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SUMMARIES OF CENTER FOR FIRE RESEARCH IN-HOUSE PROJECTS AND GRANTS - 1989

Sonya M. Cherry, Editor

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and Technology
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PREFACE

This report describes the research projects performed in the Center for Fire Research (CFR) and under its grants program during FY-1989.

The Center is nationally recognized as the focal point for fire research 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 such 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 13 groups:

Turbulent Combustion
Soot Formation
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
Technology Transfer

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.

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B. Fire Protection Technology

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

A. Turbulent Combustion

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

TURBULENT COMBUSTION SIMULATION

Professional Personnel

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

Objective

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

Part of this work, (see item 2. below) is supported by the Air Force Office of Scientific Research.

Technical Accomplishments

1. Large Eddy Simulations

A new time dependent large eddy simulation is under development, that will ultimately replace the existing three dimensional buoyancy driven flow code. The new calculation is based on "spectral" (Fourier analysis) decomposition of the flow field, which is now the dominant technique for basic computer studies of turbulent flow phenomena. The initial application, for which coding is in progress, is to a helium plume in a cylindrical enclosure. An experimental realization of this flow geometry is under construction (by W. Pitts). The numerical algorithm employed in this problem has required the development of a novel approach to spectral computations in cylindrical coordinates; the accurate and efficient use of Bessel function transforms.

A vortex dynamics simulation of wind blown turbulent plumes is also under development, with preliminary results obtained for negatively buoyant particulate plumes generated by heavily sooting fires well downstream of their point of origin. This project is expected to benefit greatly from vortex modeling capability developed by Prof. A. Ghoniem who will visit NIST this autumn.

2. Eddy Scale Combustion

The eddy scale combustion model is intended as the vehicle by which the "subgrid" chemical and physical processes are incorporated into the large eddy flow simulations. Work this year has focused on incorporating measured state relationships between the mixture fractions and major species for a "fuel library" of seven fuels. Prof. J. Gore has made a major contribution to this work. The calculations that incorporate this data require the construction of a "Pseudo-Mixture fraction" which incorporates the expansion of the gas due to the combustion energy release into the analysis. It is the spatial and temporal evolution of the pseudo-mixture fraction which is calculated theoretically. The relationship between this quantity and the actual mixture fraction depends only upon the fuel/air state relationships, and transport properties. This relationship is also calculated as part of the fuel library.

The pseudo-mixture fraction itself has been calculated in two and three space dimensions. The two dimensional calculations in the isothermal limit occupy a special place, despite their limited range of applicability. They constitute one of the few exact solutions to a multi-dimensional reacting fluid flow problem known. Among other things, they serve as a test bed for the more approximate calculations necessary for the three dimensional combustion calculations of more direct interest.

3. Computer Hardware and Software

This comprises three tasks: consolidation and execution of existing codes on the Convex computer, selection, acquisition, and installation of graphics workstations with the above and selection of field equation general purpose simulation software from a commercial vendor. Virtually all our codes are now resident on the Convex. A paper was presented (by R. Rehm) at the January Eastern Section of The Combustion Institute describing statified fire induced enclosure flows generated on the minisupercomputer. More recently, Convex Computer Corporation featured our work in its annual stockholders report for 1988. After an evaluation of several vendors' products, four Personal Iris 3-D color graphics workstations (2 for CFR and 2 for CCAM) were purchased and delivered in April. Many utilities and graphics displays for our work are under development.

Discussions were held with representatives of Cham of North America, Creare Inc., and UKAEA Harwell, all of whom market and use computational fluid dynamics (CFD) codes for use in engineering simulations of fires (among other phenomena). The necessary upgrades to the Convex and additional workstation needs have been assessed with help from D. Walton. Negotiations are continuing as of this writing.

Reports and Publications

"A Model of Three-Dimensional Buoyant Convection Induced by a Room Fire" by Rehm, R.G., Baum, H.R., Lozier, D.W. AIAA-88-3723-CP, First National Fluid Dynamics Congress, 1988.

"Smoke Plumes From Crude Oil Burns" by Evans, D., Baum, H.R., Mulholland, G., Bryner, N., and Forney, G., Proceedings of the Twelfth Arctic and Marine Oil Spill Program Technical Seminar, Min. Supply and Services Canada Cat. En 40-11/5-1989, p. 1, (1989).

"Diffusion-Controlled Reaction in a Vortex Field" by Rehm, R.G., Baum, H.R., Lozier, D.W., and Aronson, J., Combustion Science & Technology (in Press).

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.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: Factory Mutual Research Corporation

Grant No.: 60NANB7D0738

Grant Title: Radiation Modeling of Laminar Diffusion Flames

Principal Investigator: John de Ris

NIST Scientific Officer: Dr. Howard R. Baum

Technical Abstract:

Flame radiation is a particularly critical area of fire research. There is a clear need for formulating and establishing a fundamental mathematical approach which can reliably predict flame radiation in various situations of interest. At present engineers postulate that a certain fraction of the chemical heat released by combustion leaves the flame region in the form of radiation. For the turbulent burning of hydrocarbon fuels in air this fraction can vary from less than 12% to over 65% depending on the fuel and fluid dynamics. It also depends strongly on the ambient oxygen concentration. We have found empirically that the radiant fraction dependence on fuel type for buoyant turbulent fuel jet flames is closely correlated by the fuel's smoke-point laminar flame height (or heat release rate) when such comparisons are made at the same adiabatic stoichiometric flame temperature and stoichiometric oxidant to fuel mass ratio. This suggests that laminar smoke-point flames somehow encompass most of the physical-chemical processes controlling luminous flame radiation. Such laminar candle-like smoke-point flames have been extensively measured by both us and others. However, we lack quantitative predictive mathematical models describing these important classical flames.

Flame radiation originates from both the product gases and soot. Both are important when one compares theory with experiment. If the soot volume fraction were somehow to increase, the resulting increase in the soot radiation would cause the flame temperatures to decrease which in turn reduces the radiation from the gases and the radiation per unit volume of soot. The processes are strongly coupled. Similarly if one somehow extracted more heat from the flame by convection, the reduced flame temperatures cause reduced soot formation and reduced radiation from both the gases and soot. Such observed trends can be quantitatively addressed by our mathematical model.

In this project we model the pure gas-phase combustion processes as a Shvab-Zeldovich diffusion flame and thin reaction zone. Soot formation, soot oxidation and radiant heat loss are treated as distributed processes. The equation for the Shvab-Zeldovich mixture-fraction ζ has the form

$$\rho \frac{\partial \zeta}{\partial t} + \rho \vec{v} \cdot \nabla \zeta - \nabla \cdot (\rho D \nabla \zeta) = B_F \dot{m}'''_{SF} - B_O \dot{m}'''_{SO}$$

where B_F and B_O are constants and $\dot{m}'''_{SF}$ and $\dot{m}'''_{SO}$ are respectively the local soot formation and oxidation rates.

In the absence of soot and radiation the Shvab-Zeldovich concept immediately yields the local fuel, oxidant and temperature throughout the flow field. We define now a normalized variable $\chi\ (\vec{x},t)$ which describes the proportionate cooling by radiation and energetics from soot formation and oxidation. χ would be unity for complete radiant cooling, zero for no cooling and a constant equal to the overall flame radiant fraction if there were no soot energetics and if a fixed fraction of the chemical heat release were immediately radiated at the flame front. In fact, $\chi\ (\vec{x},t)$ varies throughout the flowfield and is governed by the equation

$$\rho \frac{\partial \chi}{\partial t} + \rho \vec{v} \cdot \nabla \chi - \nabla \cdot (\rho D \nabla \chi) = C_F\ \dot{m}'''_{SF} - C_o\ \dot{m}'''_{so} + \frac{\dot{q}'''_{RAD}}{h_{ad} - h_\infty}$$

which is similar to the mixture-fraction equation but with added radiation term.

The corresponding equation for the soot volume fraction, f_v, in the absence of thermophoresis,

$$\frac{\partial f_v}{\partial t} + \vec{v} \cdot \nabla f_v = (\dot{m}'''_{SF} - \dot{m}'''_{so})/\rho_c$$

lacks a diffusion term owing to the very large molecular weights of soot particles. As a result soot volume fractions are problem dependent and cannot be simply correlated by the mixture fraction.

For optically thin flame the local volumetric radiant heat loss is given by the simple formula

$$\dot{q}'''_{RAD} = 4\ (K_g + K_s)\ \sigma\ (T^4 - T_\infty^4)$$

where K_g and K_s are respectively the gas and soot absorption coefficients which are proportional respectively to the product gas mole fractions and soot volume fractions. This expression can be readily modified for optically intermediate and thick situations using our recently developed correlation formulas.

The chemistry of soot formation is not sufficiently well understood to support a detailed 'a priori' model. Instead we postulate a simple expression which we can directly test against experimental data

$$\dot{m}'''_{SF} = \begin{cases} \rho^2\ A_F\ (\zeta - \zeta_*)\ e^{-E_F/RT} & \text{for } \zeta > \zeta_* \text{ (fuel rich)} \\ 0 & \text{for } \zeta < \zeta_* \text{ (lean)} \end{cases}$$

where ξ_* is the mixture fraction corresponding to the empirical soot-point threshold of the corresponding premixed flame, while E_F is the activation energy for thermal pyrolysis of the fuel. The above model preserves the observed: first order dependence on local fuel concentration and the second order dependence on ambient pressure, as well as the very similar chemical structure diffusion and premixed flames between the positions of maximum fuel pyrolysis and heat release rate. Measurements of soot concentrations in "candle-like" flames suggest that the coefficient $A_F e^{-E_F/RT_f}$ should be inversely proportional to the observed smoke-point flame height (or heat release rate).

Measurements suggest that soot oxidation rates are proportional to the [OH] radical concentration and the soot surface area. As a result soot oxidation chemistry is very similar to CO oxidation chemistry which also is proportional to [OH]. This allows us to model soot oxidation with using conventional CO oxidation kinetics, and

$$\dot{m}'''_{so} = A_o \, f_v^{2/3} \, [OH]$$

where the soot surface area is inferred for a fixed particle size.

To test this modeling scheme we are initially computing the classical smoke-point candle flames. The model provides explicit prescriptions for all quantities except for the soot formation rate proportionality constant which must be evaluated empirically. Examination of the equations indicates that the roles of the gas and soot radiation scale quite differently with flame height or flow time. The soot radiation becomes progressively more important for longer flow times; since the local soot formation/oxidation <u>rates</u> are controlled by the local gas chemistry; whereas the product gas concentrations are directly controlled by the local gas concentrations.

The bread goal of this study is to quantify how the flame radiant fraction depends on the various controlling dimensionless groups for several idealized flame geometries "candle-like flames, opposed flow, single flames sheets, etc.).

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution:	The University of Michigan
Grant No.:	60NANB8D0833
Title:	Radiation from Turbulent Luminous Flames
Principal Investigator:	Professor Gerard M. Faeth Department of Aerospace Engineering 218 Aerospace Engineering Building Ann Arbor, MI 48109-2140
Other Professional Personnel:	M. A. Kounalakis, Graduate Assistant Y. R. Sivathanu, Graduate Assistant
NIST Scientific Officer:	Dr. Howard R. Baum

Technical Abstract:

Introduction. This investigation is considering two aspects of thermal radiation from unwanted fires, as follows: (1) the scalar structure of turbulent flames, emphasizing the radiation properties of soot in luminous flames; and (2) effects of turbulence/radiation interactions, emphasizing nonluminous flames to simplify interpretation of results. 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 papers and reports listed at the end of this report.

Luminous Flames. This portion of the study mainly involved development of the laminar flamelet concept for soot-containing luminous turbulent diffusion flames. When the laminar flamelet concept is valid for a particular scalar property, the property can be correlated solely as a function of mixture fraction (or equivalence ratio) irrespective of the position within the flame or flame operating conditions. When these correlations, called state relationships, are available, models only need to be constructed to find mixture fractions since other scalar properties follow from the state relationships; naturally, this vastly simplifies analysis to find scalar properties in flames.

Two aspects of the flamelet concept were considered during this report period: generalized state relationships for gas species in hydrocarbon/air diffusion flames and state relationships for soot volume fractions in the underfire region. Earlier work had shown the existence of universal state relationships for soot volume fractions at flame residence times roughly ten times longer than the laminar smoke point residence time.

Up to now, state relationships for major gas species had been found for a number of hydrocarbon/air diffusion flames. Finding state relationships, however, is tedious; therefore, rather than undertake measurements for a variety of fuels a method of generalizing results in the literature was sought. The reactant system was taken to be C_nH_m and the procedure involved defining generalized functions of the mass fractions of each species so that the function would correlate solely with the fuel-equivalence ratio at the limit of very low fuel equivalence ratios. This approach was very successful for N_2, O_2, the fuel, CO_2, and H_2O, and to a slightly lesser degree for H_2 and CO. Calculations of flame properties assuming local thermodynamic equilibrium

showed that the generalized functions were universal for fuel-lean conditions for H/C ratios in the range 1-4. Existing measurements agreed with predictions for fuel-lean conditions and fortuitously yielded universal functions for fuel-rich conditions where departures from equilibrium are larger. The correlations are also effective for heavily-sooting fuels like acetylene. Additional examination of the approach would be desirable, however, it appears to be a useful method for estimating gas concentrations in hydrocarbon/air diffusion flames.

The existence of soot volume fraction state relationships in the underfire region of luminous flames was studied by simultaneously measuring soot volume fractions (by laser extinction) and temperatures (by two-wavelength pyrometry) using an optical probe. Measurements were made at various points in the underfire region of relatively-large propane, ethylene, propylene or acetylene/air flames produced by a 50 mm diameter burner. The resulting correlations between soot volume fraction and temperature were essentially independent of position within the flames and flame operating conditions. Furthermore, the shapes of the correlations were in general agreement with correlations found from measurements in laminar flames for acetylene and ethylene — the only two fuels for which measurements of this type are available. Finally, the temperature range of the correlations was relatively narrow, particularly for the strongly sooting fuels, supporting the approximation of a constant-temperature soot layer for strongly-radiating flame. Thus, the main conclusion of the study is that there is strong evidence of the existence of soot volume fraction state relationships for the underfire region of soot-containing flames.

Current work involves measuring the statistics of soot volume fractions along paths through turbulent diffusion flames, and measuring spectral radiation properties in the continuum for the same paths. Given this information, and the correlations between temperatures of soot volume fractions, stochastic methods in conjunction with a narrow-band radiation model will be used to predict flame radiation properties for comparison with the measurements.

Nonluminous Flames. Past work has shown that turbulence/radiation interactions cause mean radiation levels to be biased upward from estimates based on mean scalar properties, and also result in large r.m.s. radiation fluctuation intensities. A stochastic method, based on statistical time-series techniques and the laminar flamelet concept, was developed to deal with these effects yielding encouraging agreement with measurements for hydrogen/air flames.

Work during the current report period continued development of the stochastic radiation analysis in two ways: evaluation of the method was extended to carbon monoxide/air flames, and measurements of statistical properties of mixture fraction needed for the analysis was initiated in carbon monoxide/air flames. The carbon monoxide/air system was chosen for study since it has an unusually high stoichiometric mixture fraction which simplifies measurements.

Tests of the stochastic analysis using measurements for carbon monoxide/air flames yielded results very similar to the hydrogen/air flames. Radiation fluctuation intensities were high for these flames — exceeding 100% beyond the flame tip. Predictions of fluctuating radiation properties were reasonably good with discrepancies largely attributed to errors in the flame structure analysis.

The main weakness with the stochastic radiation analysis is that little is known about the statistical properties of mixture-fraction fluctuations so that they must be estimated from a turbulence model. The second phase of the work seeks to remedy this by measuring these properties in carbon monoxide/air flames. This is being done using Mie scattering from seeding particles in the burner flow. The arrangement has two observation positions which can be traversed with respect to each other so that spatial correlations, which are very important for stochastic radiation predictions, can be measured. The measurements yield time- and Favre-averaged mean and r.m.s. fluctuating values, probability density functions, spatial correlations and temporal correlations of mixture fractions for radial paths through the flame axis.

Measurements completed thus far have been for a flame having a burner exit Reynolds number of 7,000. Favre-averaged mean values of mixture fraction are lower than time averages but both averages yield about the same r.m.s. fluctuations. Probability density functions have the general shape of a clipped-Gaussian function. Temporal correlations are crudely exponential. Spatial correlations are similar to those found in constant density jets and have the shape of Frenkiel functions, however, present measurements yield smaller negative correlations and approach zero sooner. Finally, integral scales in radial directions decrease as the edge of the flame is approached.

