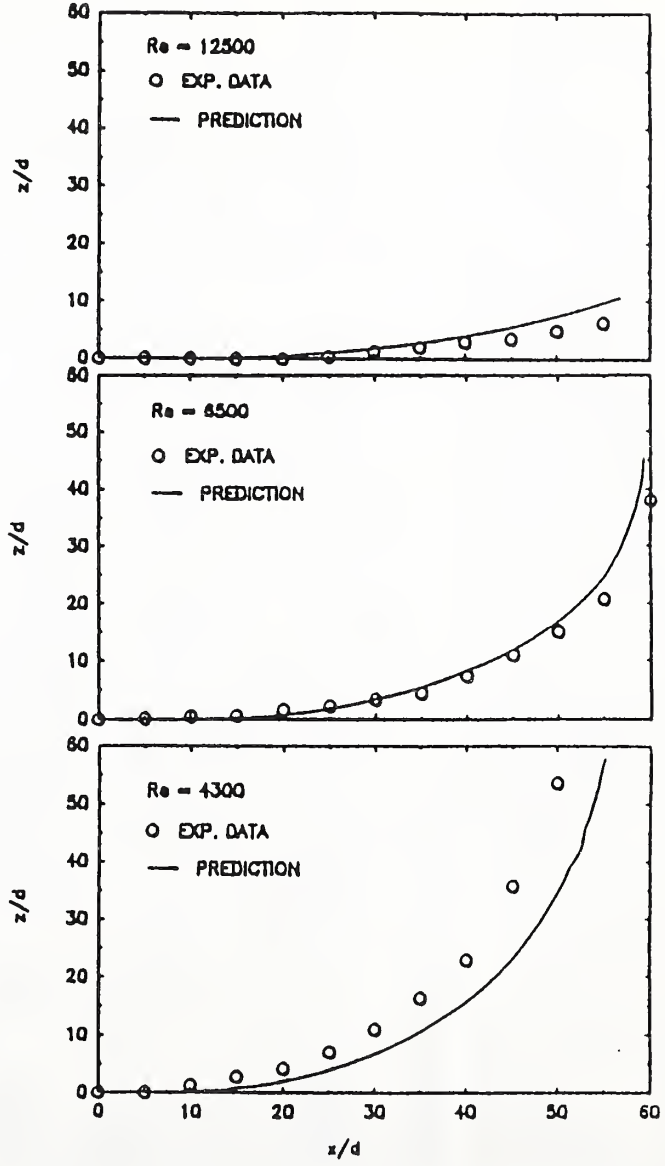

Figure 3: Centerline Trajectories of Horizontal Jet Flames.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

THE DEVELOPMENT OF SPRINKLER EFFECTIVENESS METHODOLOGY FOR THE GSA ENGINEERING FIRE ASSESSMENT SYSTEM

Funding Agency: U.S. General Services Administration

Professional Staff: Daniel Madrzykowski, Project Leader
Robert Vettori, Fire Protection Engineer

Project Objective:
To acquire data on heat release rates required as input to the GSA fire hazard assessment system and develop the methodology to incorporate sprinkler effectiveness into the system.

Technical Accomplishments:

Under the sponsorship of GSA, the Center for Fire Research has conducted several studies related to the performance of sprinkler systems in office/residential occupancies. These have included 1) investigating the applicability of quick response sprinklers in offices, 2) determining the effect of sprinkler sprays on the burning rate of idealized fuels and 3) examining the conditions effecting the operation of sprinklers. Concurrent with these studies, an engineering fire hazard assessment system (FPETOOL) was developed to evaluate hazard and fire protection strategies in GSA buildings. Although FPETOOL can be used to evaluate a wide range of conditions, it does not specifically address fire suppression. The results of these sprinkler studies are intended to provide a basis for fire suppression prediction in FPETOOL.

30 large scale fire tests were performed under an oxygen consumption calorimetry hood to determine the heat release rate (HRR) of fuel packages with and without sprinklers. Fuel packages included work stations, office furnishings, paper recycling hampers and wooden cribs. Each fuel package was tested under free burn conditions to obtain HRR curves.

The HRR measurements were repeated individually to determine the effect of water spray. The sprinkler was manually activated when the HRR of the fuel package was between 90 and 100 percent of its free burn peak HRR. The average water spray density over the fuel package floor area was 4.07 mm/min
(0.1 gpm/ft^2).

To arrive at the sprinkler effectiveness methodology, the HRRs measured during suppression were divided by their respective free burn HRRs. This yielded normalized values for the reduction of HRR for all of the fuel packages. A first order sprinkler effectiveness curve was constructed by determining the maximum normalized HRR, from all of the tested fuel packages, for the 10 minute period after sprinkler activation. Further testing will be done in FY91 to evaluate the limitations of these results as a basis for a sprinkler effectiveness methodology for use in FPETOOL.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

THE HAZARD OF FIRE GAS EXPOSURE FROM SPRINKLERED ROOMS TO CORRIDORS AND ADJOINING AREAS

Funding Agency: U.S. General Services Administration

Professional Staff: Daniel Madrzykowski, Project Leader
Robert Vettori, Fire Protection Engineer

Project Objective:

To investigate and quantify sprinklered fire exposure on an exit corridor and on spaces adjacent to that corridor.

Technical Accomplishments:

Large scale tests were performed to determine the effect of sprinklers on the hazardous effluent from a burn room. The burn room contained wooden cribs with a free burn peak heat release rate of 1 MW. The burn room was located at one end of a 40 foot long corridor with a target room adjoining the corridor at the opposite end. The target room was separated from the corridor by a simulated "normal door" with a 0.25 inch opening along both the top and one side of the door and a 0.50 inch undercut. The burn room, corridor, and target room were instrumented so that temperatures and concentrations of oxygen (O_2), carbon monoxide (CO) and carbon dioxide (CO_2) could be recorded in each area. Additionally video records of each space were made during the tests.

A sprinkler was installed in the center of the ceiling of the burn room and three sprinklers were installed along the center axis of the corridor. Both standard and quick response sprinklers were used during the testing. The sprinklers activated automatically during these tests. Tests were conducted utilizing either the sprinkler in the burn room or the sprinklers in the corridor. In either case only one sprinkler was activated. Six of the nine tests were conducted with the fuel burning under a 4 ft by 4 ft shield to inhibit suppression by the sprinkler.

During the control burns (no sprinklers) untenable conditions were measured in the corridor and incapacitating conditions were measured in the target room. However these conditions were mitigated during all the tests which had an active sprinkler. In all of the sprinklered tests, the fire or its products had a minimal effect on the conditions in the target room.

Reports and Publications:
Final Report will be issued in 1991.

Related Grants:
None

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT-1990

MEASUREMENT OF CONDITIONS RESULTING FROM A FLAMING FIRE IN A SIMULATED NIH HOSPITAL ROOM PROTECTED BY AUTOMATIC FIRE SPRINKLERS

Funding Agency: National Institutes of Health

Professional Staff: Kathy A. Notarianni, Project Leader
Doug Walton, Fire Protection Engineer
Robert Vettori, Fire Protection Engineer

Project Objective:

To generate a data bank of measured fire exposures and combustion product concentrations occurring at the patient location, as well as activation times of various automatic sprinklers and smoke detectors for NIH so that it can be determined if smoke detectors should be used to alert nursing staff prior to the activation of the sprinklers.

Technical Accomplishments:

The minimum size flaming fire in terms of rate of heat release that could cause potentially harmful conditions in a patient room was determined through propane burner tests in a simulated NIH Clinical Center Hospital room along with computer modeling using Hazard I, and FPE tool. 60 kw was determined to be the critical fire size.

Burns of various fuel packages were conducted under a calorimeter in order to identify a package with a nominal 60 kw rate of heat release. This was determined to be a wood crib approximately 18" x 24" x 6" high, weighing about 17lbs.