Measurements of the statistical properties of mixture fractions will continue in order to cover more flame conditions. This will be followed by measurements of mean and fluctuating radiation properties for the same paths as the measurements. With these results in hand, the stochastic radiation analysis will be evaluated more definitively than before by comparing predictions and measurements.

Reports and Papers:

1. M. E. Kounalakis, J. P. Gore and G. M. Faeth, "Turbulence/Radiation Interactions in Nonpremixed Hydrogen/Air Flames," *Twenty-Second Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, pp. 1281-1290, 1988.

2. G. M. Faeth, J. P. Gore and Y. R. Sivathanu, "Radiation from Soot-Containing Flames," *Combustion and Fuels in Gas Turbine Engines*, AGARD Conference Proceedings No. 422, NATO, Paris, pp. 17-1 to 17-12, 1988.

3. G. M. Faeth, J. P. Gore, S. G. Chuech and S.-M. Jeng, "Radiation from Turbulent Diffusion Flames," *Ann. Rev. Num. Fluid Mech. and Heat Trans.*, Vol. 2, Hemisphere Publishing Corp., Washington, pp. 1-38, 1989.

4. Y. R. Sivathanu, J. P. Gore and G. M. Faeth, "Scalar Properties in the Overfire Region of Sooting Turbulent Diffusion Flames," *Combust. Flame*, Vol. 73, pp. 315-329, 1988.

5. M. E. Kounalakis, J. P. Gore and G. M. Faeth, "Mean and Fluctuating Radiation Properties of Turbulent Nonpremixed Carbon Monoxide/Air Flames," *J. Heat Trans.*, in press.

6. Y. R. Sivathanu and G. M. Faeth, "Soot Volume Fractions in the Overfire Region of Turbulent Diffusion Flames," *Combust. Flame*, in press.

7. Y. R. Sivathanu and G. M. Faeth, "Temperature/Soot Volume Fraction Correlations in the Fuel-Rich Region of Buoyant Turbulent Diffusion Flames," *Combust. Flame*, in press.

8. Y. R. Sivathanu and G. M. Fath, "State Relationships for Major Gas Species in Nonpremixed Hydrocarbon/Air Flames," *Combust. Flame*, submitted.

9. Y. R. Sivathanu and G. M. Faeth, "Soot Properties in the Fuel-Rich Region of Turbulent Diffusion Flames," *Proceedings of the 1989 Spring Technical Meeting*, Central States Section of the Combustion Institute, Pittsburgh, pp. 103-110, 1989.

10. Y. R. Sivathanu, M. E. Kounalakis, J. P. Gore and G. M. Faeth, "Radiation from Turbulent Nonluminous and Luminous Diffusion Flames," NIST-GCR-88-553, 1988.

11. M. E. Kounalakis, Y. R. Sivathanu and G. M. Faeth, "Structure and Radiation Properties of Turbulent Nonluminous and Luminous Diffusion Flames," Final Report, NBS Grant No. 60NANB5D0576, October 1989.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

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) 454-8869

Other Professional Personnel: R. J. Gettings (M. S. Candidate)
M. Klassen (Ph. D. Candidate)
Dr. S. J. Fischer (N. I. S. T.)

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.

This grant started on June 1, 1989. Work during the first quarter involved: (1) measurements of burning rates and radiative heat loss fractions for small (46 mm and 76 mm diameter) pool fires burning ethanol, n-heptane, MMA (monomer), toluene and styrene in air; (2) initiation of a field model to evaluate the radiative heat flux incident on the fuel surface including the effects of large and small scale fluctuations. In the following, these two tasks are briefly summarized.

Burning Rates and Radiative Heat Loss Fractions:

The small-scale pool fires involved pyrex glass containers of heights approximately 2 times the diameters with a 6 mm diameter feed port at the bottom. The fuel was continuously injected by a gravity-feed system. The liquid level was maintained flush at the rim by adjusting a needle valve. The fuel was fed to the burner using a large tank mounted at 1400 mm above the ground. The feed rates were metered using a burette connected in parallel with a large diameter fuel-tank and a stop-watch. The height of the fuel tank and the burette was chosen to cause negligible effect of changes in the liquid level on the mass flow rates.

The radiative heat fluxes leaving the flames were measured using a wide-angle radiometer(150 ^{o} view angle). The radiometer was calibrated using a tungsten lamp source against an N.I.S.T. standard radiometer. Radiative heat fluxes leaving the flames parallel to the axis, in the plane of the pool, and in a plane well-above the visible flame-tip were measured. The points at which data were obtained can be used to define a complete cylindrical enclosure around the flames since the flames are axisymmetric in the mean. The flames are sensitive to ambient disturbances even inside the large screen enclosures. Small enclosures were not used to avoid the errors introduced by reflections from the wire screen. The radiative heat flux data were averaged over 60 seconds to obtain a smooth profile. Nominal chemical energy release for each flame was evaluated using the measurements of mass flow rates and a heat of combustion obtained assuming complete conversion to CO_2 and H_2O.

Table 1 shows various properties of the small pool flames. For each of the fuels considered, measurements of heat release rates are listed first. Then the transfer number B_T for the fuels is listed followed by moles of O_2 required per mole of fuel. These three together determine the flame size qualitatively (eg. small heat release rate, small transfer number, and small O_2 requirement indicate a small flame). The flame size in turn affects the burning rate by determining the radiative heat feedback. Table 1 shows the estimates of peak flame temperatures assuming complete combustion for the fuels followed by a listing of the measured radiative heat loss fractions.

Measured radiative heat loss fractions are remarkably close to each other(mostly between 0.3 and 0.35) for all the fuels considered here except for ethanol. The radiative heat loss fractions are essentially identical for the two pool sizes considered here. Measurements of flame heights and soot concentrations are in progress. However, visual observations confirm that the flame heights increase with: the moles of oxygen required per of mole of fuel, and the transfer number (shown in Table 1). Visual observations of soot breaking through the flame tip suggest that styrene produces the maximum soot followed by toluene, MMA, and n-heptane. Ethanol flames are clear blue. Estimates of peak flame temperatures based on complete conversion to CO_2 and H_2O and accounting for the radiative heat loss show a 10 % variation that does not correlate very well with the radiative loss fractions. Thus the reason for the small variation in the radiative heat loss fractions in spite of the large variation in soot concentrations appears to be related to optical depths and flame sizes.

The burning rate is controlled by energy and species mass balances at the fuel surface. For the same pool size styrene and toluene have the largest burning rates followed by heptane and MMA. Ethanol has the lowest burning rate mainly due to its low B_T number. The increase in burning rate with pool-size is highest for styrene and toluene followed by MMA, heptane and ethanol. Thus it appears that the effect of soot concentrations on burning rates (through radiative heat feedback) is much stronger than that on the overall radiative heat loss fractions. Theoretical models for burning rates must address all of these experimental findings.

Table 1: Properties of Small Pool Fires

Fuel	d mm	Q^a kW	$B_T{}^b$	$O_2{}^{a,c}$ Index	$T_f{}^{a,d}$ K	X_R
Ethanol	46	0.6	3.2	3	2200	0.2
	76	1.4				0.17
Heptane	46	1.4	7.4	11	1920	0.32
	76	3.2				0.32
MMA	46	1.1	7.4	7	2200	0.34
	76	2.4				0.33
Toluene	46	2.2	7.8	9	2270	0.32
	76	6.4				0.39
Styrene	46	2.2	7.3	10	2100	0.31
	76	5.6				0.31

[a] assuming complete combustion to CO_2 and H_2O

[b] defined as $C_p(T_f-T_b)/h_{fg}$; C_p = 1.5 kJ/Kg-K
T_b = Normal boiling point; h_{fg} = heat of vaporization.

[c] moles of oxygen per mole of fuel

[d] estimated based on specific heat at 2000 K

The small flames described above are laminar with small well-defined buoyancy-induced oscillations in the flaming region. Practical fires are larger than these and are turbulent. The purpose of the baseline tests is to isolate the fuel structure effects in a relatively simple environment.

Field Model for Radiative Feedback from Turbulent Fires:

Practical fires are turbulent. Experiments with a large multi-ring pool burner developed by Dr. Kashiwagi are being conducted and planned in collaboration with Dr. Fischer to obtain: total heat feed back to the fuel surface as a function of radius, infrared and visible absorption profiles, and radiative component of the heat feedback to the fuel surface. These data will be used to evaluate a field model of radiative feed back currently being developed. The model treats the effects of large scale and small scale fluctuations in scalar properties of the fire separately. Frequencies associated with the large scale fluctuations in turbulent pool fires are known from the literature. Detailed flow visualization studies of others have revealed that the flame shape and height undergo reasonably well-defined cyclic variations.

The radiative heat feedback model being developed will be compatible with numerical simulations of fluid mechanics, mixing and chemical reactions. In addition the model must address the fuel property effects observed in the small scale pool fires. Fuel property effects are also expected to affect large scale fires. Comparisons with existing models that are based on flame shape, size and apparent emissivity and temperature are also planned.

Reports and Papers:

This is the first quarter of the grant and papers based on the early results are still in preparation.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: University of California, Berkeley

Grant No.: 60NANB7D0737

Grant Title: Fire Propagation in Concurrent Flows

Principal Investigator: Professor A. Carlos Fernandez-Pello
Department of Mechanical Engineering
University of California
Berkeley, CA 94720
Telephone: (415) 642-6554 - Fax: (415) 642-6163

Other Professional Personnel: L. Zhou, Doctoral Graduate Student

NBS Scientific Officer: Mr. Kenneth Steckler

Technical Abstract

Research is being conducted to study the effect of flow turbulence on the spread of flames over the surface of a solid combustible. During this reporting period, a parametric study of the effect of flow velocity and turbulence intensity on the opposed mode of flame spread has been completed. The results obtained provide insite on how turbulence affects the spread of flames in an opposed flow and the extinction of the flame. Currently, we are conducting experiments on concurrent flame spread, which are yielding results that are potentially significant not only in the flame spread modeling but in other aspects of fire development such as flame length and soot, flame interaction with combustible surfaces and possibly burning rates.

I. Flame Spread in an Opposed Turbulent Flow:

The experiments are conducted in a facility specifically designed to perform flame spread experiments consisting of a small scale combustion tunnel and supporting instrumentation based primarily on optical and thermocouple measuring methods. 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.

I.1 Thick PMMA sheets

The measurements of the flame spread rate over PMMA sheets as a function of the opposed air flow velocity are shown in Fig. 1 for several values of the turbulence intensity. It is seen that the spread rate first increases sharply as the flow velocity is increased and then decreases. The initial sharp increase appears to be due to the under-ventilated conditions that the flame encounters at very low flow velocities. As the flow velocity increases, mixed flow (buoyant and forced) conditions determine the transition to a flame spread rate that decreases as the gas velocity increases. The decrease of the flame spread rate with the opposed flow velocity at higher air velocities has been observed and explained in other studies. This effect is observed to occur at all turbulence intensity levels.

The effect of turbulence intensity on the flame spread rate can also be deduced from the results of Fig. 1. It can be seen that for all flow velocities the flame spread rate first increases and then decreases as the turbulent intensity increases. The maximum occurs at approximately 6% of the turbulent intensity. This result may reflect the differences in the boundary layer that take place during the transition from laminar to turbulent flow. For PMMA, heat conduction through the solid is an important flame spread mechanism. Thus, the transition from laminar to turbulent should result in an increase of the flame spread rate because the heat transfer to the solid increases. At low turbulence intensities, this effect appears to be more important than the enhancement of the fuel convective cooling that should occur as the flow becomes more turbulent.

I.2. Thin paper sheets

The results of the measurements of the variation with the air flow velocity and turbulence intensity of the flame spread rate over thin paper sheets are presented in Fig. 2. In this case, the flames do not propagate (extinguish) in gas flows with velocities larger than 1.5 m/s. The low flow velocities at which the tests had to be conducted limited the maximum range of turbulence intensities attainable to 15%. From the results of Fig. 2 it is seen that for all turbulence intensities the spread rate decreases as the opposed gas velocity increases. The decrease in the low velocity region, however, is small. The stronger decrease of the flame spread rate with the flow velocity observed for the larger turbulence intensities appear to be the combined effect of convective cooling and weakening of the chemical reaction that take place as the turbulence intensity increases.

An interesting result obtained in these experiments is the effect of flow turbulence intensity on the extinction of the flame. This is also shown in Fig. 2 where the gas velocity at which extinction occurs is indicated for the different turbulence intensities used in the experiments. It is seen that flame extinction occurs at lower flow velocities when the turbulence intensity is increased. This result, although it is in general agreement with the other flame spread results, is somewhat unexpected since turbulence is often viewed as a means to enhance fuel combustion processes.

II. Flame Spread in a Concurrent Turbulent Flow

Experiments are currently being conducted to study the effect on the spread of flames over thick PMMA of the turbulence intensity of an air flow moving in the direction of flame propagation. The experimental procedure is basically the same as that described in the previous section.

The measurements of the flame spread rate as a function of the concurrent air flow velocity are shown in Fig. 3 for several values of the turbulence intensity. It is seen that the spread rate increases approximately linearly with the flow velocity and that the slope becomes smaller as the turbulence intensity is increased. The effect of the turbulence intensity on the flame spread rate can also be deduced from the result of Fig. 3. It is seen that the rate of flame spread decreases as the turbulence intensity is increased, and that this trend is more noticeable for large flow velocities. This result, which is somewhat unexpected, is important not only because it introduces 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 and material flammability tests.

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 indicates that the spread rate is of the form $V_f \sim q^2 l_f$ where q is the surface heat flux, l_f the flame length. 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 this work the heat flux is calculated from the surface temperature histories and the flame length from the time lapsed from the instant the surface temperature starts to increase to the instant it reaches the pyrolysis temperature. The results show that for low turbulence intensities, the flame length increases with the flow velocity and for large turbulence intensities, it decreases. This effect seems to be due primarily to the convective cooling of the reaction zone by the cold air induced toward the flame by the turbulent eddies. This conclusion was reached through the qualitative information provided by interferograms of the flame and the visual observation of an apparent increase of the flame soot when the turbulence intensity is increased. The results for the variation of the heat flux with the turbulence intensity show that the heat flux is only weakly affected by the flow turbulence, decreasing slightly with the turbulence intensity for large flow velocities and increasing slightly for low flow velocities. All of the above results have been combined in Fig. 4 where the ratio $V_f/(Ul_f)$ is plotted versus the flow turbulence intensity. It is seen that this ratio is independent of the flow velocity and turbulence intensity, which indicates that the effect of the flow turbulence on the flame spread rate takes place primarily through the flame length. 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.

III. Publications and Presentations

Amos, B., Kodama, H. and Fernandez-Pello, A.C., "An Analysis of the Ignition by Vapor Radiation Absorption of Vaporizing Fuel at Zero Gravity," Progress in Astronautics and Aeronautics, 113, p. 115 (1988).

Amos, B. and Fernandez-Pello, A.C., "Ignition and Flame Development of a Vaporizing Combustible Surface in a Stagnation Point Flow," Combustion Science and Technology, 62, 4-6, p. 331 (1988).

Di Blasi, C., Crescitelli, S., Russo, G. and Fernandez-Pello, A.C., "Predictions of the Dependence on the Opposed Flow Characteristics of the Flame Spread Rate Over Thick Solid Fuels," 2nd International Symposium on Fire Safety Science, p. 119, (1988).

Di Blasi, C., Crescitelli, S., Russo, G. and Fernandez-Pello, A.C., "Model of the flow Assisted Spread of Flames Over a Thin Charring Combustible," 22nd International Symposium on Combustion, The Combustion Institute, p. 1205, (1988).

Zhou, L., Fernandez-Pello, A.C. and Cheng, R., "Flame Spread in an Opposed Turbulent Flow," submitted for publication in Combustion and Flame (1988).

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).

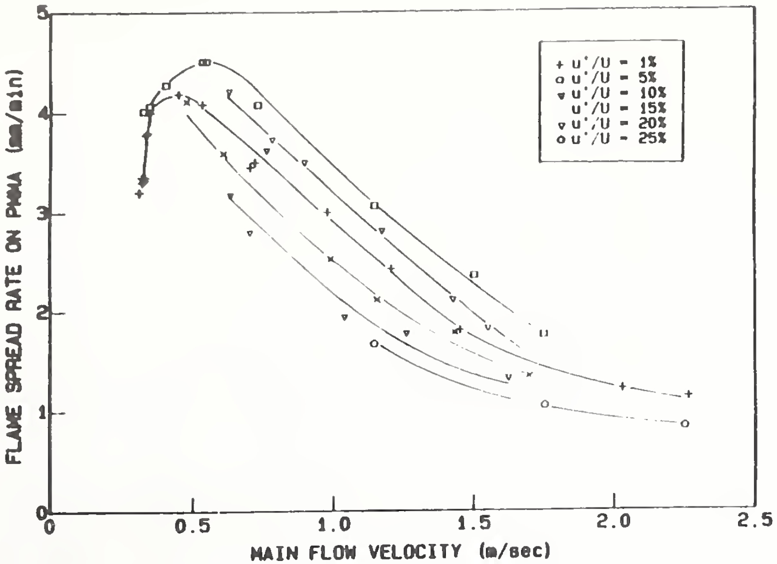

FIG.1. Opposed Flow. PMMA.

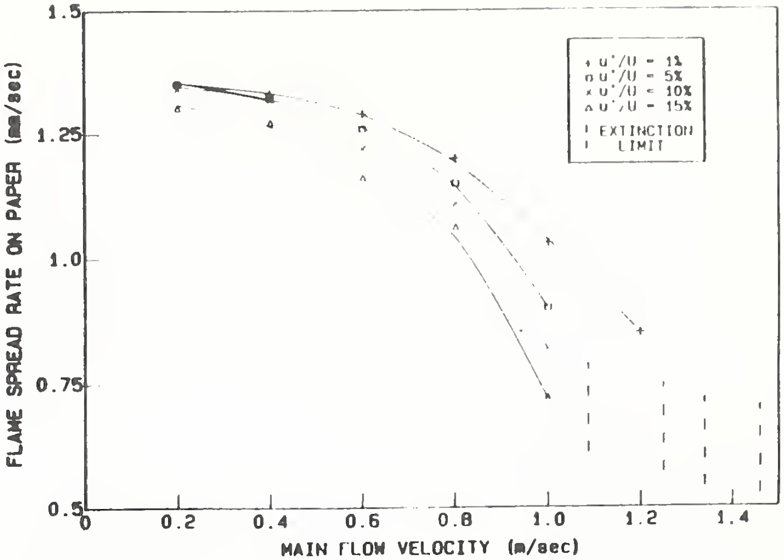

FIG.2. Opposed Flow. Paper

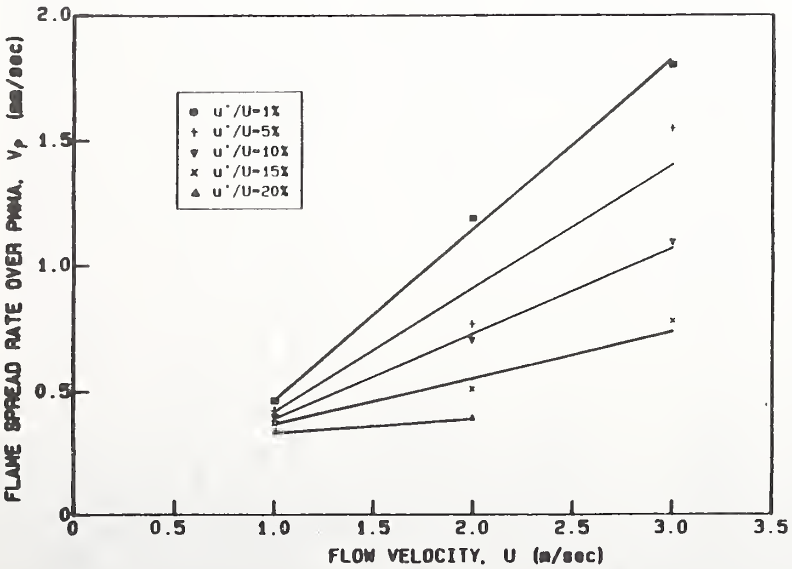

FIG.3. Concurrent Flow. PMMA

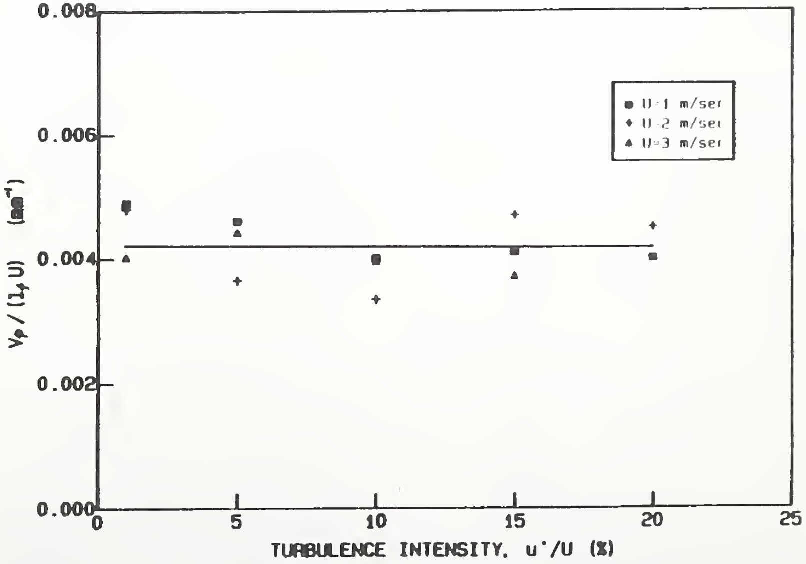

FIG.4. Concurrent Flow. PMMA

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution:	University of California at Berkeley
Grant No.	60NANB8D0848
Grant Title	Fire Modeling
Principal Investigator:	Professor Patrick J. Pagni Mechanical Engineering Department University of California Berkeley, CA 94720 Telephone: (415) 642-0729 FAX: (415) 642-6163
Other Professional Personnel:	Aruna Joshi (Ph.D. Candidate) Charles Fleischmann (Ph.D. Candidate) Joseph Viray (M.S. Recipient) Javier Trelles (M.S. Candidate) Sidney Huey (B.S. Recipient)
NBS Scientific Officer:	Dr. Howard R. Baum

Technical Abstract:

The overall goal of this project is to develop chemical, physical and mathematical models of the detailed combustion phenomena which control a fire's growth. Our emphasis recently has been on measurement of pool fire phenomena such as coherent structure shedding frequency and soot volume fraction, and on window breaking in compartment fires with subsequent combustion of accumulated excess pyrolyzates.

Pool Fire Vortex Shedding Frequencies:

Pool fires are defined as diffusion flames stabilized on a burning horizontal surface. Usually the fuel is solid or liquid phase and the mass transfer rate at the surface is controlled by heat transfer feedback from the flame. However, the data described here also include gas phase fueled flames on sintered burners at variable flow rates. A variety of pool shapes is also included from circular to rectangular.

It has been known for twenty years (1-17) that such fires pulsate with a regular frequency, releasing large annular vortices (coherent structures) from their bases, see e.g. Ref. 17. The unanswered question is:

> "Why does $f = 1.5D^{-0.5}$, where f is in Hz and D is in m, or $f(D/g)^{0.5} = 0.48$, describe the shedding frequency over three orders of flame base diameter, $5\text{cm} < D < 50\text{m}$?"

This fit is shown in Fig. 1, which contains all data pertinent to this question known to the author. Since the data shown in Fig. 1 represent a wide variety of fuels from methane to JP4, with no clear dependence on fuel type, the answer to this question may lie in the convective fluid mechanics rather than the combustion aspects of the problem.

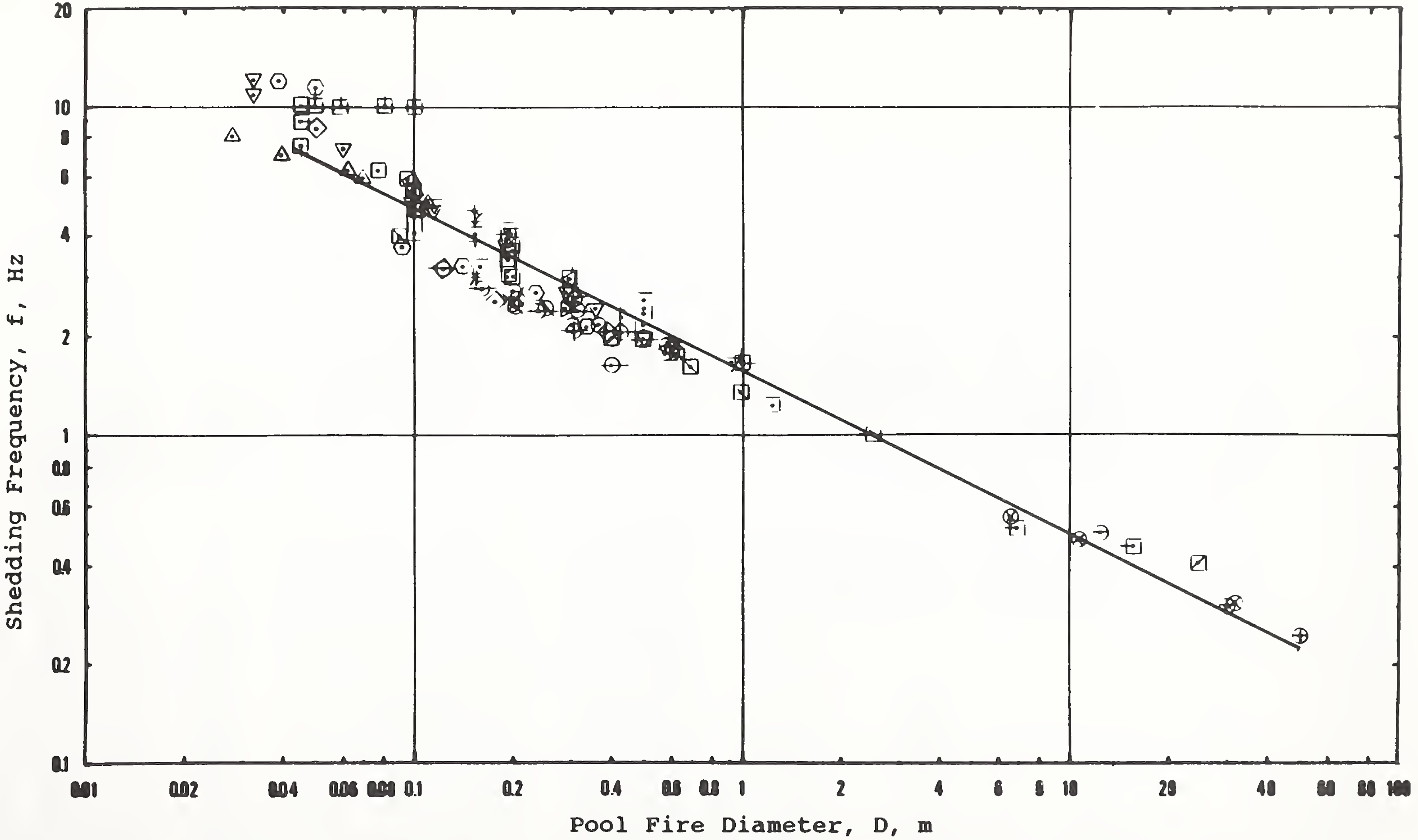

Fig. 1 Shedding frequencies as a function of diameter for the following fuels (ref. no.): Liquids - Ethanol ▽(3), □(2), ◇(7), ⦶(15); Methanol ○ (5), ○(13), □(14); JP4 ⊟(14), ⊖(16); Oils∗ +(1), ⊗(9); Gasoline + (1); Kerosene ⊕(9); Acetone ⊘(17); Heptane ⧅(10); Hexane □(14); and Pentane ⧄(14): Solids - PMMA △(4); Polyurethane -○-(13); and Wood ○(13): Gases - Natural Gas +(1), ⊘(6), ◁(8), ▯(11), ⊟(14); and Propane ▷(12), ○(13).

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3. Portscht, R., "Studies on Characteristic Fluctuations of the Flame Radiation Emitted by Fires," *Comb. Sci. Tech., 10,* 73-84, 1975.
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5. Hertzberg, M., et al., "The Diffusion Flame in the Free Convection," US Bureau of Mines Report RI8263, Washington, D.C., 1978, 33 pp. And private communication, February 6, 1989.
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12. Gengembre, E., et al., "Turbulent Diffusion Flames with Large Buoyancy Effects," *Comb. Sci. Tech., 41,* 55-67, 1984.
13. Beyler, C. L., "Fire Plumes and Ceiling Jets," *Fire Safety J., 11,* 53-75, 1986. See also "Entrainment in Pool-type Buoyant Diffusion Flames," Eastern States Section Meeting of the Combustion Institute, 1983.
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15. Joulain, P., Grosshandler, W., and Duparc, B. H., "Thermal Structures of Ethanol Pool Fires," Joint Meeting of the French and Italian Sections of the Combustion Institute, Paper 6.11, 1987.
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Other Activities:

Previous summaries have described our experimental results for the mean soot volume fraction, f_v, in a variety of fires. The two-laser apparatus for measuring f_v in pool fires has been reconstructed and connected to a Mac IIcx for data collection and interpretation. We are gathering data now to explore the range of application of our previously suggested correlation to pool fire f_v's.

Glass breaking in fires is a crucial pheomenon which we are examining both experimentally and analytically. Current results will be presented at this meeting. To date we have used the "FIRST" version of the Harvard V room fire model to predict the time of glass breaking by calling the windows remote objects with an ignition temperature of 360°K (a 60°C (108°F) glass temperature rise usually causes windows to break and become vents). Once the break time is known, "FIRST" is rerun with vents, of the same size and location as the windows, opening at the break time. Improving on this first approximation is the subject of our effort during this grant period.

We hope eventually to include a statistical approach to how much of a vent is actually created when the window glass breaks. It is also our goal to write a subroutine specifically describing glass breaking for "FIRST" and/or other compartment fire model programs. It is clear from real fire experience, particularly in hotels, that the introduction of fresh oxygen, when a window breaks, into a room charged with accumulated excess pyrolyzates has dramatic consequences. We are trying to model the flow, mixing and combustion processes as a gravity current moving from the new opening toward the fire plume followed by a turbulent premixed flame propagating throughout the compartment.

Finally, during this grant period, I was elected to the Executive Committee of the International Association of Fire Safety Science and we had the opportunity to host the very successful Eleventh Meeting of the United States-Japan Conference on Development and Utilization of Natural Resources (UJNR) Panel on Fire Research and Safety at the University of California at Berkeley in October 1989.

Books:

1. T. Wakamatsu, Y. Hasemi, A. Sekizawa, P. G. Seeger, P. J. Pagni, and C. E. Grant, eds., *Fire Safety Science - Proceedings of the Second International Symposium,* Hemisphere Publishing Co., New York, 1989.

Papers and Presentations:

1. P. J. Pagni, "Fire Physics - Promises, Problems and Progress," *Fire Safety Science - Proceedings of the Second International Symposium,* pp. 49-66, Hemisphere Publishing Co., New York (1989).
2. P. J. Pagni, "Glass Breaking in Fires," invited presentation at the Eleventh Meeting of the UJNR Panel on Fire Research and Safety, Berkeley, California, October 1989.
3. P. J. Pagni, "Pool Fire Vortex Shedding Frequencies," to be presented in the session "Open Questions in Fluid Mechanics" at the American Society of Mechanical Engineers Winter Annual Meeting, San Francisco, California, December 1989.

B. Soot Formation

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

SOOT FORMATION AND EVOLUTION

Staff

Kermit C. Smyth, Project Leader
George W. Mulholland, Project Leader
Nelson P. Bryner, Chemical Engineer
J. Houston Miller, Visiting Scientist

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 process of particles sticking and forming a cluster. The agglomerate structure consists of a number of primary particles with diameters of about 30 nm connected in a rather open structure. The light extinction coefficient and light scattering coefficient, both of which affect the visibility through smoke, are not well characterized for agglomerate structures. The aerodynamic properties, which control smoke deposition in the respiratory tract, are also poorly 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, carried out jointly with the Thermal Processes Division and the Chemical Kinetics Division at NIST. 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. The results show that acetylene plays the major role in surface growth on particles (as also found in premixed flame studies). Furthermore, direct tests of proposed models of chemical growth can now be made which strongly suggest that a pathway involving vinyl radical addition to acetylene is the fastest route to form benzene. Experiments have also investigated fuel structure effects on chemical growth pathways by the addition of small amounts of ethylene, butadiene, and toluene to the base methane flame.

Recently we have made the first quantitative OH· concentration measurements in a hydrocarbon diffusion flame. These 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. New results have also been obtained for detection of H·, O:, C:, CH·, O_2, and CO by means of multiphoton ionization spectroscopy. Profiles of these species (especially H·, O:, and CO) are being measured in our methane/air diffusion flame. Future work will focus on establishing reduced chemical mechanisms for hydrocarbon oxidation and growth processes.