A series of 5 full-scale fire tests were conducted to measure temperatures, radiation, and carbon dioxide, carbon monoxide, and oxygen concentrations resulting from the flaming wood crib fires within the simulated NIH Clinical Center Hospital room protected with automatic sprinklers. Extensive records of test measurements were taken which include measured time for activation of smoke detectors and "dry" sprinkler heads located throughout the room.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

COMPARTMENT FIRE MODEL TO SIMULATE THE EFFECT OF
ROOF VENTS, SPRINKLERS, AND THEIR INTERACTIONS

Funding Agency: AAMA Research Foundation

Professional Personnel: Leonard Y. Cooper, Project Leader
William Davis, Physicist

Program Objectives

Development of a computer fire model for engineering analysis of roof vents, sprinklers and their interactions during fire-generated environments.

Technical Accomplishments

The generic fire scenario to be analyzed is depicted in Figure 1. The analysis and the corresponding computer code must capable of simulating smoke layer growth in a curtained area of a building space. The action of fusible-link-actuated ceiling vents on the fire environment is taken into account. The model also takes account of first sprinkler actuation by a fused link and the effect of subsequent sprinkler-spray cooling of the accumulating ceiling-

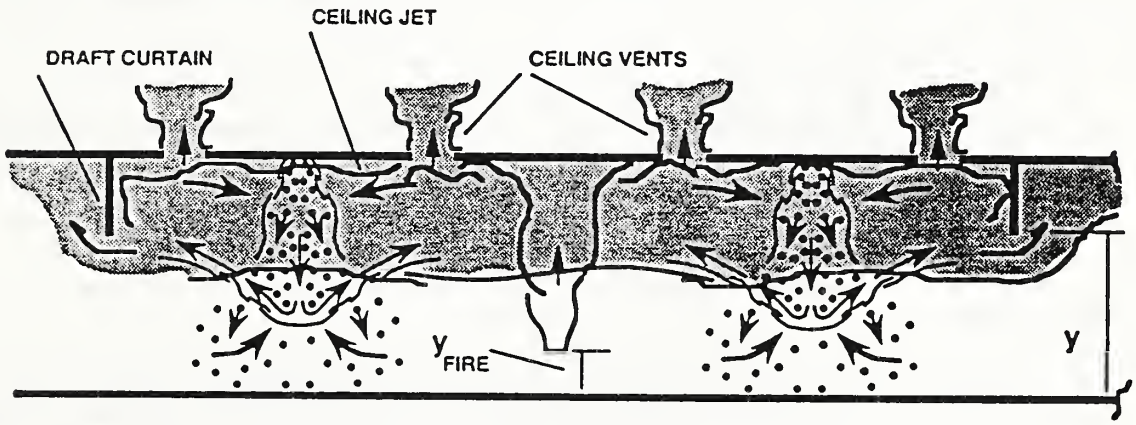

Figure 1. Fire in a building with draft curtains and fusible-link-actuated ceiling vents and sprinklers.

level smoke layer on subsequent sprinkler link responses. The fire is assumed to be specified. The goal is to predict the effects of various vent deployment and actuation schemes within the sprinkler-operating environment.

The work of developing the computer model has been divided into two major stages. Each stage involves the formulation of mathematical algorithms for particular aspects of the problem, the development of their solution in terms of computer code, and the demonstration of the computer code to yield sound and consistent results over a range of parameters.

Stage 1: The effect of roof venting on the actuation of sprinkler links.

Stage 2: Stage 1 with the added effect of sprinkler spray discharge.

Work on Stage 1 was completed last year. This resulted in the user-friendly computer code LAVENT (Link Actuated VENTs) and a comprehensive User Guide (NISTIR 89-4122). This code implements the model equations developed and presented in [1]. LAVENT simulates the fire environment and the response of arbitrarily deployed fusible-links, as depicted in Figure 1, up to the time of actuation of the first sprinkler. Reference [2] describes a parametric study of fusible-link actuation which was carried out with LAVENT. The Stage-2 effort has led to an improved version of LAVENT which can receive a modular subroutine for simulating the interaction of an isolated sprinkler and an upper layer of arbitrary temperature and thickness. A preliminary submodel for the sprinkler/layer interaction phenomenon was completed [3]. Combining a computerized version of the final submodel and the improved LAVENT will lead to the fire model computer code LAVENTS (Link-Actuated VENTs and Sprinklers).

Reports and Publications

1. "Estimating the Environment and the Response of Sprinkler Links in Compartment Fires with Draft Curtains and Fusible Link-Actuated Ceiling Vents - Theory," Cooper, L.Y., Fire Safety Journal 16 (1990) pp. 137-163.

2. "A Computer Model for Estimating the Response of Sprinkler Links to Compartment Fires with Draft Curtains and Fusible-Link-Actuated Ceiling Vents, Davis, W.D. and Cooper, L.Y., submitted for outside publication.

3. "Sprinkler/Hot Layer Interaction - A Preliminary Model," Heskestad, G., FMRC Report to NIST under Grant 60NANBOD1006, June 27, 1990.

Related Grants

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

2. Sprinkler/ Hot Layer Interaction, Heskestad, G. Factory Mutual Research Corporation.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 90

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

Grant No.: 60NANB7D0743

Grant Title: Flow Through Horizontal Vents as Related to Compartment Fire Environments

Principal Investigator: Professor Yogesh Jaluria
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New Brunswick, NJ 08903
Telephone: (908)932-3652

Other Professional Personnel: A. Abib (Ph.D. Student)
Q. Tan (M.S. Student)
K. Kapoor (Visiting Investigator)

NIST Scientific Officer: Dr. Leonard Y. Cooper

Technical Abstract:

Introduction The flow through horizontal vents, such as ceiling or floor vents in a multi-room compartment, is of considerable importance in the mathematical modeling of fires in such enclosures. The flow of the combustion products out of the room and the mass flow rate of oxygen being added to the room due to the flow through the vent are important inputs for studying the changing environment in the room. A density difference $\Delta\rho$, with heavier fluid overlying lighter fluid, arises across the opening due to the heating up of the gases in the enclosure containing the fire. Similarly, a pressure difference Δp is generated across the vent, with the pressure in the enclosure higher than the atmospheric pressure. Therefore, the resulting flow rate through the vent as a function of $\Delta\rho$, Δp and the thickness to diameter ratio L/D of the vent is of direct relevance to fire research.

The flow through horizontal vents, as related to enclosure fires, has been considered in terms of available literature on such flows. However, though work has been done on buoyancy-driven vent flows for the special case of $\Delta p=0$, very little information is available for a nonzero pressure difference, which is of particular interest to vented room fires. Work has also been done on flows due to an applied pressure difference Δp, with no buoyancy effects. The present study was initiated on September 29, 1989, to determine the flow exchange across horizontal vents for arbitrary $\Delta\rho$, Δp and L/D, in order to provide the necessary inputs for fire modeling studies.

Experimental Approach An experimental system has been designed and fabricated, employing a fresh-water/salt-water flow arrangement, to determine the flow through a horizontal vent for circular and rectangular vents, over wide ranges of the variables $\Delta\rho$, Δp and L/D. Figure 1 shows a schematic of the experimental arrangement. The upper region of the tank is filled with the higher density salt water, or brine, and the lower region with fresh water. The tank is 0.74 m long, 0.44 m wide and 0.62 m high, with

the horizontal partition at 0.31 m from the bottom. The tank is made of Plexiglas so as to allow flow visualization, for which a dye or a shadowgraph is used. Plexiglas tubes of different lengths and diameters are used to yield a variety of L/D ratios. The density difference ratio $\Delta\rho/\bar{\rho}$, where $\bar{\rho}$ is the mean density, can be varied up to around 0.2. This value is approximately the same as that obtained by a temperature difference of 100K in gases, with 500K as the average temperature.