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. Recently we have upgraded the instrument by using low temperature coefficient feedback resistors for the operational amplifiers associated with the Si detectors, by replacing optical flat beam dividers with wedges, and by fabricating rigid mounts for the optical components. These changes have reduced the drift in the ratio of transmitted to incident light intensity by a factor of about 10 to a few parts in 10,000 over ten minutes. This improvement will allow the characterization of optical properties of smoke at concentrations as low as 0.2 mg/m^3. Preliminary results with the improved system indicate that the optical properties of acetylene soot are changed by exposing the soot to a slight water supersaturation of a few percent.

A Smoke Aging/Dilution chamber has been used in the past year to measure the agglomeration rate of smoke and the effect of agglomeration on the light extinction coefficient. The 1 m^3 chamber was rapidly filled with smoke from a 0.6 meter crude oil pool fire. The number and mass concentration of the smoke particulate were monitored over a one to two hour period as the smoke aged. By controlling the wall temperature of the chamber, data were obtained for smoke near ambient temperature and smoke at about 100°C. The measured agglomeration rate was $8 \pm 4 \times 10^{-10}$ cm^3/s at 25°C and $13 \pm 7 \times 10^{-10}$ cm^3/s at 100°C. The light intensity transmitted through the chamber was monitored at three wavelengths, 450, 630, and 1000 nm. The value of the extinction coefficient per unit mass did not change by more than a few percent over the 90 minute aging period for either the ambient temperature smoke or the hot smoke. The results for the specific extinction coefficient are 5.1 ± 0.4 m^2/g (1000 nm), 7.8 ± 0.6 m^2/g (630 nm), and 9.7 ± 0.7 m^2/g (450 nm).

Publications

P. J. H. Tjossem and K. C. Smyth, Chemical Physics Letters 144, 51 (1988). Multiphoton Ionization Detection of CH, Carbon Atoms, and O_2 in Premixed Hydrocarbon Flames.

G. J. Rosasco, A. D. May, W. S. Hurst, L. B. Petway, and K. C. Smyth, Journal of Chemical Physics 90, 2115 (1989). Broadening and Shifting of the Raman Q Branch of HD.

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

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

G. W. Mulholland, The SFPE Handbook of Fire Protection Engineering, edited by P. DiNenno, C. Beyler, R. Custer, W. Walton, and J. Watts, published by the Society of Fire Protection Engineers, Boston, 368 (1988). Smoke Production and Properties.

G. W. Mulholland, R. J. Samson, R. D. Mountain, and M.H. Ernst, Energy and Fuels 2, 481 (1988). Cluster Size Distribution for Free Molecular Agglomeration.

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R. D. Mountain and G. W. Mulholland, Langmuir 4, 1321 (1988). Light Scattering from Simulated Smoke Agglomerates.

P. Meakin, B. Donn, and G. W. Mulholland, Langmuir, in press. Collisions between Point Masses and Fractal Aggregates.

Related Grants

1. Soot Morphology and Radiation in Turbulent Flames, Richard A. Dobbins, Brown University.
2. Products of Incomplete Combustion: Formation and Emission from Diffusion Flames, J. Houston Miller, George Washington University.
3. Soot Particle Formation and Destruction in Diffusion Flames, Robert J. Santoro, Pennsylvania State University.
4. Kinetics of Aggregates, James A. Gentry, University of Maryland.

Center For Fire Research
National Institute of Standards and Technology
FY 89

Institution: Brown University

Grant No.: 60NANB6DO643

Grant Title: Soot Morphology in Flames

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

Other Professional Personnel: Dr. C. M. Megaridis, Post Doctoral Research Investigator through June 1988.

NIST Scientific Officer: Dr. George W. Mulholland

Technical Abstract:

The object of this research has been to examine the morphogical properties of soot particles within flames or released from flames, and to gain from this examination a deeper understanding of the soot properties and the history of its formation and oxidation or release to the surroundings.

1. **Experimental Results:** During the past year the thermophoretic sampling technique developed earlier was used to probe the smoking flame for purposes of comparing the vertical variation of primary particle diameter with the nonsmoking flame. The vertical survey of the primary diameters of these two flames is given in Fig.1 where it is apparent that the sizes in the lower 40 mm. of both flames are identical. Furthermore, the primary diameters in the smoking flame (solid symbols) are nearly identical to the sizes displayed by the nonsmoking flame (open symbols). These observations support the view advanced by others that the taller smoking flame allows more cooling of the soot field by radiation. This lower temperature results in a lower oxidation rate that permits the soot to escape to the surroundings. A detailed discussion of these results is given in an impending publication listed below (Ref. P4).

Examination of our data on these two ethene diffusion flames has lead us to conclude that the growth of the soot particles in flame is well described in terms of the growth of fractal aggregates. In particular it is found that the growth of the primary particles by heterogeneous reactions can be described by monomer-cluster aggregation which results in compact structures with a fractal dimension of 3. The aggregates experience growth through collisions resulting in cluster-cluster aggregation that form tenuous structures of fractal dimension equal to 1.7 to 1.9. These points have been discussed in our article on flame generated fractal materials where comparisons are made on the results of a number of investigations of pyrogenic soot and silica. In a wide range of experiments involving many hydrocarbon fuels it is found that the primary particle diameters, when they are determined through examination by electron microscopy, lie in the range of 10 to 40 nm.

The fractal dimensions for both carbonaceous soot and silica fume, where reported, are in the range of 1.7 to 1.9 as is typical when cluster-cluster aggregation is also present a growth mode. This information [Ref. P5] provides very important leads in the formulation of the optical properties of these materials in more detail than has previously been possible.

2. **Formulation of Optical Cross Sections of Aggregated Material:** The optical cross sections for differential scattering, for total scattering, and for absorption have been formulated in terms of the properties which describe the aggregate morphology, viz., fractal dimension, radius of gyration, and primary particle diameter. Our formulation also includes the polydispersity of the aggregate population that is the inevitable result of the cluster formation process. In Figs. 2 and 3 we show the C_{vv} differential cross section (for vertically polarized both incident and scattered light) and the total differential cross sections (for natural light), respectively. The quantities $\overline{I^A}$ and $\overline{\vartheta^A}$ are the average cross sections normalized by the Rayleigh differential cross section for the primary particle, $\overline{n^2}$ is the second moment of the aggregate size distribution function, $\overline{R_g^2}$ is the mean square radius of gyration, k is the wave number and $q = 4\pi \sin(\theta/2)/\lambda$ is the modulus of the scattering vector. The open symbols in Figs. 2 and 3 represent the results of calculations using our porous sphere model for 45 sets of polydispersions of narrow, moderate and wide of distribution functions and for $\pi d_p/\lambda$ varying from 0.01 to 0.1, where d_p is the primary particle diameter. The points in these figures represent the computer simulations of Mountain and Mulholland (Ref. R1). The smooth lines are equations that are based on the considerations given above. Two applications of these results to fire research are given below. A publication with the details of these developments is in progress (Ref. P7).

3. **Applications to Smoke Obscuration:** The optical cross sections are used to formulate the aggregate albedo, specific extinction and volumetric extinction P_{ext}. The latter is the extinction cross section times the wavelength divided by the volume of the aggregate. This quantity has often been presented as calculated from the Mie theory for spheres even when the primary interest is the highly nonspherical chained aggregate. In Fig. 4 we compare P_{ext} for a sphere and for an aggregate of variable chain lengths and volume-equivalent diameter D when the refractive index m = 2-i1, the primary size d_p = 40 nm and the wavelength of light λ is the midpoint of the visible range at λ = 555 nm. In the small size limit both curves coincide with the Rayleigh results. At intermediate and large values of $\pi D/\lambda$ the two curves are dramatically different. The results similar to those depicted in Fig. 4 explain the aging smoke tests conducted by Bryner and Mulholland at the NIST, and permit the calculation of smoke obscuration with a greater confidence than has been possible in the past.

4. **The Applications to Laser Diagnostics:** The widespread use of laser scattering techniques to monitor the formation, transport, and oxidation of soot in flames in the past has been based on the the assumption of sphericity of the scattering particles. As a result of the formulation of the morphology of polydispersions of aggregates and their scattering properties, we are now in a position to devise and apply a more realistic data reduction process for the laser scattering experiment. This has been accomplished using the data reported previously (Ref. R2), and a journal article on this subject is in preparation (Ref. P8). The analysis yields the usual quantities (aggregate volume fraction, volume-equivalent diameter, and number concentration) and, additionally variables describing the aggregate morphology (primary particle diameter, mean square radius of gyration, average number of primary particles per aggregate, and number

concentration of primary particles). The values of these quantities that are derived from the coannular ethene flame are consistent with the growth of the aggregate structures by the combined effects of surface reactions and cluster-cluster aggregation.

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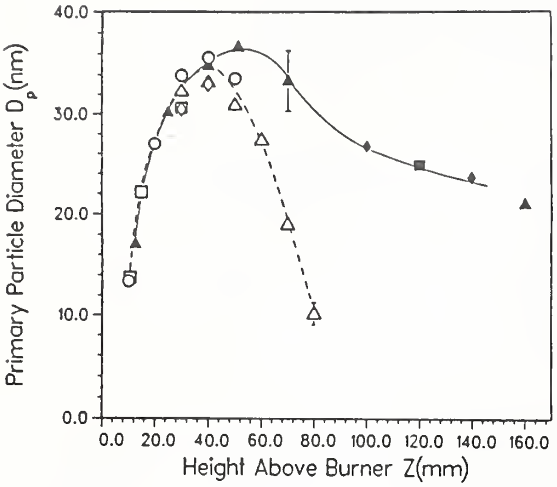

Fig. 1. Primary Particle Diameter vs. Height Above the Burner for Nonsmoking Flames.

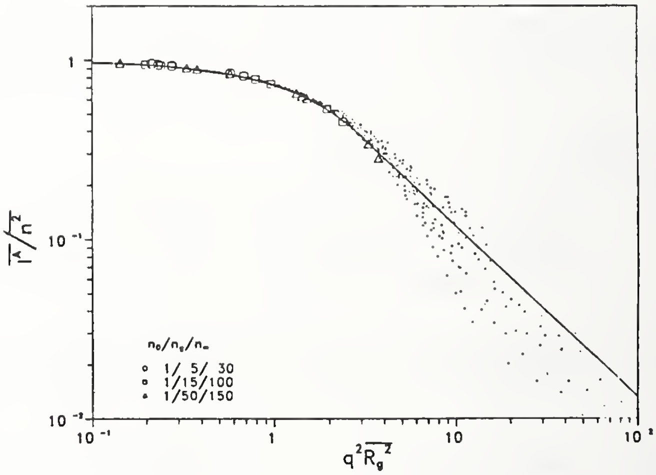

Fig. 2. Dimensionless Differential Scattering Cross Section vs. $\overline{(qR_g)^2}$. See text for symbols.

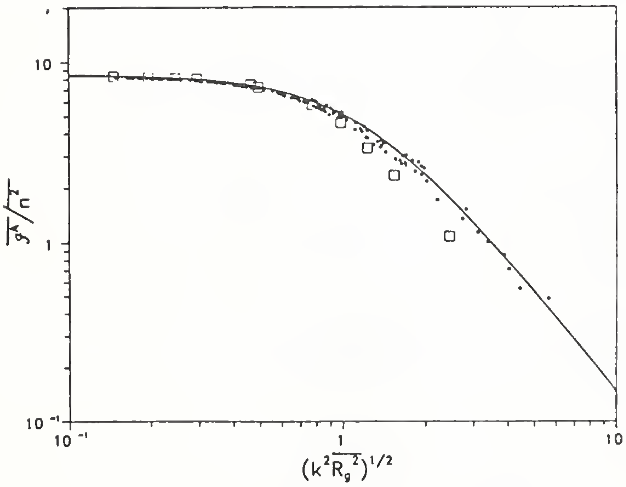

Fig. 3. Dimensionless Total Scattering Cross Section vs. $\left[\overline{(kRg)^2}\right]^{1/2}$. See text for symbols.

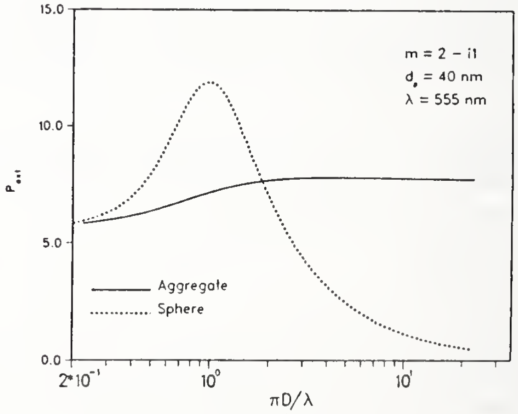

Fig. 4. Volumetric Extinction vs. $\pi D/\lambda$ for Sphere and Aggregate of Volume Equivalent Diameter D.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: The George Washington University
Grant Number: 60NANB6DO625
Grant Title: Chemical Pathways to Soot Formation in Diffusion Flames
Principal Investigator: Professor J. Houston Miller
Department of Chemistry
The George Washington University
Washington, DC 20052
(202) 994-7474

Other Professional Personnel: Dr. Anthony Hamins, Postdoctoral Research Assoc.
NBS Scientific Officer: Dr. Kermit C. Smyth

Technical Abstract:

Hydroxyl Radical Measurements and Chemistry

Over the course of the past year our group has combined with workers within the Center for Fire Research to make quantitative determinations of hydroxyl radical concentrations in our methane/air laminar diffusion flame [1]. Hydroxyl radical is a very important species to add to our data base for two reasons. First, hydroxyl radical has been the greatest success of the ten years of effort expended in the development of laser diagnostics for combustion. Second, hydroxyl radical is a very important flame species. Because it is involved in fast radical shuffle reactions, its concentration may fix the concentrations of other flame species such as hydrogen atom and some of the hydrocarbon radicals. Further, hydroxyl radical destruction of carbon monoxide is the dominant loss mechanism for this species (R5). Profiles of hydroxyl concentration may allow a greater understanding of the limits of carbon monoxide oxidation (and thus emission) in hydrocarbon diffusion flames. Some comments on hydroxyl radical and carbon monoxide chemistry appear below.

In our analysis of the hydroxyl radical data, we spent a considerable amount of effort in exploring the validity of equilibrium (both full and partial) assumptions in our flame system. It is appropriate to review these findings.

Partial vs. Total Equilibrium

Bimolecular Reactions:

R1) $H\bullet + O_2 \rightleftharpoons OH\bullet + O:$
R2) $O: + H_2 \rightleftharpoons OH\bullet + H\bullet$
R3) $OH\bullet + H_2 \rightleftharpoons H_2O + H\bullet$
R4) $2OH\bullet \rightleftharpoons H_2O + O:$
R5) $CO + OH\bullet \rightleftharpoons CO_2 + H\bullet$

Recombination Reactions:

(a) $H\bullet + OH\bullet + M \rightleftharpoons H_2O + M$
(b) $H\bullet + O: + M \rightleftharpoons OH\bullet + M$
(c) $H\bullet + H\bullet + M \rightleftharpoons H_2 + M$
(d) $O: + O: + M \rightleftharpoons O_2 + M$
(e) $CO + O: + M \rightleftharpoons CO_2 + M$

Box 1: Radical Reactions Near the Flame Front.

Near the high temperature reaction zone of a diffusion flame, there are two important classes of radical reactions: bimolecular shuffle reactions, in which radical character is maintained in the products of the reaction; and recombination reactions, where radicals are lost. Near the high temperature reaction zone of a diffusion flame, these reactions include those shown in Box 1. At temperatures as high as those encountered near the flame front, the gas density is relatively low and third body reactions such as the recombination processes are slow compared with bimolecular processes. Under these conditions, radical concentrations in excess of those calculated assuming full equilibrium, can be observed. On Figure 1, the experimental hydroxyl radical concentration is compared with the calculated full equilibrium value. At the location of the peak hydroxyl concentration, the experimental value exceeds the full equilibrium value by a factor of 3.

If the bimolecular radical reactions listed in Box 1 are fast relative to other chemical or transport processes in the flame, then it is possible that these reactions are equilibrated; i.e. the rate forward is exactly balanced by the reverse rate. This hypothesis can be checked by comparing radical concentrations calculated assuming partial equilibration with experimental values. For example, a linear combination of R1 and R2 suggests the following expression for the hydroxyl radical concentration:

$$[OH\bullet] = (K_1 \cdot K_2 \cdot [H_2] \cdot [O_2])^{1/2} \qquad \text{(Eq. 4)}$$

where the Ks refer to the equilibrium constants. The predicted profile assuming equilibrium in reactions R1 and R2 is shown in Figure 1. As this data suggests, these reactions are not equilibrated near the high temperature reaction zone of our diffusion flame.

Carbon Monoxide Chemistry

As a result of our effort in collecting and analyzing the hydroxyl radical data, we can now offer some preliminary observations concerning CO formation and oxidation in the methane/air flame. A brief review of the literature of carbon monoxide chemistry in diffusion flames reveals that a common theme has been *simplification*. A few of the schemes devised for CO chemistry have been:

- mixture fraction correlations
- the water-gas shift reaction
- global oxidation kinetics.

These approaches share a common strategy: each is based on assumptions of equilibrium, which may not be valid in our flame system.

Assume R5 dominates CO destruction

$$d[CO]/dt = -\, k_5\, [CO]\, [OH]$$

Estimate [OH] from partial equilibrium

$$\text{R4)} \quad 2OH\bullet = H_2O + O{:}$$

$$\text{(d)} \quad O{:} + O{:} + M = O_2 + M$$

$$[OH] = K_d^{1/4}\, K_4^{1/2}\, [O_2]^{1/4}\, [H_2O]^{1/2}$$

$$d[CO]/dt = -\, k_{overall}\, [CO]\, [O2]^{1/4}\, [H2O]^{1/2}$$

Box 2: Equilibrium assumptions implicit in global oxidation kinetics for carbon monoxide.

Mixture Fraction Correlations

For a number of years it has been known that the concentrations of many species in a diffusion flame (including CO) can be collapsed onto a single curve when plotted against a non-dimensional parameter of the local stoichiometry, such as either mixture fraction or equivalence ratio [3,4].

There has been some dispute as to why this approach should work. Our working hypothesis has been that the mixture fraction correlation is appropriate when the controlling chemical rates for a particular species are fast relative to transport phenomenon. This condition will be met when the flame chemistry is either fully or partially equilibrated. However, rarely do flame species come close to their full equilibrium values, and further, the mixture fraction correlation may still be applied to species whose concentrations are not even in partial equilibrium. We will return to the *why* of mixture fraction correlations at the end of this report, but for the moment it is sufficient to note that this correlation does *not* imply equilibrium.

Global Oxidation Kinetics

Another common simplification of CO chemistry recognizes the dominant role reaction R5 has in carbon monoxide oxidation. As shown in Box 2, implicit in this scheme are two critical assumptions: first, the hydroxyl radical concentration can be estimated from partial equilibrium. As we have seen above, this is a somewhat dubious assumption even for bimolecular processes. The argument is made even weaker by requiring one of the reactions in the partial equilibrium assumption to be a recombination process. The second assumption is that R5 is an irreversible reaction. This assumption will fail when hydrogen atom concentrations are on the same order as hydroxyl radical, which our calculations suggest is true near the flame front of our flame.

To check the validity of the global oxidation scheme, Figure 2 compares the experimental rate for carbon monoxide disappearance with those predicted from three different values for the overall oxidation rate constant [5]. Note that oxidation rates are plotted on a log plot covering six orders of magnitude. None of the calculated curves adequately describes the experimental data. The reversibility of R5, which contributes to this disagreement is explored below.

Water-Gas Shift Reaction

In both real fires and in practical combustors, the relative concentrations of carbon monoxide and carbon dioxide is often used as an indicator of the completeness of the combustion process. On a more fundamental level, many researchers have used the water gas shift equation (Box 3) as an indicator of the combustion efficiency. Further, this reaction is often used as a test of equilibrium in flame environments. As shown in Box 3, the water gas shift equation is really a linear combination of two of the bimolecular processes shown in Box 3. Our analysis of partial equilibrium in the methane flame suggests that one of the reactions which makes up the water-gas reaction is equilibrated near the high temperature reaction zone (R3). Our calculations show that, within the accuracy of the experimental measurements, the water-gas reaction can be considered in or near equilibration. This result suggests that R5 must be near equilibrium. Because equilibrium of R5 requires a substantial reverse reaction rate, the global oxidation of CO would fail under these flame conditions.

Water-Gas Shift Reaction

R3) $OH\bullet + H_2 = H_2O + H\bullet$

R5) $CO + OH\bullet = CO_2 + H\bullet$

R5-R3 $CO + H_2O = CO_2 + H_2$

Box 3: Partial equilibrium assumptions of the water-gas shift equilibrium.

The Right Way to Think About Diffusion Flames

As discussed earlier, mixture fraction correlations are appropriate when a species' dominant chemistry is faster than transport processes. This would be true when a species is partially equilibrated, but also seems to be true even when a species does not participate in a single, equilibrated, elementary reaction.

In the last few years, there have been a number theoretical attempts made to understand the laminar flamelet concept [6]. The most intriguing of these have been able to reduce complicated chemical codes to just a few composite processes which adequately describe the chemistry of the major species and accurately predict the state relationships. To make complicated chemistry computationally easier, it is necessary to reduce the number of species in the calculation (the computation time goes as the number of species squared, but is more or less independent of the number of reactions relating these species to one another). This can be accomplished by assuming partial equilibration for some reactions (for example, hydrogen atom concentrations can be written in terms of $OH\bullet$, H_2O and H_2 via R3) or by imposing the steady state assumption on some species. In our work, we have used the species conservation equation

$$R_i = \nabla(Ni(V + v_i)) \qquad \text{(Eq. 5)}$$

to develop chemical insight into the chemistry of our flame. In this work, the transport rates (both convection and diffusion) are set equal to chemical rates. For the steady state assumption to be valid, contributions to the chemical rates (individual forward and reverse reactions) must be much faster than their sum, i.e. much faster than transport processes. For example, the forward and reverse rates for reactions R1-R3 have been calculated to be on the order of 10^{-2} - 10^{-1} mole/cc·sec. However, the sum of transport rates calculated for hydroxyl radical was much smaller, with a peak of only 10^{-5} mole/cc·sec. Therefore, for hydroxyl radical near the flame front, the steady state assumption would be valid.

It is obvious that there are some species and some places in a laminar diffusion flame where the mixture fraction correlations will work. It is just as obvious that these state relationships are not universal: subtle changes in the local chemistry can upset the steady state conditions. For example, oxygen atoms, assumed to be in steady state in the reduced kinetic schemes, react rapidly with acetylene, a species present in high concentrations in hydrocarbon diffusion flames. In a turbulent flame, it is likely that large concentrations of acetylene could mixed into a reaction zone and upset the oxygen atom steady state balance.

Understanding diffusion flame chemistry requires quantifying the limits of these simplifying assumptions. As this report has illustrated, even the most complex simplification schemes have definitive limits of application.

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Recent Publications:

"Concentrations and Production Rates of Hydroxyl Radical in a Laminar Methane/Air Diffusion Flame.", K.C. Smyth, P.J.H. Tjossem, A. Hamins, and J.H. Miller, Combust. Flame, in press.

"Partial Equilibrium in Laminar Hydrocarbon Diffusion Flames." J.H. Miller and K.C. Smyth, Chem. Phys. Processes Comb. 1988, paper .

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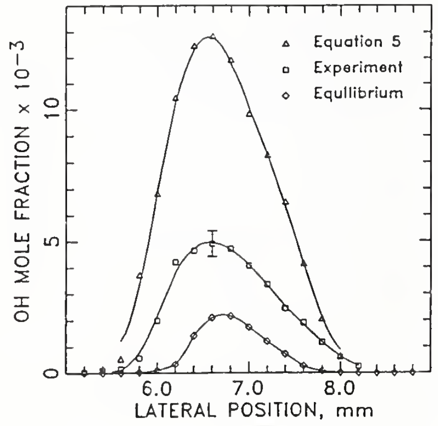

Figure 1 Comparison of experimental hydroxyl radical profile with predictions of full and partial equilibrium.

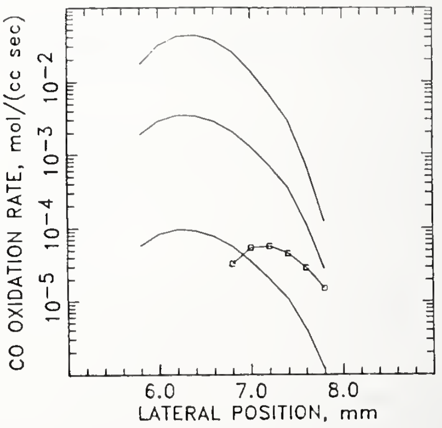

Figure 2 Comparison of global oxidation rates for carbon monoxide with experimental loss rate.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution:	The Pennsylvania State University
Grant No.:	60NANB7D0706
Grant Title:	Soot Particle Formation and Destruction in Diffusion Flames
Principal Investigator:	Dr. Robert J. Santoro Department of Mechanical Engineering 313A Mechanical Engineering Building 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 formation of soot particles has important effects on energy transfer and combustion product emissions from fires which dramatically impact loss of life and property. The objective of the present study is to provide a fundamental understanding of the soot formation and destruction processes which impact fire growth, spread and emissions. The approach adopted emphasizes two elements of the problem. The first element concentrates on the processes responsible for the conversion of fuel carbon to soot (i.e. particle inception and surface growth) and particularly stresses the importance of fuel molecular structure. The second element examines the destruction stage of the process which reduces the soot concentration in the latter parts of the flame. In particular, specific information on the relationship between soot and CO production is sought. A basic thrust of the work is to identify the overall mechanism relating the emission of CO and soot particles from flames. In addition, fundamental information on soot oxidation processes as well as the role of soot particles in the competition for oxidizing species such as O_2 and OH may be forthcoming.

The results of this study are of direct relevance to the problems of fire research. Soot particle formation and destruction along with other basic phenomena such as ignition, hydrocarbon chemistry, turbulence, radiative transfer and plume dynamics constitute the fundamental elements of the fire problem. Soot particles, once formed, are not passive species in the evolution of the fire situation. Through their radiative properties, soot particles can strongly enhance flame spread rates or the conditions necessary for "flash over" to occur. Soot particles present other complications through their role in visual obscuration and potential effects on carbon monoxide formation. These effects represent serious problems in terms of victim escape from fire situations and significantly contribute to fire mortality rates. However, with a proper understanding of the fundamental controlling mechanisms, significant improvements in the predictive capabilities of fire science modeling can dramatically improve the present situation.

Experimental Approach These studies are carried out using a coannular diffusion flame facility to which extensive laser-based diagnostics can be applied for particle and velocity measurements. The burner, which has been previously described in detail [1], consists of a 1.1 cm diameter fuel tube surrounded by a 10 cm diameter air annulus. The fuel flow can consist of up to three metered gases which provides for the study of fuel mixtures. The burner is mounted on computer controlled motorized stages which traverse the burner to obtain measurements over the cross section of the flame at a particular height.

In order to accomplish the objectives of this study, a number of measurement capabilities are required. These include laser light scattering for particle sizing, laser velocimetry for velocity measurements and intrusive probing for temperature and species concentration measurements. Figure 1 shows a schematic representation of the laser scattering/extinction system used to characterize the soot particle field throughout the flame. This facility provides measurements at three angles (45°, 90°, 135°) as well as determination of the light extinction. Polarization rotation capability allow measurements as a function of the laser polarization to be obtained as well. The individual photodetectors are connected to separate lock-in amplifiers which are interfaced to a laboratory computer. A similar arrangement is used for the laser velocimetry measurements. Gas sampling measurements are obtained using water cooled metal sampling probes. Two probes have been constructed during the last year having sampling orifices of 0.8 and 2.0 mm. For sampling in highly sooting flames, the probes have a high voltage applied to repel soot particles from the sampling orifice and, thus, impede soot clogging of the probe tip. Experience with these probes will be described below. Analysis of the gas samples is achieved on-line using NDIR analyzers for CO and CO_2 or off-line using gas chromatography (GC). Recently, GC analysis has been more prevalent in order to provide a more complete analysis of the gases present in the samples. For the GC analysis, samples are taken and stored in a multiport sampling loop. This procedure allows up to sixteen samples to be obtained for analysis.

Technical Accomplishments The present research program emphasizes the understanding of soot formation as it relates to important fire phenomena. The effect that fuel molecular structure has on the production of soot particles has been a major element of the current effort. Results regarding the effects on surface growth and precursor formation have been described previously [2]. Recent work has emphasized the formation of CO in the region above the flame under conditions where the soot concentration is systematically varied. The objective of these studies is to determine the mechanism by which increased amounts of CO can be emitted from diffusion flames. In particular, the effects of temperature decreases resulting from increased soot radiation as opposed to competition from soot particles for oxidizing species such as O_2 and OH are to be addressed.

The study of CO emission as a function of soot production, presents several measurement challenges. First a systematic, well characterized variation of the soot particle field is required. Secondly, a means to obtain gas sampling measurements in regions in which substantial amounts of soot particles are present is necessary. The first condition has been addressed by using a fuel mixture approach to provide a series of laminar diffusion flames in which the concentration of soot is varied by adding fuels exhibiting different sooting propensities to a methane baseline flame. In this approach the overall flame shape and size is maintained approximately the same, while the soot concentration and emission characteristics from the flame change significantly. To accomplish this variation, butane, 1-butene and 1,3-butadiene have been selected for study.

In order to measure CO and CO_2 in these flames, the previously mentioned gas sampling approach utilizing water cooled probes has been employed. To overcome problems associated with plugging of the probe, a high potential (1000-2000 volts) is applied to the probe to repel soot particles from the orifice region. This technique has worked sufficiently well with both the 0.8 and 2.0 mm orifice probes to allow sampling in the 1-butene/methane flame which is observed to emit copious amounts of soot. During the current year of this study, an investigation of the charged probe technique has been undertaken. The region over which the probe allows suitable sampling has been examined. An evaluation of perturbations introduced by the charging of the probe for locations inside the flame as well as above the flame is also underway. In general, the charged probe has been observed to operate satisfactorily in the region above the flame to heights approaching 20 cm from the burner exit. Above this height, probe clogging for the 0.8 mm orifice occurs. This is likely a result of the presence of large agglomerated particles which are not charged in these cooler regions. For samples obtained inside the flame, application of the sufficiently high voltages needed to repel the particles (500-1000 volts) often result in a flame oscillation. Thus, the occurrence of this phenomena limits the application of the charged probe technique within the flame. Measurements have been obtained over an extensive region of the flame and present efforts are focussing on quantitative effects regarding the emission of CO from the flame.

Figure 2 shows the measurements of the CO concentration along the centerline in a series of laminar diffusion flames. The flames burning solely methane or ethene show very similar profiles with the CO concentration rapidly decreasing with the distance above the flame. These ethene and methane flames correspond to non-soot emitting conditions with the exception of the ethene flame with a fuel flow rate of 4.9 cm^3/s. This flame is just slightly above the soot point. The results for a more heavily sooting butene/methane flame are also shown. For this case the rate of decrease of the CO concentration is significantly reduced and, in fact, does not reach zero within the measurement region of these flames.

Two processes are responsible for the decrease in the CO concentration with increasing distance along the flame. One is due to mixing of the surrounding flow with the flame products, while a second is the result of reaction of CO with oxidizing species to form CO_2. An estimate of the effect of mixing can be obtained from the CO_2 concentration profile along the centerline. Although some increase in the CO_2 concentration does result from the oxidation of CO, its contribution is small. Figure 3 shows the CO_2 concentration profiles for the methane and butene/methane flames, while figure 4 shows the profile of the CO concentration corrected for mixing effects. The results shown clearly indicate that the oxidation rate for CO is significantly reduced in the butene/methane flame. As to the source of the difference in the observed rate, analysis is presently proceeding to evaluate the effect of temperature differences in the flames on the oxidation process. The temperature in the butene/methane flame is 200-300 K lower than the methane flame. Analysis based on global reaction rates for moist CO oxidation are presently being evaluated for comparison with the present results. Based on this analysis, the potential effect from competitive reactions with soot particles for OH and O_2 will be evaluated.

The above results clearly demonstrate that soot production can have significant effects on chemical reaction rates occurring in flames. The source of the observed effect must still be established since both temperature and competitive reaction mechanism are relevant. Clearly, soot particle effects can dramatically effect the fire emission scenario and, thus, impact loss of life in fire situations.