The pressure difference Δp is imposed by moving the storage tank for fresh water, shown in the figure, up or down. The resulting pressure difference across the vent, in the quiescent environment far from the flow region, is measured by means of a low pressure differential transducer made by Omega. The flow rate across the vent over a given time interval is obtained by opening the vent over the specified period of time, mixing the fluid in the upper region after closing the vent and measuring the density with a hydrometer, employing hydrometers with different ranges for accurate results. Thus, the average flow rate across the vent over the given time interval is obtained. The velocity level can also be measured with a hot film anemometer, which is suitably calibrated.

Preliminary Results Some of the important preliminary results obtained are discussed here. 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 Δp was increased, this downward flow was found to decrease, ultimately leading to a unidirectional upward flow. This purging, or flooding, pressure difference Δp_c is of order $g\Delta\rho L$, where g is the magnitude of gravitational acceleration. Thus, for typical values of L=0.1 m and $\Delta\rho=100$ kg/m^3, $\Delta p_c=98$ N/m^2. This is a very small pressure differential and accurate measurements are difficult. Differential pressure transducers of around 250 N/m^2 full scale are being used for these measurements.

Figure 2 shows the measured variation of the density ρ_H of the heavier fluid with time t, for $\Delta p=0$. With increasing time, the density difference $\Delta\rho$ decreases and this is reflected in a decrease in the flow rate Q across the vent into the upper region. This flow rate Q is proportional to the rate of decrease in ρ_H, averaged over a chosen time interval. The average values of the gradient over the duration of the entire experiment are given in the figure. A comparison with earlier work on this circumstance indicated good agreement, as seen in Fig. 3. The dependence of Q on L/D follows the trend predicted by analysis in the earlier studies, lending support to these measurements.

For the nonzero pressure case, Fig. 4 shows a few results. The pressure Δp_s given here is the static pressure measured across the vent before the vent is opened. The pressure difference Δp that arises after the vent is opened is much smaller due to head loss in the pipes and the system is being instrumented for an accurate measurement of Δp. For large values of Δp the flow across the vent is unidirectional upward or downward, depending on the pressure imposed across the vent. The flow is unidirectional, upward, in both the cases shown. At small pressure differences, less than the purging pressure as mentioned earlier, a bidirectional flow exchange arises. The flow rate across the vent in this case is obtained from a measurement of the variation in the density ρ_H of the denser fluid, knowing the initial densities and volumes of the two regions and the measured volume inflow into the lower region. Some experiments have been conducted for this case. For the unidirectional flow circumstance, Q has been obtained as a function of the physical variables of the problem. As seen in Fig. 4, Q increases with Δp_s. This is reflected in a higher rate of decrease in ρ_H at a larger imposed pressure difference.

Further work is presently being continued on this interesting and important flow circumstance to characterize the flow rate across horizontal vents as a function of $\Delta\rho$, Δp

and L/D. The results will be obtained in dimensionless terms so as to allow their applicability to a wide range of situations arising in compartment fires.

Reports and Papers

1. Y. Jaluria and L,Y. Cooper, "Negatively Buoyant Walls Flow Generated in Enclosure Fires," Prog. Energy Combust. Sci., 15, 159-182, 1989.
2. Y. Jaluria and K. Kapoor, "Downward Turning of a Ceiling Jet in an Enclosure Fire," Proc. Fall Tech. Meeting, Eastern Sect. Combust. Inst., Albany, NY, Paper No. 56, 1989.
3. Y. Jaluria and K. Kapoor, "Wall and Corner Flows Driven by a Ceiling Jet in an Enclosure Fire," submitted, 1990.
4. K. Kapoor and Y. Jaluria, "Flow Characteristics of a Downward Turning Buoyant Ceiling Jet," submitted, 1990.
5. K. Kapoor and Y. Jaluria, "Thermal Transport from a Heated Ceiling Jet Near the Corner of a Compartment," submitted, 1990.

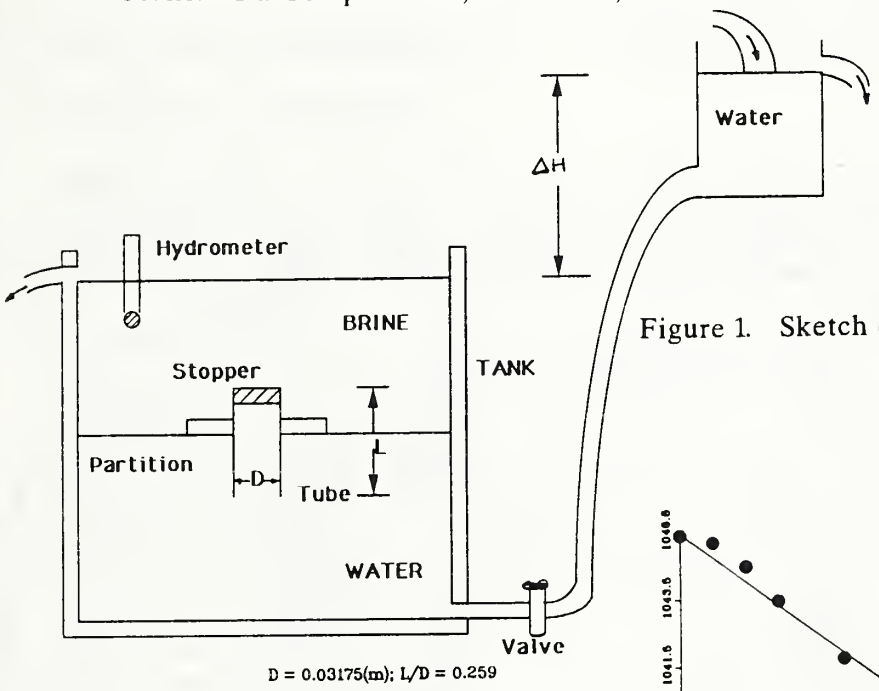

Figure 1. Sketch of the experimental arrangement.