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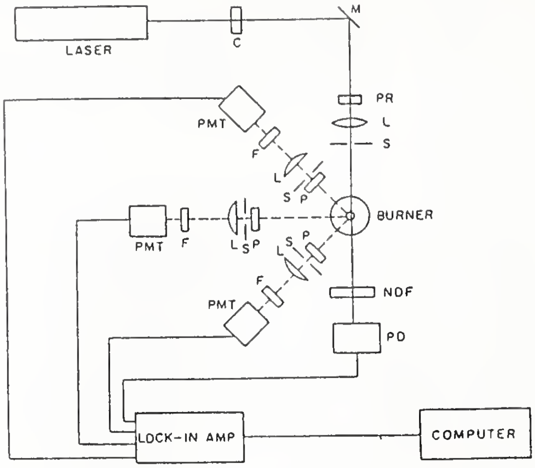


Figure 1. Schematic of laser scattering/extinction system: C = chopper, M = mirror, PR = polarization rotator, L = lens, S = spatial filter (circular aperture), NDF = neutral density filter, PD = photodiode, P= polarization, F = narrowband filter, PMT = photomultiplier

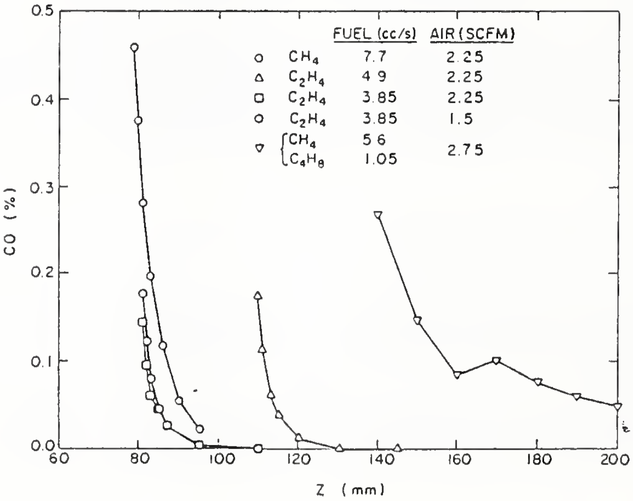
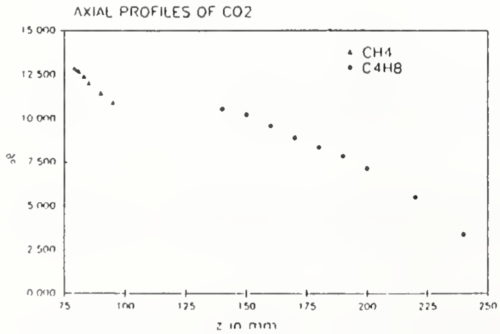


Figure 2. Centerline profiles of the CO concentration in a series of laminar diffusion flames.



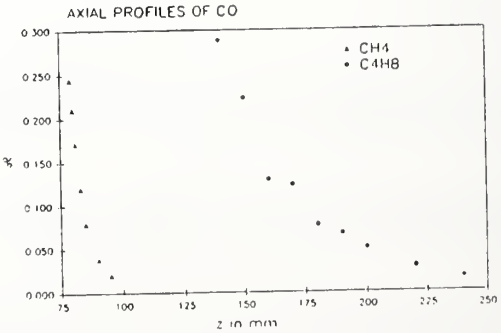


Figure 3. Centerline profiles of the CO_2 concentration in the methane and 1-butene/methane laminar diffusion flames (see figure 2 for flow conditions).

Figure 4 Centerline profiles for CO in the methane and 1-butene/methane flames corrected for the effect of mixing

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution : University of Maryland

Grant No. : 70 NANB8H0852

Title : Kinetics of Aggregates

Principal Investigator : Professor James W. Gentry
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Other Professional Personnel : Thomas G. Cleary

NIST Scientific Officer : Dr. George Mulholland

Technical Abstract :

The overall goal was to relate the aerodynamic, electrical, and optical properties of soot clusters with their geometric structure. Secondly to relate the aerosol formed to the parameters characterizing the soot flame. The use of fractals to characterize the soot clusters was investigated both theoretically and experimentally. It was found necessary to introduce three and possibly four dynamic regimes to describe different operating regimes of the burner.

Combustion Regimes

All of the quantitative experiments were with aerosols of soot formed from the partial oxidation of acetylene in a Santoro type diffusion burner. The acetylene flow rate was varied from 0.02 to 0.08 l/min. This covered the range from no visible soot (although the luminescence of the flame suggested the formation of carbon particles), to very large aggregates of several mm size. The mode of formation for the clusters was controlled by the acetylene flow rate. Below 0.04 l/min there was no visible formation of soot and the clusters appeared to consist only of primary particles. In a narrow intermediate zone of 0.04-0.045 l/min. the aerosol consisted of small agglomerates of 10^2 to 10^4 primary particles. These agglomerates appeared to be fractal. For acetylene flow rates > 0.045 l/min the clusters were no longer fractal but were porous aggregates. There appeared to be a transition zone between the fractal-like agglomerates and the aggregates, but this was not unambiguously established.

Formation of Primary Particles

When the flow rate was less than 0.04 l/min. there was no visible ribbon of soot formed, but the concentration of nuclei increased by four orders of magnitude. The size of the clusters was measured by two methods. The particle concentration before and after a diffusion battery was measured as a function of flow rate through the battery. The aerosol had a very narrow size distribution with a mean diameter of 10-12 nm. This diameter was independent of acetylene flow rate. This implies that below the sooting limit, increased acetylene concentration results in more particles of the same size. The mean size was decreased by 2-3 nm when the burner was redesigned to operate at an elevated pressure. The size was also determined by counting (with a CNC) the number of particles passing through a differential mobility classifier. The mean particle size from this determination was 12 nm , consistent if slightly higher than the diffusion battery measurement.

Formation of Agglomerates

As the concentration passed through the sooting zone, the number of nuclei dropped by a factor of four and the mass of soot increased by 2-4 orders of magnitude over a narrow band of acetylene flow rates. Clusters in this size range were sampled and examined by transmission electron microscopy. Log-Log plots of the number of primary particles with radius of gyration or other measures of the optical diameter show fractal behavior with a slope well below 2.0. Similarly comparisons of the optical diameter from electron microscopy with the mobility equivalent diameter from the differential mobility classifier indicate that the aerodynamic diameter of the cluster is related to the number of primary particles by a relation :

$$D_{AE} \approx (N_p)^k$$

where k should be approximately (1/f). The data are consistent with this conjecture and exclude the aerodynamic diameter being proportional to N (the friction factor being proportional to $N^{(1/3)}$.

Formation of Aggregates

When the acetylene flow rate is greater than 0.045 l/min. the number of nuclei does not increase but the clusters are much larger. It is no longer possible to count the individual primary particles. The key experiment consisted of collecting a sample on different stages of an Andesen inertial impactor. The particles per stage were then sized. The "aerodynamic" diameter on a log-log plot. The slope of unity indicated that the aggregates were no fractal, but had a Hausdorff-Besicovitch dimension of three. The clusters were porous with densities of 0.08 g/cc. It is interesting to note that for the largest agglomerates in the transition regime the H-B dimension was approaching 2 for the projection, which may be consistent with a dimensionality of 3 for the cluster. It will be necessary measurement and analysis techniques with greater sensitivity to quantify the transition.

Reports and Papers

1. Cleary, T.G., "Measurement of the Size Distribution and Aerodynamic Properties of Soot", Master Thesis, 1988.

2. Samson, R., "Structural Analysis of Soot Agglomerates", Master Thesis, 1986.

3. Samson, R., G. Mulholland and J.W. Gentry, "Analysis of Soot Agglomerates and Their Physical Properties", ed., H. Fissan, C. Helsper, in Aerosol Formation and Reactivity, pp. 413-416 (1986).

4. Samson, R., G. Mulholland and J.W. Gentry, "The Fractal Analysis of Soot Agglomerates", Langmuir, 3, pp.272-281 (1987).

5. Cleary, T., R.J. Samson, R.J. Mulholland and J.W. Gentry, "The Relationship Between Structure and Aerodynamic Measurements for Clusters", to be published J.Aerosol Science (1988)

6. Cleary, T., G. Mulholland and J.W. Gentry, "The Experimental Measurements of Clusters Formed from Soot Agglomerates near the Sooting Limit", to be published in Atmospheric Aerosols and Nucleation, ed. P. Wagner, Lecture notes in Physics, Springer-Verlag (1988).

7. Cleary, T., J.R. Pao, G. Mulholland, and J.W. Gentry, " The Use of Simulated Fractals in the Correlation of Aerodynamic Properties with the Structure for Agglomerates submitted to J. Aerosol Science (1988).

8. Gentry, J.W., G. Mulholland, R. Samson and T. Cleary, " Methodology for Fractal Analysis of Combustion Aerosols and Particle Clusters", accepted pending revision in J. of Aerosol Science and Technology, (May 1988).

C. CO Prediction

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

CARBON MONOXIDE PRODUCTION AND PREDICTION

Professional Personnel

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

Project Objective

Develop scientifically-sound principles, metrology, experimental data, and calculational procedures for measurement and prediction of carbon monoxide (CO) production by fires and to utilize this information to assess the hazard due to this toxic species.

Scope

This program is designed to assess the importance of CO in fire toxicology 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

1. Project Planning

A long-range plan has been formulated which is designed to improve the understanding of and predictive capabilities for the formation of high CO concentrations in enclosure fires. This plan is based on an extensive review of the literature and the findings of a workshop entitled "Workshop on Developing a Predictive Capability for CO Formation in Fires" which was held in Clearwater, FL on December 3-4, 1988. Both fundamental and engineering approaches to the problem are recommended. Tables are included in the planning document which list major research components and required funding levels. Efforts are included to:

- develop the global equivalence ratio as a means for correlating the amount of CO produced in fire,
- experimentally and theoretically explore the physical and chemical processes responsible for the generation of high levels of CO in fires,
- investigate the possible importance of burning outside of a fire room on the amount of CO transported to remote locations,
- develop fundamental models for the prediction of CO generated by underventilated burning, and

- incorporate findings of the study into existing and future CFR fire models.

Internal reports describing the findings of the workshop and the research plan have been prepared.

2. CO Production in a Full-Scale Enclosure Fire Test

In September 1988, CFR researchers staged a full-scale fire reconstruction of a fatal fire which occurred in Sharon, PA on September 26, 1987. Since occupants of the structure were known to have succumbed to flame gases, a premium was placed on the production and measurement of high CO concentrations during the test. This data has been analyzed and the results compared with a simple two level model for CO production. The model assumes that 0.002 g CO/g wood burned are produced for wood burning under pre-flashover fire conditions and 0.3 g CO/g wood burned for post-flashover conditions. The CO concentrations measured in the reconstruction were generally consistent with this simple model, but the average levels fell somewhat below those predicted.

3. Effects of Vitiation on Production of CO

The cone calorimeter is widely utilized for investigating the combustion of small fuel samples under conditions of heat irradiation characteristic of large fires. Combustion products produced are collected and analyzed. The CO/CO_2 ratio is one of the parameters which is determined. In the past, measurements have been performed under fully ventilated conditions which generally produce low levels of CO. During the past year such measurements have been made in a cone calorimeter redesigned to allow investigations of burning under vitiated conditions. The new design features include an adjustable total flow through the chamber with flow straightening, variable O_2 concentration, load cell separated from combustion chamber, overpressure panel on back of cone, and a radiation shield for the specimen. Measurements of the CO yield from burning Douglas fir were performed at nominal oxygen concentrations of 21%, 17%, and 14% and for radiant fluxes of 25, 50, and 75 kW/m^2. From a preliminary review of the data it is apparent that for all flux levels investigated the CO yield increases by a factor of about 3-5 as the air is vitiated from 21% to 14%.

4. Fundamental Investigations of Turbulent Combustion

The production of CO is ultimately due to the entrainment, mixing behavior, and chemical reactions occurring within the turbulent buoyant plume of a fire. Due to the heat release there is a strong coupling of the reactions occurring in the fire and the turbulent structure of the plume. This part of the CO priority project is an effort to characterize the turbulent structures responsible for mixing within buoyancy-driven plumes. Measurements are to be made in isothermal, buoyancy-driven flows generated using gases which are lighter than air (e.g., helium or methane). A cylindrical enclosure having a height and diameter of 2.4 m has been designed and constructed especially for these studies. Air for the enclosure is passed through a system of high efficiency particle filters to create a dust-free environment where previously-developed Rayleigh light scattering diagnostics can be utilized to investigate mixing in the buoyant plumes. The results of the experimental measurements will be compared with predictions of a model for similar flows currently under development by Drs. Howard Baum and Ronald Rehm of NIST.

Reports and Publications

"Executive Summary for the Workshop on Developing a Predictive Capability for CO Formation in Fire," W. M. Pitts, National Institute of Standards and Technology Internal Report, NISTIR 89-4093, May, 1989.

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

"Importance of Isothermal Mixing Processes to the Understanding of Lift-Off and Blowout of Turbulent Jet Diffusion Flames," W. M. Pitts, Combustion and Flame 76 (1989) 197-212.

"Assessment of Theories for the Behavior and Blowout of Lifted Turbulent Jet Diffusion Flames," W. M. Pitts, Twenty-Second Symposium (International) on Combustion, The Combustion Institute, 1989, pp. 809-816.

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
FY89

Institution: Virginia Polytechnic Institute & State University

Grant No.: 60NANB8D0829

Grant Title: Compartment Fire Combustion Dynamics

Principal Investigators: Richard J. Roby
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Cincinnati, Ohio 45239

Other Professional Personnel: Michael J. Skelly (M.S. Candidate)
Daniel J. Gottuk (Ph.D. Candidate)

NIST Scientific Officer: Dr. Henry Mitler

Technical Abstract:

This abstract covers the first year of a new 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 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.

The major goal of the first year of the project was to develop and test a new scale size compartment for fire dynamics studies and to demonstrate that the compartment can operate in a manner which allows for measurement of both fuel and air inflow without disturbing the compartment outflow. The development of this compartment test facility is an integral part of the research program. To this end, the first year of work has been devoted to design, construction

and testing of the test compartment and renovation of the hazardous test facility which is being used as the test site.

Facilities Development

The test facility being used for this project is a hazardous test facility previously used for solid rocket propellant testing. The facility consists of a 10 foot cube, concrete block test building equipped with a steel overhead door and a blowout roof. The test building is separated from a measurement trailer by a steel reinforced concrete wall. Renovation of the building has included the installation of an exhaust system which includes a 5' by 5' exhaust hood and an orifice meter for exhaust flow measurements.

The test compartment consists of an angle-iron frame with insulating ceramic board on the inside. The bottom 0.4 meters of the compartment serve as the air inlet plenum and will house a sensor for measurement of fuel weight-loss rate. The overall height of the compartment is 1.5 meters and it contains an opening which can be as large as 0.5 meters on a side. The test compartment is placed in the test building under the hood during testing so that the effluent from the compartment can be collected and sampled. Fresh air for the compartment is inducted into the base of the compartment through a 12 inch inlet duct open to the outside which is instrumented for accurate measurement of air inflow.

Currently, an FTIR analyzer and the two NDIR analyzers are installed to measure production rates of chemical species including CO, CO2, HCN and HCl. The analyzers have been specified so that they can be used to analyze samples directly from the compartment or the more dilute samples obtained from the exhaust. A schematic of the compartment and sampling system is shown in Figure 1.

Compartment Testing

After construction of the scale compartment was completed, several open-air test burns were performed using hexane pool fires. These tests were made to determine if the compartment would function with one directional, unforced flow. These tests have proven successful. A two-layer environment has been achieved in the compartment using a 40 cm by 40 cm opening with a 20 cm soffit height. The fuel for the fires was supplied by a 2.5 cm deep by 22 cm in diameter pan of hexane. Total burn times were five to seven minutes. After an initial period of one to two minutes, the layer level was below the bottom of the compartment opening and flow (as indicated by smoke) was only out of the window opening. Under these conditions, there was no sustained flame out the opening.

These results demonstrate the suitability of the compartment design for obtaining a two-layer room fire environment with no inflow in the window. These results also demonstrate the viability of supplying air from underneath the compartment in a way that allows for measurement of compartment air inflow. The ability to carefully measure air inflow is critical to the experiments to be performed. These tests constitute a major milestone in demonstrating the suitability of the experimental design.

Window Breakage Experiments

A second set of experiments to test the value of this compartment for fire dynamics studies were conducted. These tests consisted of installing a 25 cm by 40 cm window frame in a wall of the compartment in order to test conditions of window breakage in a fire. Since failure of windows in a fire contribute to establishment of toxic gas levels either by providing a ventilation path or by providing a route for spread of the gases, these experiments are important to modeling the overall environment for toxic gas generation.