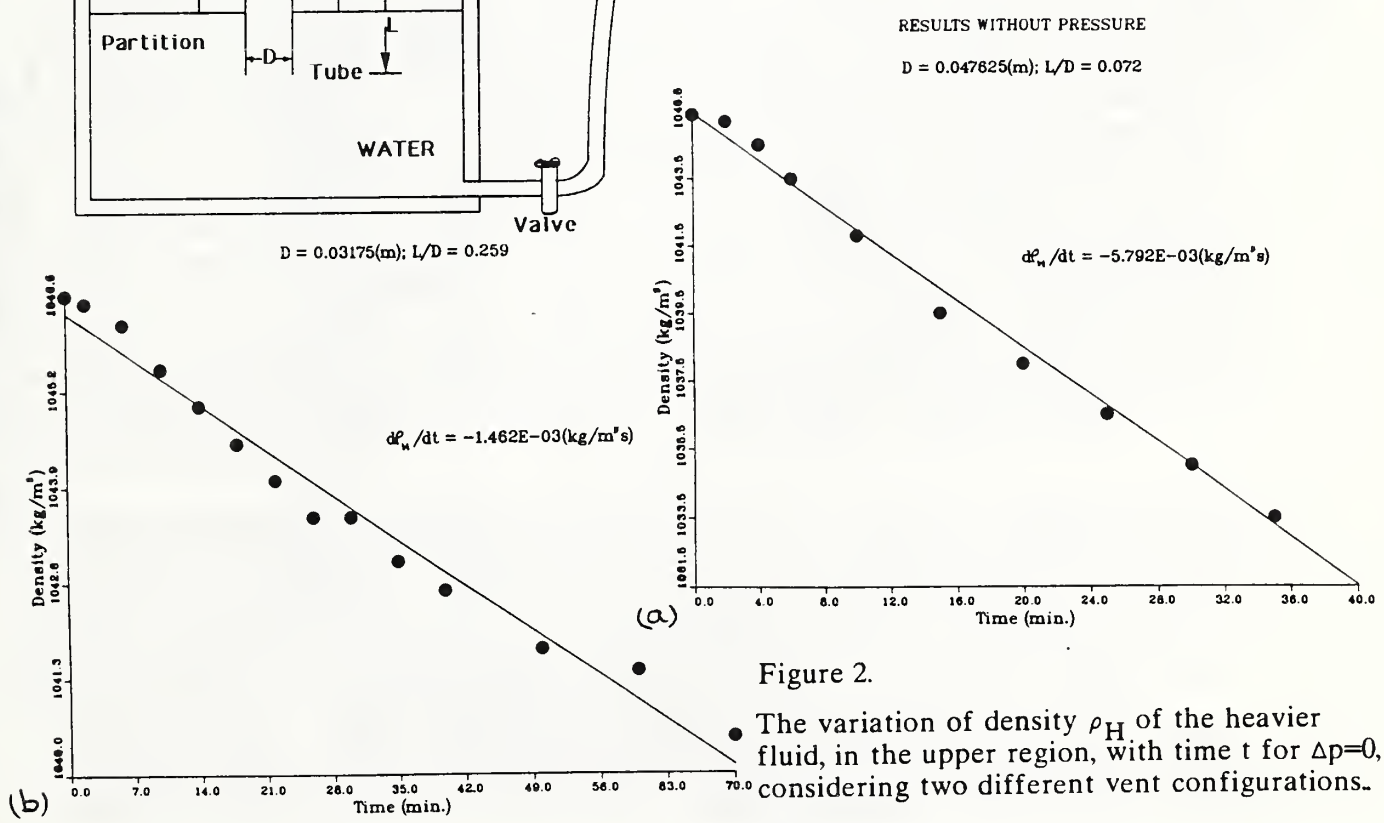

Figure 2.

The variation of density ρ_H of the heavier fluid, in the upper region, with time t for $\Delta p=0$, considering two different vent configurations.

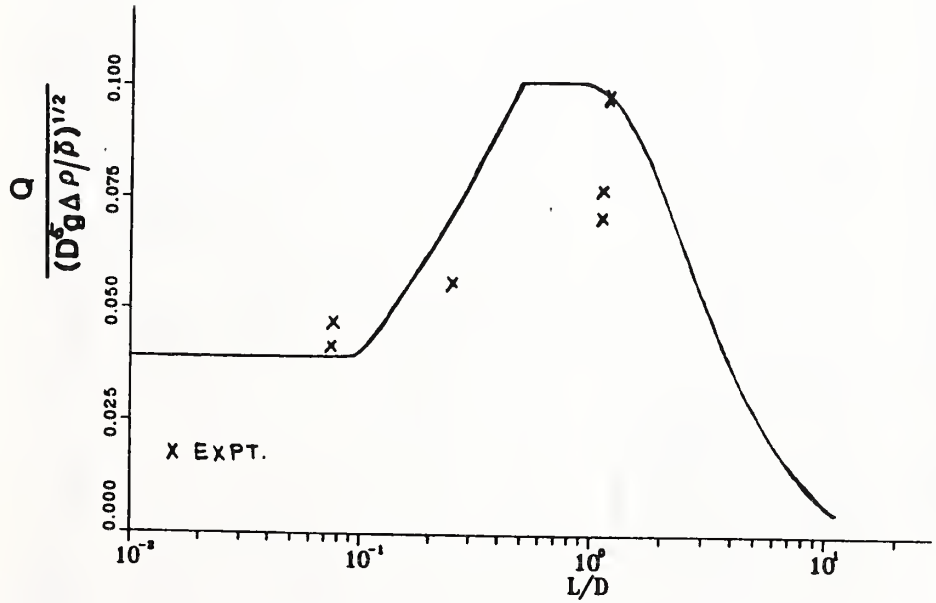

Figure 3. Flow rate Q across a horizontal vent for $\Delta p=0$ as a function of L/D. The curve shown is from Epstein (J. Heat Transfer, 110, 885-893, 1988).

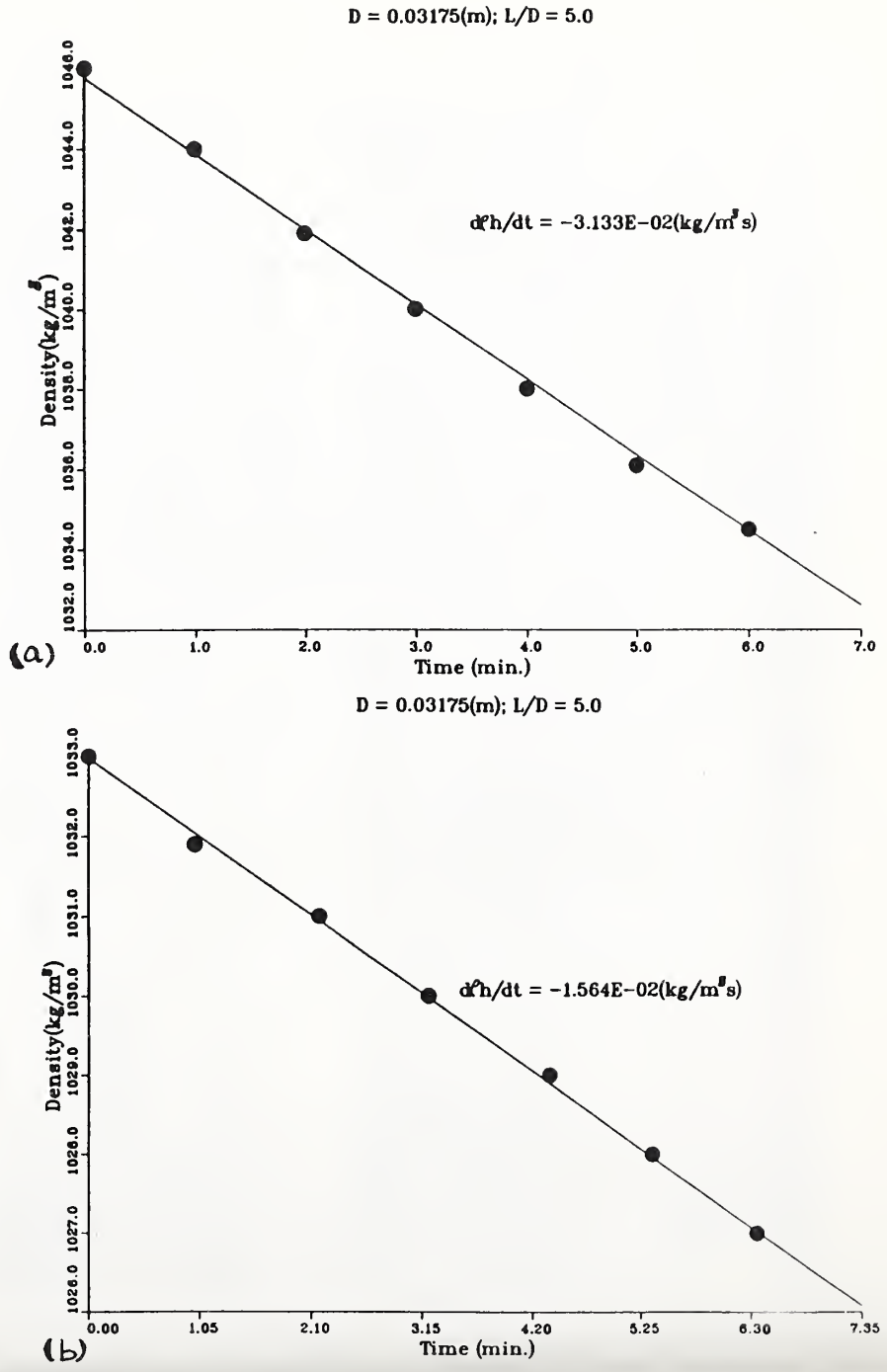

Figure 4. The variation of density ρ_H with time t for nonzero pressure difference Δp_s. (a) $\Delta p_s = 867.3$ N/m^2; (b) $\Delta p_s = 458.1$ N/m^2.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY90

Institution:	Factory Mutual Research Corporation
Grant No:	60NANB0D1006
Grant Title:	Sprinkler/Hot Layer Interaction

Principal Investigator: Dr. Gunnar Heskestad
Factory Mutual Research Corporation
1151 Boston-Providence Turnpike
Norwood, MA 02062

NIST Scientific Officer: Dr. Leonard Y. Cooper

Technical Abstract:

The Objective is to develop a submodel, to be incorporated in a two-layer zone model, for the evaporation of water from a sprinkler spray with associated cooling effects and for mass transfer, generated by the spray, between the two layers.

Introduction It is visualized that there is an upper layer of hot fire gases of uniform temperature under the ceiling of the compartment and a lower layer of relatively cool gases of uniform temperature extending to the floor. A single sprinkler operates near the ceiling within the upper layer. The spray entrains hot gases from the upper layer, producing a vertical jet toward the layer interface. The gases in the jet have increased water content and reduced temperature relative to the quiescent hot layer because of evaporation of water drops. After the jet penetrates the interface, it is surrounded by cool air and experiences an upward, buoyant force which eventually reverses the downward flow back into the upper layer, in the process entraining air from the lower layer. The basic information required includes the evaporation rate of water and associated cooling effect, together with the mass transfer rate from the lower layer to the upper layer from which the contribution to cooling of, and mass addition to the upper layer can be calculated.

Accomplishments Entrainment of gas (air) into a water spray has been treated by Heskestad et al. [1,2] Penetration of a jet across a density interface has been investigated by Turner[3], and entrainment of fluid of the penetrating jet into the layer from which it projects from the other side of the density interface, has been studied by Baines.[4] Finally, Yuen and Chen[5] have established heat-transfer correlations for evaporating liquid drops which make it possible to calculate evaporation and cooling rates. The various pieces have been adapted and assembled to produce the required prediction method.

Jet penetration and air entrainment from the lower layer are governed by a Froude number, the latter based on the velocity and width of the spray-entrained gas flow at the interface level and the density difference between the gas in the spray and the lower layer. Sample calculations are presented in Figures 1 and 2 for a 1/2 in. standard sprinkler discharging 1.89 l/s (30 gpm) at ceiling level, with nominal characteristics of spray angle, initial spray momentum, and drop size. Figure 1 presents penetration depth δ_p versus the difference in temperature between the gas phase in the spray (T_s) and the lower layer (T_ℓ). Various smoke layer depths are reported: 0.35 m, 0.71 m, and 1.41 m. Except for the smallest depth, temperature differences are rather small for significant penetrations. Once penetration begins to occur as temperature differences decrease, the penetration depth increases rapidly with further decreases. Figure 2 presents associated volumetric entrainment rates from the lower layer ($\dot{V}_e$), including a brief table for reference showing entrained flow rates in the spray at the interface level ($\dot{V}_s$). Significant entrainment rates from the lower layer develop as the temperature differences between the gas in the spray and the lower layer is reduced.

The evaporation and cooling model assumes that the bulk of the contributing water drops are evaporating in a quasisteady state, thermodynamically, so that the heat transfer results only in drop vaporization. Best agreement with experimental cooling data is obtained assuming an effective drop diameter equal to 55 percent of the volume mean diameter of the drop population. Figure 3 presents a comparison of calculated and experimental[6] spray cooling rates, Q_s. The experiments represented in the figure involved two sprinkler sizes, three water discharge rates, and three heat release rates. Input parameters for the calculations included upper layer thickness and temperature in freeburn, lower layer temperature, sprinkler diameter and discharge rate, and spray diameter at the interface to the lower layer.

Some refinements of the model remain.

References

1. Heskestad, G., Kung, H.C. and Todtenkopf, N.F. "Air Entrainment into Water Sprays and Spray Curtain," ASME Paper 76-WA/FE-40, American Society of Mechanical Engineers, 1976.
2. Heskestad, G., Kung, H.C. and Todtenkopf, N.F., "Air Entrainment into Water Sprays," RC77-TP-7, Factory Mutual Research Corporation, November 1977.
3. Turner, J. S., "Jets and Plumes with Negative or Reversing Buoyancy," J. Fluid Mech., 26 (1996), pp. 779-792.
4. Baines, W.D., "Entrainment by a Plume or Jet at a Density Interface," J. Fluid Mech. 68 (1975), pp. 309-320.
5. Yuen, M.C. and Chen, L.W., "Heat-Transfer Measurements of Evaporating Liquid Drops," J. Heat Mass Transfer 21 (1978). pp. 537-542.
6. You, H-Z, Kung, H-C and Han, 2, "Spray Cooling in Room Fires," Twenty-First Symposium (International) on Combustion, The Combustion Institute, 1986, pp. 129-136.

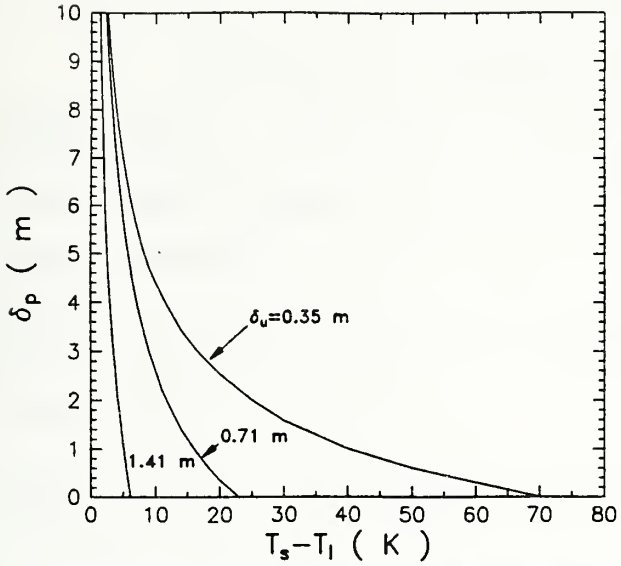

FIGURE 1 INFLUENCE OF THE TEMPERATURE DIFFERENCE BETWEEN GAS IN SPRAY AND LOWER LAYER ON JET PENETRATION DEPTH BENEATH LAYER INTERFACE FOR VARIOUS LAYER DEPTHS, δ_u. (½ IN. STANDARD SPRINKLER DISCHARGING 1.89 l/s AT CEILING LEVEL.)

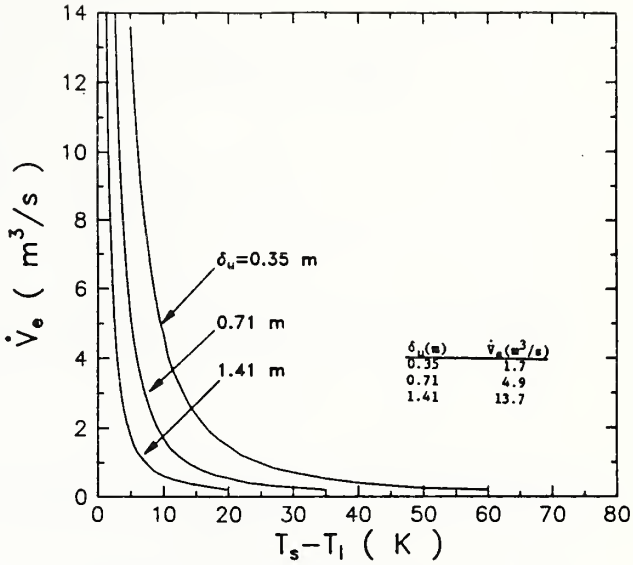

FIGURE 2 VOLUMETRIC ENTRAINMENT RATES FROM LOWER LAYER ASSOCIATED WITH FIGURE 1.