For these experiments, glass panes were installed either with their edges protected from direct fire gas impingement (as in a typical window installation) or with the edges fully exposed to the compartment fire. A thermocouple was used to measure the temperature of the center of the glass pane on the inside. For the protected pane, the glass edge temperature was also measured. Figure 2 shows a comparison of the time to breakage and the temperature history for a typical set of tests. As the figure shows, the glass pane with a protected edge breaks much sooner and at a significantly lower temperature than the pane whose edges are fully exposed. Futhermore, visual observation of the two cases showed that in the edge protected cases, the window shatters in less than 0.1 seconds with multiple bifucated cracks throughout the pane. By contrast, the fully exposed pane fails by developing one or several cracks at the edge which slowly propogate across the pane on a time scale of tens of seconds. These results where obtained for a hexane pool fire in a 20 cm by 20 cm square pan. Similar results were obtained for both a 50% larger and a 50% smaller pan.

In agreement with the analysis of both Emmons and Pagni, the protected glass pane consistenly shattered with bifucating cracks at a temperature differential between the center and protected edge of 90C. These results confirm previous analysis by both Emmons and Pagni that window glass fractures in a fire at a relatively low temperature due to the thermal stresses near the edge of the glass. The stresses are the result of the differential heating between the exposed part of the glass and the protected edge.

Future Work

Oxygen and hydrocarbon analyzers will be added to the continuous gas analysis system. Experiments in which the area and location of the fuel, as well as the ventilation are systematically varied will be performed to establish the effects of compartment fire flows on species yields. Measurements will focus on composition (carbon monoxide, carbon dioxide, oxygen and hydrocarbons) of the upper layer and exhaust gases, but will include fuel volatilization rate, air inflow rate, temperature profiles in the compartment, and temperature, flow rate and extinction coefficient of the exhaust gases.

Gas (particularly CO) and smoke production will be correlated with the fuel-to-air ratio and will be compared to previous correlations. The effects of layer mixing, transom height, vent area and residence time will be systematically studied. In addition, the effectiveness of external flames in destroying products of incomplete combustion, especially toxics, will be investigated. In particular, the effect of external flames on overall yield of carbon monoxide, carbon dioxide and oxygen will be studied.

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.

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 and window breakage, it will provide information about the spread of toxic species from the compartment of fire origin. Since this 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.

Reports and Papers:

Skelly, M. J., Roby, R. J. and Beyler, C. L., "An Experimental Investigation of Window Breakage in Compartment Fires," submitted to The Journal of Fire Protection Engineering, August 1989.

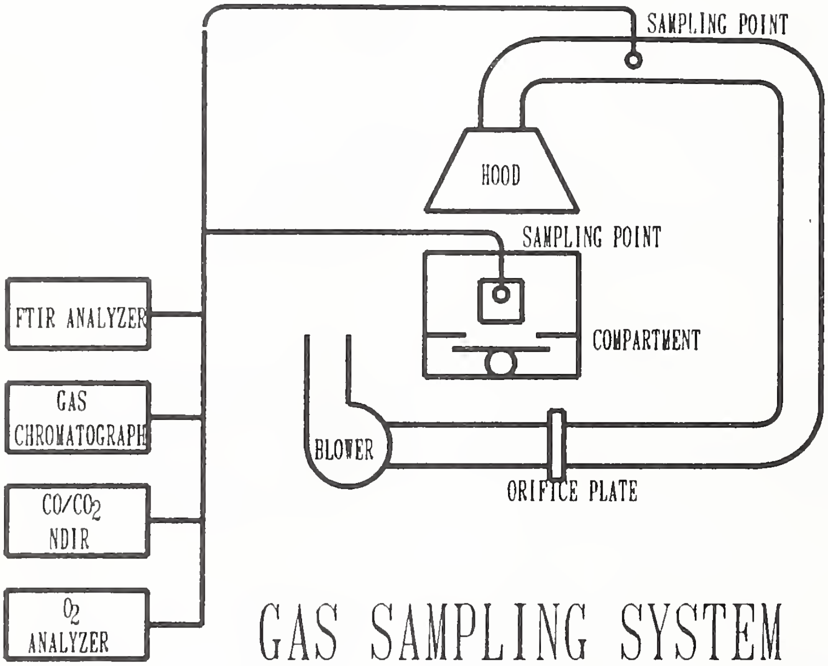

Figure 1. Schematic of the gas sampling system for the test compartment.

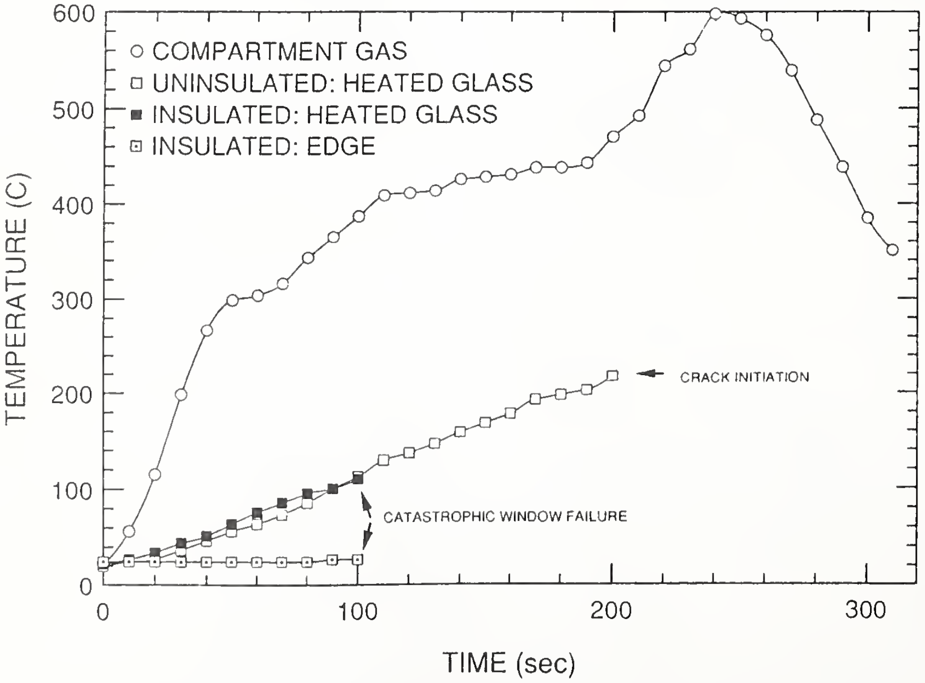

Figure 2. Plot of time versus temperature for for glass breakage experiment.

D. Polymer Gasification

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

POLYMER GASIFICATION/POOL BURNING

Professional Personnel

T. Kashiwagi, Project Leader
J. Brown, Research Chemist
Stephen Fischer, NRC Post Doctorate
K. Kanemaru, Guest Researcher
H. Nambu, Guest Researcher

Project Objectives

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

Scope

The study of the polymer gasification process consists of three parts: thermal degradation chemistry, heat transfer, and mass transport processes through polymer samples. After each part is separately studied in detail, an overall model consisting of simplified models for each part will be developed. An energy feedback rate and a flame heat transfer process are studied using a pool burning configuration with well defined liquid fuels simulating the burning of the polymer degradation products. A global energy feedback model will be developed after the effects of the fuel structure and pool size on the energy feedback rates are understood.

Technical Accomplishments

I. Polymer Gasification

1. Experimental Study of Polymer Gasification Rate

Measured non-flaming gasification rates of polystyrene, PS, and poly(methyl methacrylate), PMMA, samples at external radiant fluxes from 1.7 to 3.9W/cm^2 show that the thermal stability of the polymer sample affects the gasification rate, but the transport process of the in-depth degradation products through the molten polymer to the sample surface appears to have and insignificant affect on the gasification rate except at low external radiant flux. The results are shown in Fig. 1 using two PS samples having nearly the same thermal stability with two different initial molecular weights (The higher molecular weight sample has higher melt viscosity of molten polymer). The global heat of gasification based on the energy balance at the polymer surface without including energy loss into the polymer sample is sensitive enough to differentiate the effects of the thermal stability of the sample, but its value also depends on external radiant flux; in addition, it decreases with an increase in exposure time as shown in Fig. 2. A paper based on this study has been written and submitted to a technical journal.

2. A Global Gasification Model

Two analytical solutions to the time-dependent non-flaming gasification rates are derived; one is based on the assumption that external radiation is absorbed at the sample surface and the other is an approximate solution which includes in-depth absorption of external radiation. The principle assumptions in both models are that there is a well-defined vaporization temperature and chemical heat of vaporization. Both models include reradiation loss from the sample surface, time-dependent external radiation and variable thermal properties. The sample is assumed to be thermal thick for the two models. Since the solutions include an integral form, iteration and mathematical functions, the results are calculated using a PC.

II. Pool Burning

1. Pool Burning Experiments

A 38cm diameter pool burning facility was constructed. The system consists of five concentric rings and each ring is fed independently by five different liquid feed systems to maintain the liquid level at the specified location close to the rim. Preliminary experiments are being conducted with heptane. Other fuels such as methyl methacrylate, toluen and others will be used to study the effects of the fuel structure on the energy feedback rate. The transmission measurements through pool flames at broad infrared wavelengths using a gray body source and the He-Ne laser line will be conducted at various flame locations. The total energy feedback rates will be determined from the measured gasification rates multiplied by the heat of the vaporization of the liquid fuels. The taking of the measurements of temperature, CO, CO_2, H_2O in flames are planned.

2. A Pool Burning Rate Model

A global time-dependent pool burning rate model consisting of (1) the above described gasification rate model based on the surface absorption for a polymer sample and (2) a gas phase energy feedback model based on the Froude number (Orloff and de Ris, 1983) has been developed. The preliminary calculations are being conducted using a PC; typical computation time is less than ten minutes.

<u>Reports and Publications</u>

Kashiwagi, T., Omori, A. and Brown, J.E., "Effects of Material Characteristics on Flame Spreading", Proceedings of Second International Symposium on Fire Safety Science, Hemisphere, p.107, 1989.

Kashiwagi, T. and Omori, A., "Effects of Thermal Stability and Melt Viscosity of Thermoplastics on Piloted Ignition", Twenty-Second International Symposium on Combustion, The Combustion Institute, p.1329, 1989.

Kashiwagi, T., Inaba, A. and Hamins, A., "Behavior of Primary Radicals During Thermal Degradation of Poly(methyl methacrylate)", Polymer Degradation and Stability, in press.

Kashiwagi, T., Omori, A. and Nambu, H., "Effects of Melt Viscosity and Thermal Stability on Polymer Gasification", submitted to Combustion and Flame.

Related Grants

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

"Interaction of Radiation and Conduction in Polymeric Materials", Win Aung, University of Maryland.

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

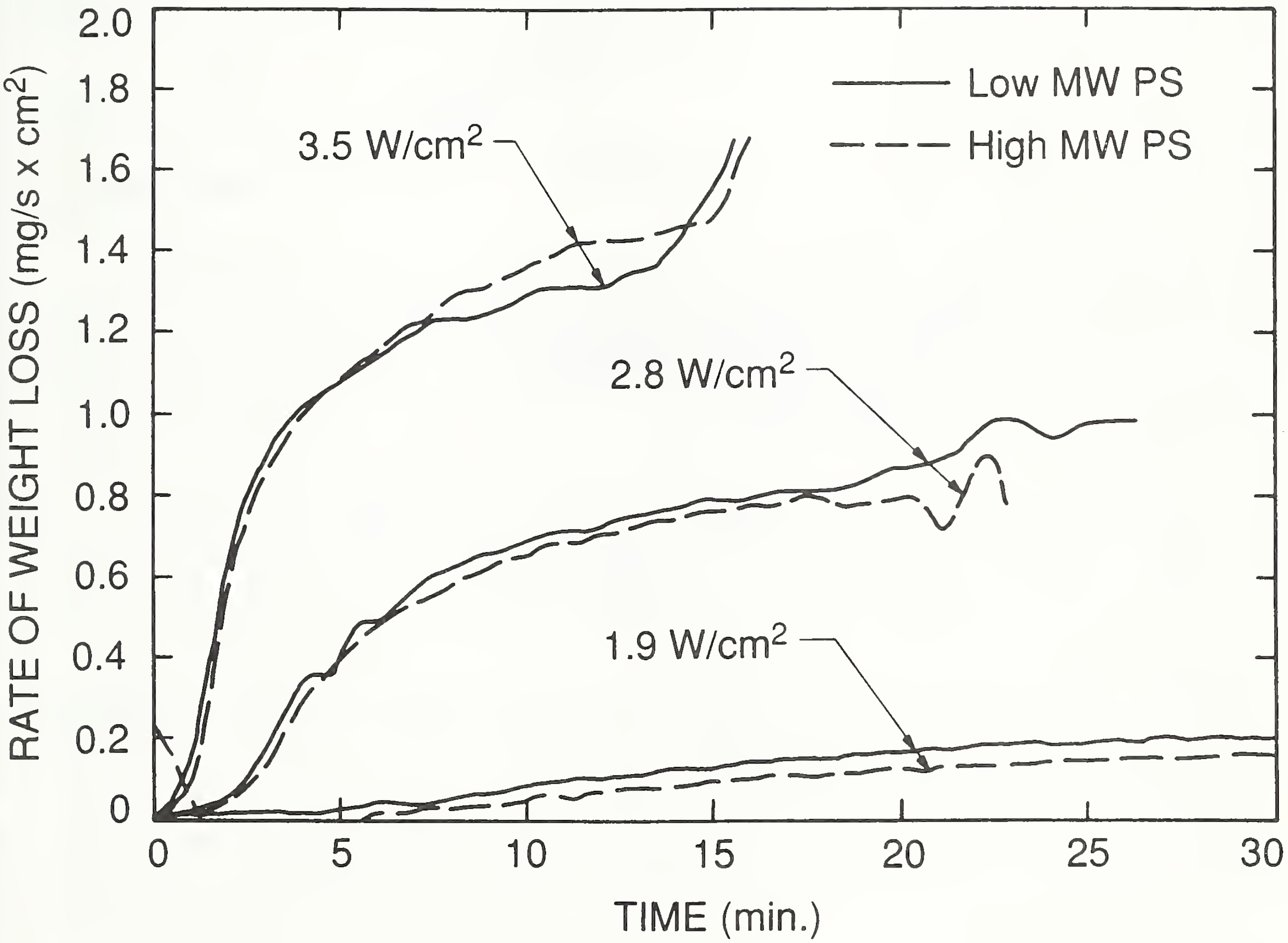

Fig.1 Comparison of non-flaming gasification rates of two different PS samples with two different initial molecular weights at three different external radiant fluxes in nitrogen.