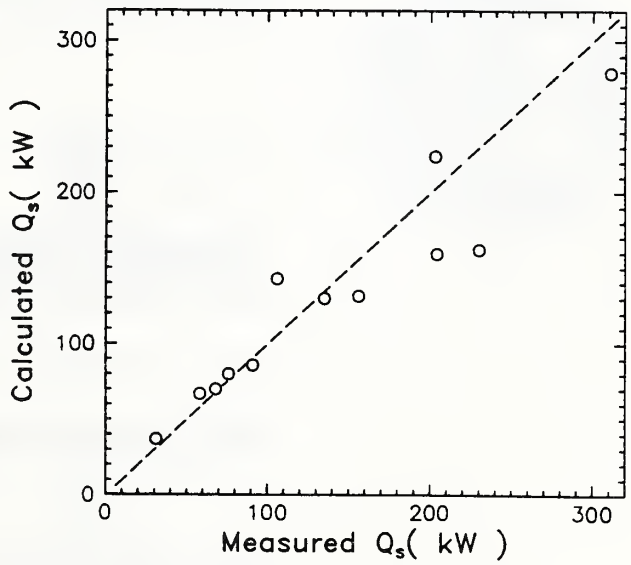

FIGURE 3 COMPARISON OF CALCULATED AND EXPERIMENTAL[6] SPRAY COOLING RATES.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

FIRE AND SMOKE SPREAD IN SHIPS - CEILING/FLOOR VENTS

Funding Agency: Naval Research Laboratory

Professional Personnel: Leonard Y. Cooper, Project Leader

Program Objectives

Develop a capability for modeling of flow through horizontal vents in multi-room zone-type fire model computer codes.

Technical Accomplishments

Work was completed on development of an algorithm and associated computer subroutine for calculating the characteristics of the flow across a horizontal vent which connects two adjacent spaces of a multi-room facility involved in a

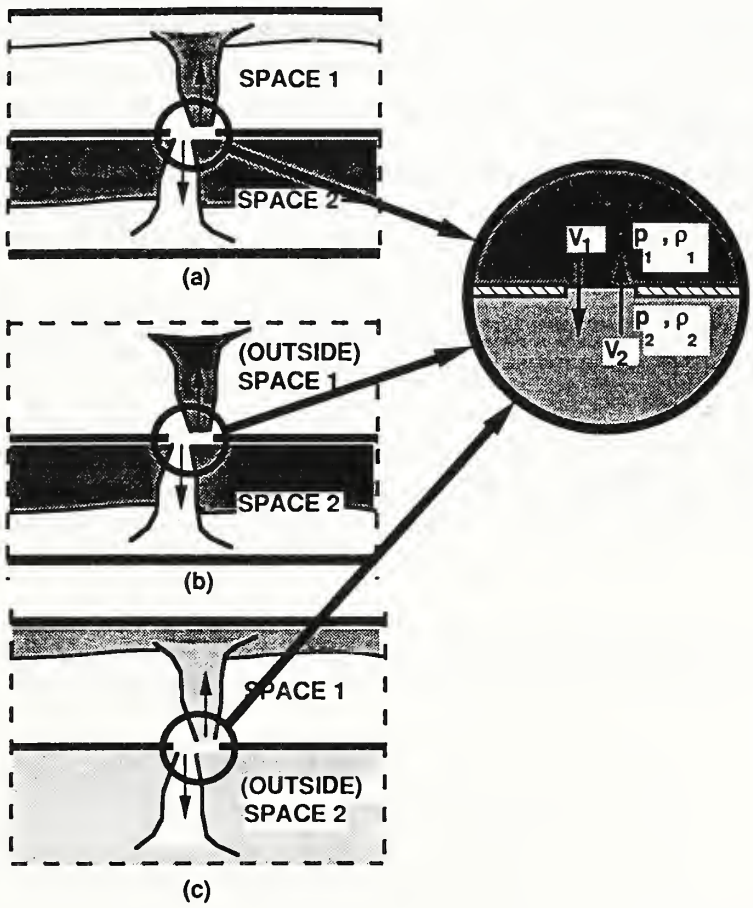

Figure 1. The possible configurations of the two spaces joined by a horizontal ceiling/floor vent with space 1 above space 2: a) two inside rooms; b) an outside space above an inside room; c) an inside room over an outside space.

fire. The algorithm and subroutine will appear and be discussed in reference [1]. As depicted in Figure 1, the two spaces joined by the horizontal vent can be either two inside rooms of a multi-room facility or one inside room and the outside ambient environment local to the vent. The description of the flow through the vent is determined by combining considerations of 1) the unidirectional-type of flow driven by a cross-vent pressure difference and, when appropriate, 2) the exchange-type of flow induced when the fluid configuration across the vent is unstable, i.e., when a relatively cool, dense gas in the upper space overlays a less dense gas in the lower space. In the algorithm, calculation of the rates of flow exchange between the two spaces is based on a previously reported theory [2]. Characteristics of the geometry and the instantaneous environments of the two spaces are assumed to be known and specified as inputs. The outputs calculated by the algorithm/subroutine are the rates and the properties of the vent flow at the elevation of the vent as it enters the top space from the bottom space and/or as it enters the bottom space from the top space. Rates of mass, enthalpy, and products of combustion extracted by the vent flows from upper and lower layers of inside room environments and from outside ambient spaces are determined explicitly. The algorithm/subroutine is called VENTCF. The computer subroutine is written in FORTRAN 77. The subroutine is completely modular, and it is suitable for general use in two-layer, multi-room, zone-type fire model computer codes. It has been tested over a wide range of input variables and these tests are described in the NISTIR.

Reports and Publications

1. "An Algorithm and Associated Computer Subroutine For Calculating Flow Through a Horizontal Ceiling/Floor Vent in a Zone-Type Compartment Fire Model," Cooper, L.Y., to appear as NISTIR 4402, National Institute of Standards and Technology, Gaithersburg MD.

2. "Buoyancy-Driven Flow Through a Horizontal Vent," Cooper, L.Y., submitted for outside publication.

Related Grants

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

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

Fire Risk Assessment

Funding Agency:

National Fire Protection Research Foundation

Staff:

Walter W. Jones and C. Lynn Forney

Objective:

To provide users of the risk assessment methodology with the software, and documentation which will allow them to utilize this software.

Scope:

The fire risk assessment project is an application of the Fire Hazard Methodology Project. This particular aspect is supported by the National Fire Protection Association to provide a means of implementing the Hazard Methodology for several prescribed situations. The intent of this project is to provide a document which describes the usage of the software on a Concurrent Computer, and a computer tape which contains the source for said implementation.

Technical Accomplishment:

This project consisted of the following two tasks: (1) Provide a tape containing the software used in the Risk Project, as developed for phases I and II; (2) Provide a report which describes the software in task #1, and how to use it. This will include a sample calculation, such as provided in the earlier reports. To the extent possible, the code will be annotated, and directions given, to indicate where system specific information exists, and how it could be modified. This is to facilitate transfer to other computers, such as a DEC Vax. NIST will not undertake such a conversion, however.

Publications:

Forney, C. L. and Jones, W. W., Fire Risk Assessment Method: Guide to the Risk Methodology Software, NISTIR 4401 (1990).

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

EVALUATION OF STAGING AREAS FOR THE HANDICAPPED

Funding Agency: General Services Administration

Professional Personnel: John Klote, Project Leader
Leonard Cooper, Danial Alvord,
and Harold Nelson

Project Objective

Develop the capability to evaluate the fire safety of the staging area approach for protection of the handicapped during building fires.

Scope

The fire safety of the handicapped in multi-story buildings is a matter of considerable concern, and staging areas are one approach that has gained considerable attention for providing fire safety. The evaluation consists of development of methods for analysis of smoke transport into staging areas during a fire and determination of the resulting tenability conditions. Field tests of six GSA buildings will be conducted to determine if the methods of smoke transport analysis are appropriate, and to gain data about these systems. Human behavior studies will be conducted to gain information about the extent to which these systems will be accepted and used as intended. The system concepts may be revised due to the human behavior studies. This new information will be applied to the six GSA buildings.

Technical Accomplishments

A method of building smoke transport has been developed which is applicable to sprinklered fires. This method is based on an idealized building network consisting of floors with negligible leakage, shafts, and staging areas for the handicapped. Based on an initial field trip to GSA buildings, this idealized network appears to be appropriate. The analysis incorporates stack effect and wind. This analysis is selected as a worst case for design calculations. The method is being extended for unsprinklered fires. In addition to analytical equations of smoke transport, the possibility of using a computer fire model such as FAST or CCFM is being investigated. There are numerous obstacles to overcome, but the advantages of this approach would be significant.

Reports and Publications None

Related Grants None

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

Expert System & Fire Protection Design Assessment System

Funding Agency: Air Force

Professional Personnel

R. Smith (Project Leader), H. Nelson

Project Objective: To develop an artificial intelligence expert system program that will perform as an expert consultant for the determination of fire safety specifications for the design of buildings and thereby will significantly reduce the cost of design and construction of buildings.

Technical Accomplishments

The concept of the Calculus of Fire Safety was developed as a declarative programming language. This calculus will enable users to specify what fire safety question is to be answered without specifying how the answer is to be obtained. Advances in Artificial Intelligence programming techniques will enable the implementation of the Calculus of Fire Safety on widely available workstations. This will provide a very powerful tool to anyone interested in determining the fire safety of buildings.

The knowledge based system (or expert system) EXPOSURE was completed. EXPOSURE offer advice on how to design a building so as to prevent fire from spreading from one building to another. A procedure was developed for the determination of the maximum radiation at various regions of a vertical wall due to N-openings in a wall of a burning building. This allows EXPOSURE to deal with building which have nonparallel walls, various materials, and arbitrary positions for openings. It will allow a designer to fully utilize unique building material properties for fire safety and thereby lower the cost of fire protection.

The knowledge representation for EXPOSURE consists of flavors (a Lisp object oriented programing system), production rules, procedural code, and predications. The graphic editor show the single line floor plans and the wall elevation view.

Reports and Publications

Smith, Richard L., EXPOSURE80A: A Computer Program Version of NFPA 80A.
National Instiute of Standards and Technology, NISTIR 4372: 1990

Smith, Richard L. EXPOSURE: An Expert System Fire Code.
National Institute of Standards and Technolology NISTIR-4373; 1990

Smith, Richard L., A Program for Calculating the Maximum Radiation on a Wall. National Institute of Standards and Technolology NISTIR to be published

Smith, Richard L., The Concept of the Calculus of Fire Safety, National Instiute of Standards and Technology, NISTIR to be published

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

LIVE FIRE TESTING

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

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

Project Objective: Support Critical Review of Live Fire Test Plans and Analysis

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

This program is in its early phases. Most emphasis to date is on a new submarine design that will be "all up" tested in 1995, and on "HULLVUL" surface ship tests performed by the Royal Navy in 1990.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

EFFECTS OF FIRE SUPPRESSANTS ON SAFETY RELATED EQUIPMENT

fUNDING AGENCY: Nuclear Regulatory Commission

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

Project objective: Collect data on the effects of fire suppressants used in nuclear power plants on equipment important to safety, in support of the SNL/INEL work on Generic Issue 57.

Technical accomplishments: Nuclear power plants have many installed fire suppressant systems. If operated inadvertantly, the suppressant may damage operating equipment and/or interfere with safety circuits or create spurious signals. This project will examine Navy experience with the large variety of operating systems on ships to gain insight on the effects that might occur.

This is a new project, just starting as this is written.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

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:
Measure compartment air and wall temperatures, atmospheric composition, radiant fluxes, vent flows, and other pertinent characterists of prototype trainers at Mayport Naval Station, New London Submarine Station, Great Lakes Naval Station (recruit trainer), Treasure Island (San Francisco), and San Diego. Measurements are made with the CFR instrument van, and the results are reported to the sponsors. Gas and water analyses are performed as required to obtain site permits from the local Environmental Protrection Agencies.

On occasion, special analyses are carried out, using NIST personnel, to obtain information of importance to solving developmental problems in the trainers. This includes, for instance, metallurgical analysis of slag from a failed smoke generator component to discern the cause of the failure.

It is planned to evaluate the FPETOOL compartment fire model as a design tool for future trainers. Previously, FIRST 9X was found to be useful, but it is difficult to run and requires significant computer capability.

The project leader participates in design reviews 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."

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

PRELIMINARY SCREENING PROCEDURES AND CRITERIA FOR HALON ALTERNATIVES

Funding Agency: U.S. Air Force, Engineering and Services Center

Professional Staff: Richard Gann, Project Leader
John Barnes, Research Physicist (Division 440)
Sanford Davis, Research Chemist
Richard Harris, Research Chemist
John Herron, Research Chemist (Division 582)
Barbara Levin, Research Biologist
Fred Mopsik, Research Chemist (Division 440)
Kathy Notarianni, Fire Protection Engineer
Marc Nyden, Research Chemist
Richard Ricker, Research Materials Engineer (Division 450)

Project Objectives:

(a) Determine the most appropriate, currently available screening methods for: fire suppression efficiency, residue level, and electrical conductivity; ozone depletion potential, greenhouse warming potential, metals corrosion, materials compatibility, storage stability, and toxicity; and (b) establish reasonable figures of merit by which the test results will be judged.

Technical Accomplishments:

With the current halogenated fire suppressants [halons 1301 (CF_3Br) and 1211 (CF_2ClBr)] now marked for phaseout, there is an urgent need to identify alternative chemicals, halons or others, that satisfy the most critical properties of the current halons: fire suppression efficiency, low residue level, low electrical conductivity, low metals corrosion, high materials compatibility, stability under long-term storage, and low toxicity (inhalation and contact) of the chemical and its combustion products. In addition, the new chemicals must make low contributions toward stratospheric ozone depletion and global warming. This project is a first step in a government/industry program to identify and qualify candidate replacements for halons 1301 and 1211 that will satisfy the needs of the major users for existing applications.

A team of specialists in each of the areas of testing has surveyed the existing methods in their fields and compiled descriptions of the protocols. Each procedure was analyzed, considering at least the following factors:

- ease of operation for these types of chemicals,
- number of locations having the capability to perform the test,
- amount of chemical required, and
- relevance of the figure(s) of merit to this program.

In several cases, adaptations were needed to improve the fit to this application. In some cases, no standard methods existed and procedures were derived from the most appropriate current practice. Where a standard method has been modified or a non-standard method is recommended, operating procedures are described. Multiple laboratories are available for performing each of these tests, but few can perform them all.

Each method was performed for at least halons 1211 and 1301. Since it was likely that these compounds would perform similarly in the test, a third chemical that would behave differently was selected and tested. Screening tests emphasize accurate indication, rather than high precision. Thus, we have reported the results of each test in a series of Performance Classes. These are related either to the performance of halons 1211 and 1301, or to some accepted criterion for practical use. The interpretation of the data from this battery of screens requires the expertise of persons knowledgeable in each of the fields described. Weak performance in any given area may not be the basis for eliminating any material from further consideration. These methods and performance classes have been developed for screening purposes only and should not be used for final acceptance of an agent without more extensive evaluation.

The full battery of tests requires about 4 moles of chemical and can be performed in about 8 days for less than $15,000. Lower costs would result for concurrent testing of a large number of chemicals. High purity of the samples of chemicals to be tested is critical.

Reports and Publications:

Gann, R.G., Barnes, J.D., Davis, S., Harris, J.S., Harris, R.H., Herron, J.T., Levin, B.C., Mopsik, F.I., Notarianni, K.A., Nyden, M.R., Paabo, M., and Ricker, R.E., "Preliminary Screening Procedures and Criteria for Replacements for Halons 1211 and 1301," Technical Note TN-1278, National Institute of Standards and Technology, September, 1990.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990

EXPLORATORY LIST OF POTENTIAL REPLACEMENTS FOR HALONS 1211 AND 1301

Funding Agency: U.S. Air Force, Engineering and Services Center

Professional Staff: Richard Gann, Project Leader
Gary Mallard, Research Chemist (Division 582)
Marc Nyden, Research Chemist
William Pitts, Research Chemist
Wing Tsang, Research Chemist (Division 582)

Project Objective:

Identify ≈100 gases and/or liquids, covering a range of chemical and physical principles thought to affect flame suppression capability.

Technical Accomplishments:

With the current halogenated fire suppressants [halons 1301 (CF_3Br) and 1211 (CF_2ClBr)] now marked for phaseout, there is an urgent need to identify alternative chemicals. Replacements for the current halons must have a large number of critical properties. These constraints are expected to complicate the search.

Our strategy focussed on principles for efficient fire suppression and low contribution to stratospheric ozone depletion. The widest range of chemical families were researched for their potential to test these principles. Some of these families have not previously been considered for fire suppression. Some included compounds are clearly not candidates as alternatives, but test principles of fire suppression or ozone depletion.

A chemical can quench a flame by (a) physical mechanisms (smothering or blanketing, cooling and dilution, mechanical means (e.g., blowing out a match), or flame radiation blockage) or by (b) chemical action (interference with the chain reactions that propagate flames). All agents have physical effects on a fire. Agents which also have a chemical mechanism, such as the currently-used halons, are more effective due to the additional pathway for flame suppression. There have been several studies of the effectiveness of specific chemicals. Very few of those separate the contribution of physical and chemical mechanisms.

The means for altering a chemical to decrease its contribution to ozone depletion also fall under two headings: (a) elimination of all bromine, chlorine, and iodine atoms; and (b) and increased reactivity in the lower atmosphere. The latter results from enhanced reaction with OH radicals, dissociation due to absorption of solar radiation, and enhanced rain out due to increased polarity. Assessment of ozone-depletion effectiveness is based only on atmospheric modeling.

We identified nine families of chemicals with potential for testing the above principles.

- Saturated halocarbons, or halons: ($C_nF_oCl_pBr_qI_r$ where $o+p+q+r=2n+2$). These are analogs of the currently-used halons and include totally fluorinated compounds, photosensitive compounds, and analogs to the HCFCs.
- Halogenated ketones, anhydrides, and esters. These contain C=O bonding and may be more prone to solar dissociation in the troposphere.
- Unsaturated halocarbons. These contain C=C bonding and may be more reactive with OH in the troposphere.
- Halogenated ethers. These contain an O-C-O linkage, which is thought to promote solar dissociation in the troposphere.
- Halons containing iodine. These are likely to be more reactive in the troposphere.
- Sulfur halides. These are analogs to the halons.
- Compounds containing phosphorus. These are non-ozone-depleting, possibly highly efficient fire suppressants.
- Silicon and germanium compounds. These are tropospherically-reactive analogs to the halons.
- Metallic compounds. These are extremely efficient fire inhibitors that are non-ozone-depleting.
- Inert gases. These are baseline chemicals: less-efficient, only physically active agents with zero ozone-depletion potential.

The list of 103 chemicals from these families will enable testing the principles and identifying optimal candidates. Some of the chemicals can be considered candidates themselves. The final report contains detailed data sheets for each of the selected compounds.

Reports and Publications:

Pitts, W.M., Nyden, M.R., Gann, R.G., Mallard, W.G., and Tsang, W., "Construction of an Exploratory List of Chemicals to Initiate the Search for Halon Alternatives," Technical Note TN-1279, National Institute of Standards and Technology, September, 1990.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1990
MASS FIRE RESEARCH

Funding Agency: Defense Nuclear Agency

Project Leader: James Quintiere

Other Staff: H. Baum, D. Corley, H. Mitler, T. Ohlemiller

Project Objective: To coordinate and conduct studies related to mass fires; specifically, (1) determine the energy output and ground level flow field associated with the Hill Township mass fire experiment of 1989, (2) to prepare a summary report of the Hill fire experiment, and (3) to conduct a literature review on research and methods for predicting aspects of mass fires in an urban environment.

Technical Accomplishments: Three draft reports associated with each of the three specific objectives have been completed and are in review. A summary of the Hill Township fire results are presented below:

Working with Forestry Canada and the Ontario Ministry of Natural Resources, the Defense Nuclear agency carried out an extensively instrumented experiment of a prescribed burn in forest debris to simulate conditions of a mass fire. In addition to the Canadian team, a multi-institutional US team made both ground and airborne measurements of the fire and smoke conditions. The fire reported on was in Hill Township, Ontario and covered nearly 480 ha in its overall burning area. The experimental prescribed burn began with prevailing winds from the west of 3 m/s. The fire in Block A1 caused a plume to rise to 6.5 km in 20 minutes, and achieve a nominal diameter of 1 km in a flaming and smoldering condition. The PSRC had some success at predicting the plume rise. The fire began in Block A approximately 25 minutes later and began to trigger the ground instruments. The Block A fire achieved an energy release rate of nearly 50,000 MW in 15 minutes which is believed to have been dominated by smoldering combustion. Fire whirls and water spouts were observed.

Ground level horizontal winds increased as a result of the fire to 12 m/s (approximately 25 mph) suggesting the potential destructive nature of mass fire including the possibility of fire whirls and brand transport. The NIST team exercised a model which gave fair to good results for predicting the ground wind field from the fire configuration.

The fire spread rate through the forest debris fuel bed achieved levels as high as 1 m/s under these wind conditions. Flames reached as high as 12 m. However ground level oxygen concentrations in the region surrounding the flame only dropped to 19 % at least. The relative levels of CO/CO_2 and the specific extinction area of the smoke particulates suggest that the combusting products of this fire were significantly influenced by smoldering combustion.

The cloud effects caused precipitation, lightning, and even snow flakes. The estimation of the cloud processing in removing smoke (carbon) particulates below 1 um is nominally 40 % and perhaps higher. LIDAR data suggest that the smoke detrained at an altitude of 4 km from the capping cloud despite its ascent to nearly 7 km. Airborne trace specie samples show an interesting array of components that bear generally on global environmental effects.

APPENDIX

ALPHABETICAL LISTING OF
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5. AUTHOR(S)

Sonya M. Cherry

6. PERFORMING ORGANIZATION (IF JOINT OR OTHER THAN NIST, SEE INSTRUCTIONS)

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NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
GAITHERSBURG, MD 20899

7. CONTRACT/GRANT NUMBER

8. TYPE OF REPORT AND PERIOD COVERED

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (STREET, CITY, STATE, ZIP)

same as above

10. SUPPLEMENTARY NOTES

11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

This report describes the research projects performed in the Center for Fire Research and under its grants program during October 1, 1989 to October 1, 1990.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

charring; combustion; fire models; flame spread; hazard; ignition; polymers; smoke; soot; toxicity

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