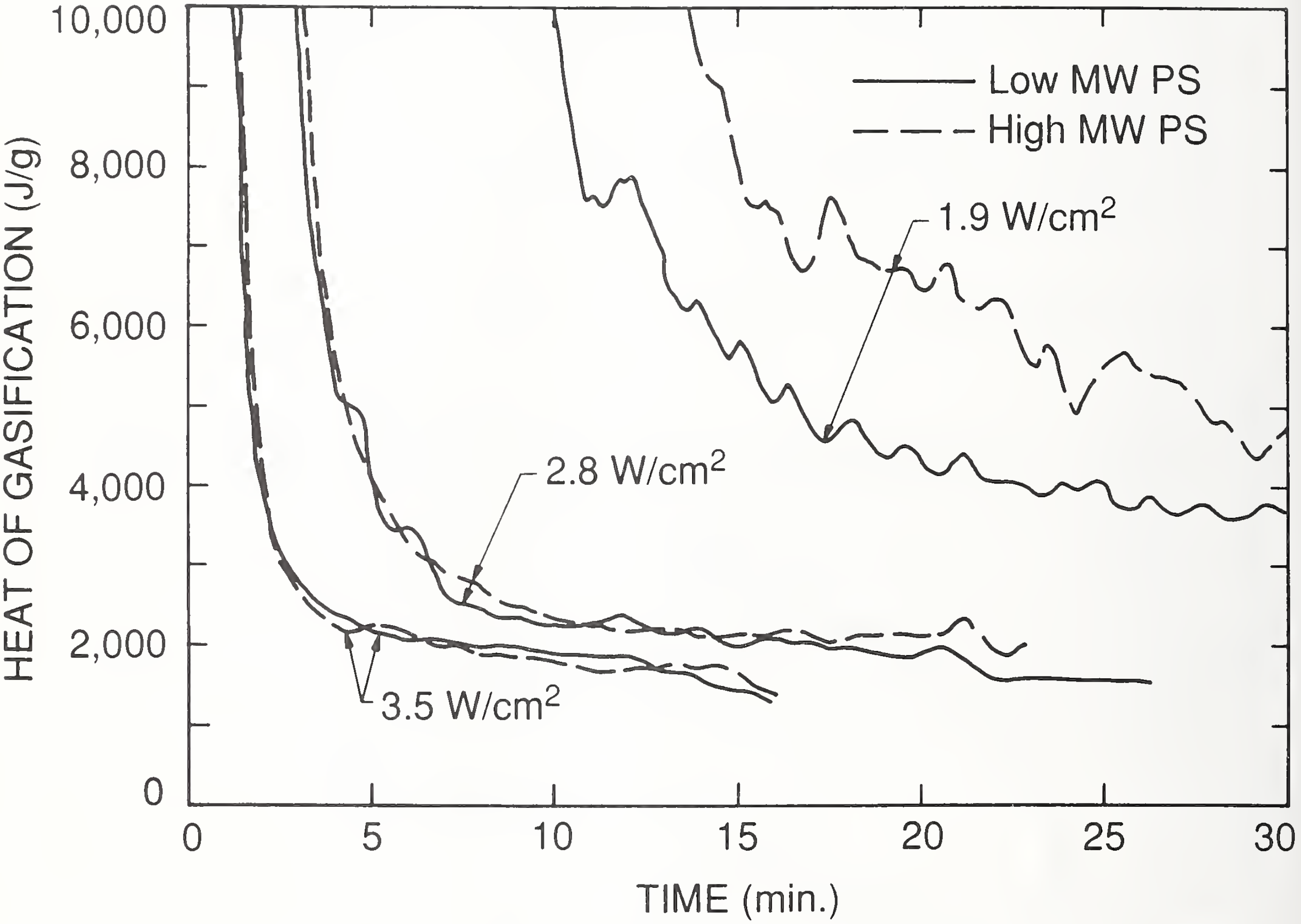

Fig.2 Comparison of global heat of gasification of the two PS samples of two different initial molecular weights at three different external radiant fluxes in nitrogen.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: University of California--Berkeley/Irvine

Grant Number: 60NANB4D0827

Grant Title: Flame Radiation

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S. H. Park, Ph.D student
A. Tuntomo, Ph.D student

NIST Scientific Officer: Dr. Takashi Kashiwagi

Technical Abstract:

Introduction. The objective of this research program is to establish a simple analytical framework for the accurate calculation of radiative heat transfer in fires while retainingthe fundamental physics of the problem. From both the experimental investigation and the theoretical analysis, approximate relations have been developed for practical engineering applications. Three primary topics are addressed: (1) measurement and correlation of the infrared radiation properties of hydrocarbon gases pyrolyzed from burning condensed fuels, (2) development of an accurate radiation model for large pool fires, and (3) determination of the effects of the gas-phase radiation absorption on the ignition mechanism of plastic solids.

Radiation Properties of Hydrocarbon Gases. Due to the infrared absorption capability of hydrocarbon gases evolved from condensed fuels, the fuel ignition delay time is greatly shortened, while the evaporation rate is significantly reduced. Therefore, the infrared radiation properties of the pyrolyzed hydrocarbon gases are critical for a rigorous study of fire safety enforcement.

During the past year, the infrared radiation properties of ethylene (C_2H_4), which is one of the important pyrolysates in plastic fires, have been determined experimentally [1]. The spectral absorptivities for each of the four infrared-active bands of ethylene have been measured at low resolution for temperatures between 300K and 700K. These measurements have been used to correlate both the spectral-mean narrow-band parameters and the wide-band parameters for each band. The wide-band parameters have been further employed to develop both total emissivity and Planck mean absorption coefficient charts. The total emissivity chart for ethylene is presented in Fig. 1, while the Planck mean absorption coefficient chart for various gases, including ethylene, is presented in Fig. 2.

Thermal Radiation in Large Pool Fires. A fluctuating cone model has been developed for accurate prediction of the dynamic characteristics in realistic pool-fire situations [2]. The vertex of a fire cone is moved off-axis to simulate the randomized movement of a tilted cone within a cylindrical envelope.

The variation in radiative heat flux emitted from a fluctuating flame is due to the variation of its shape factor, or mean beam length, which is purely a geometric consideration. Therefore, the algebraic mean of radiative heat fluxes determined from the fluctuating cone model is very close to the radiative flux calculated from the mean position of the tilted cone. The quantitative results of the radiative flux obtained from various considerations are presented in Fig. 3. In the case of a fire which is tilted by ambient air movement, the difference in radiative heat flux to the upwind and to the downwind sides of the fire is of the order of 40 percent or more. This is sufficient to cause preferential ignition and flame spread on the downwind side of the fire.

Radiation Induced Ignition of Solid Plastics. A comprehensive analysis on the radiation induced ignition of a solid 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 [3]. The absorbed radiant energy is calculated in the radiation flux-type transfer equation. The natural convection effect is considered through the assumptions of a thin gas-phase layer and an effective thermal conductivity within the layer.

The study reveals that the radiation absorption in the gas phase is one of the major mechanisms inducing the ignition of plastics. For less favorable physico-chemical conditions for ignition, the ignition is mainly governed by the radiation absorption in pyrolyzed gases. In general, the ignition delay times for absorbing gases are shorter than those for non-absorbing gases. The ignition delay times versus the radiation source temperatures for various gases with the absorption coefficient k_g ranging from 0 to 5 $atm^{-1}cm^{-1}$ are presented in Fig. 4. The effect of the absorption by the gas phase on the ignition delay time is even prominent for high source temperatures.

Reports and Papers:

1. A. Tuntomo, S. H. Park and C. L. Tien, "Infrared Radiation Properties of Ethylene," Experimental Heat Transfer (in press).

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

3. S. H. Park and C. L. Tien, "Radiation Induced Ignition of Solid Fuels," (to be published).

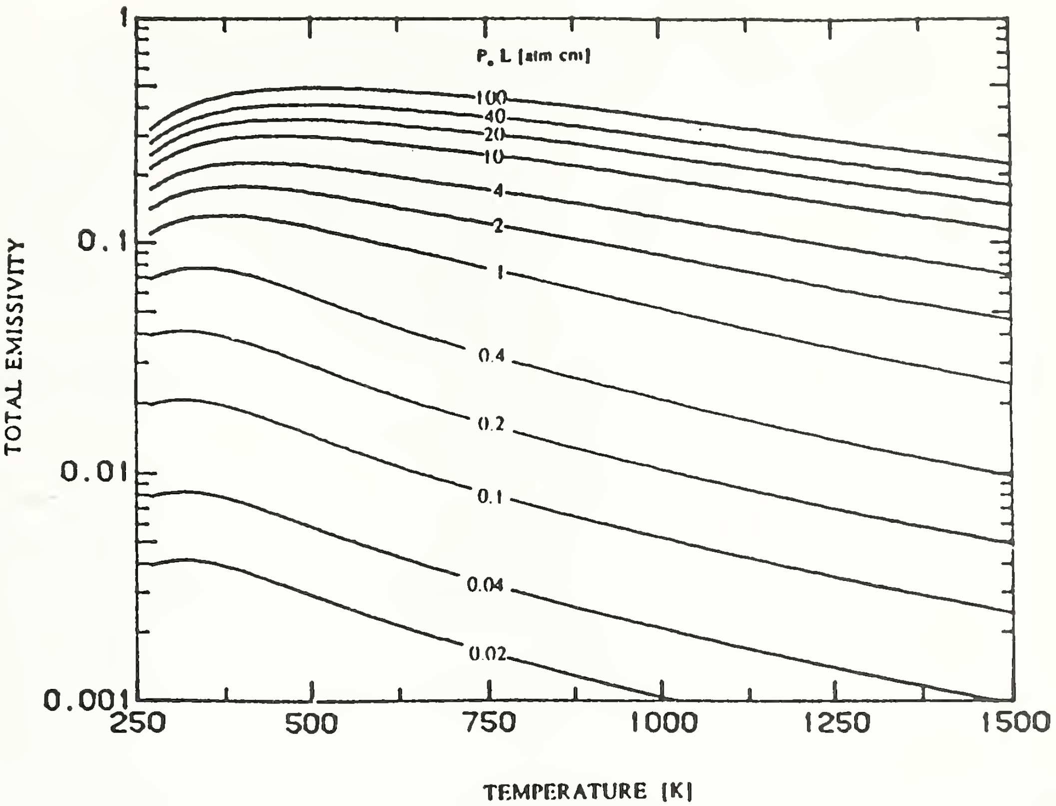


Fig. 1 Total emissivity for ethylene

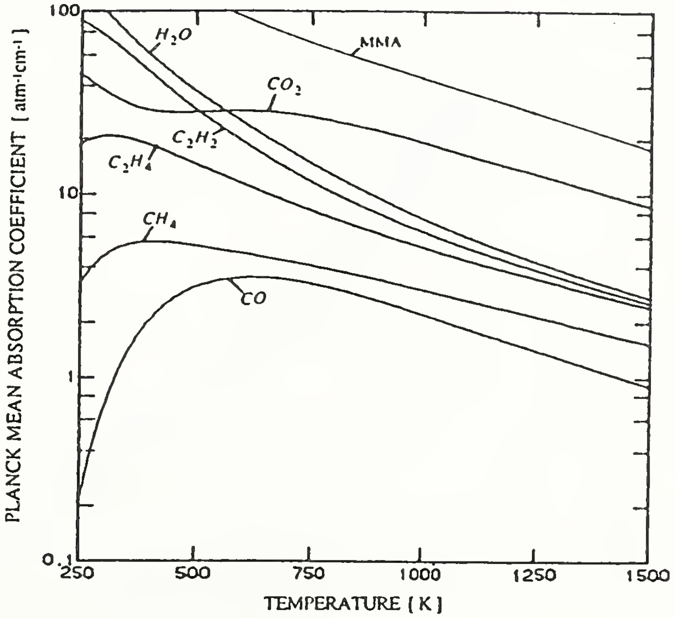


Fig. 2 Planck mean absorption coefficient of various gases

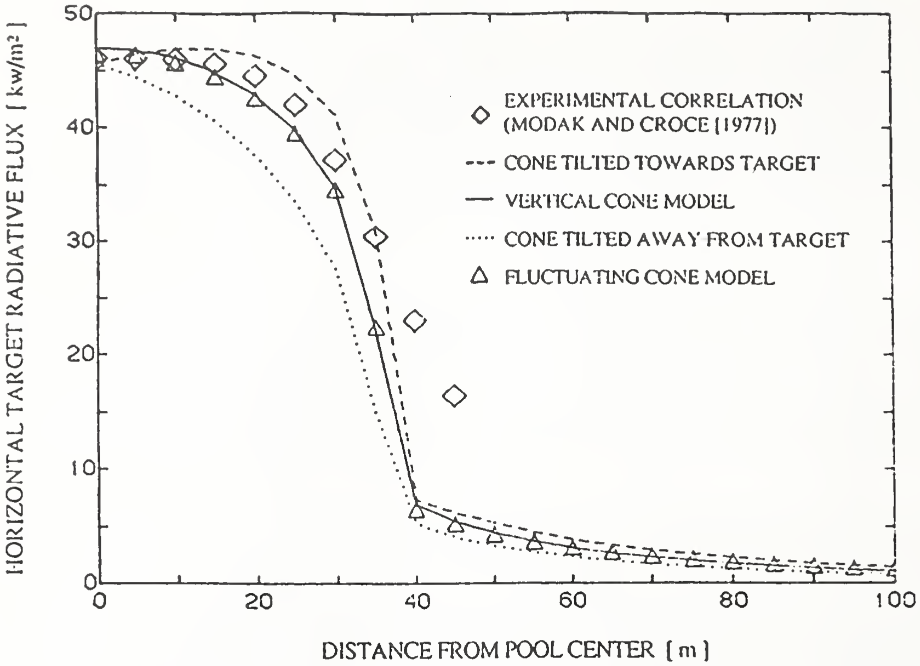


Fig. 3 Effect of the fluctuating cone on the radiative flux to the ground plane

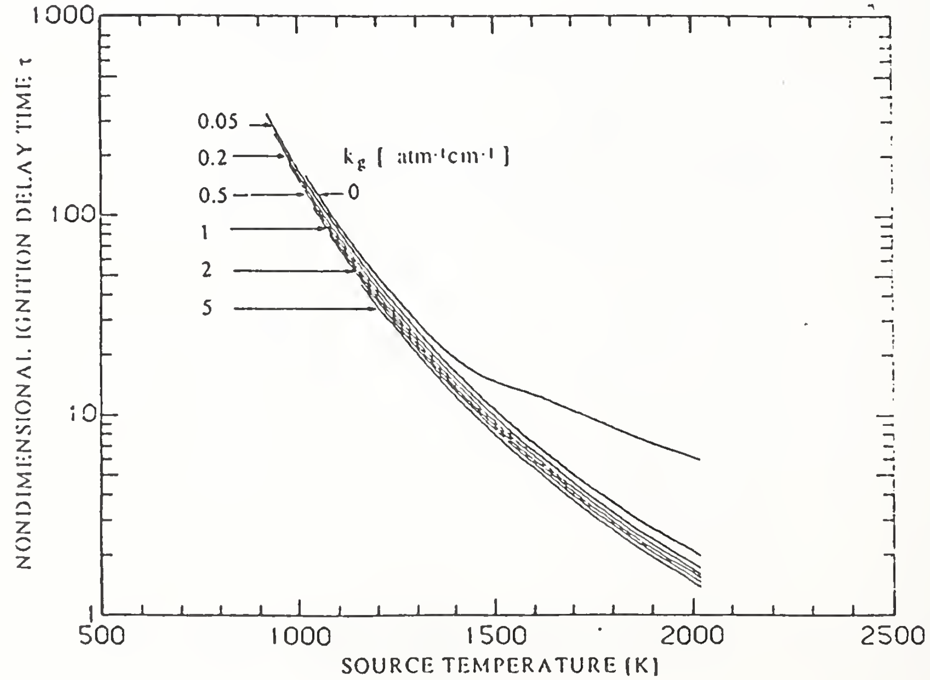


Fig. 4 Effects of absorption coefficient and radiation source temperature on ignition delay

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: University of Maryland

Grant No.: 70NANB8H0853

Grant Title: Interaction of Radiation and Conduction in Polymeric Materials

Principal Investigator: Dr. Win Aung (Adjunct Professor)
Mechanical Engineering Department
University of Maryland
College Park, MD 20742

Other Professional Personnel: Yen-hao Pan, Ph.D. Student

NIST Scientific Officer: Dr. Takashi Kashiwagi

Technical Abstract:

Introduction

The flammability of polymeric materials, of great interest in studies related to fire safety, is governed by complex phenomena that aries in both the gas phase and the condensed phase. From the heat transfer standpoint, the complete non-flaming, transient heating cycle for a polymeric solid consists of an initial, combined radiative-conductive heating phase involving a homogeneous solid, followed by heating with phase transition and gas-product liberation. The heat and mass transfer has a significant effect in the transient heating polymers prior to ignition. We consider the radiant heating of a semitransparent polymeric material in the condensed phase. The heating may be viewed as caused by a remote source during the pre-ignition stage. The objective of this research is to analyze the transient heating of semitransparent polymeric materials exposed to radiant fluxes from high temperature sources.

To simplify the analysis, we have focused on a one-dimensional problem. The vertical solid plane is exposed to a high temperature radiant flux. The solid is in local thermodynamic equilibrium and with negligible scattering. The collimated radiant flux which reaches the solid at normal incidence is a known quantity. The specific heat and thermal conductivity is assumed to be functions of temperature only. The reflectivity is determined by Snell's law. The boundaries of the solid lose energy to the surrounding by surface re-emission and convection. The convection heat transfer coefficient is obtained from a simplified correlation for laminar flow past a vertical plate.

We initially focused on a reradiating model (Finlayson, Aung and Kashiwagi, 1987), which solves the coupled nonlinear energy equation and equation of transfer. This proved to require long calculation time, thus diminishing the model's usefulness in the development of the eventual thermochemical model for the second phase heating process. More recently, we applied Rosseland approximation and derived a model with correction terms (RAC) (Pan, Aung and Reiss, 1989a, 1989b). This has been shown to be very effective and accurate when compared with the reradiating model. In the RAC model, the correction terms are identical to those from the cold model. When compared against experimental data for fused silica, the RAC model is almost identical to the reradiating model.

The present paper provides a summary of the general (dimensionless) results obtained using the RAC model.

Results and Discussion

Figure 1 shows the effect of dimensionless optical thickness on dimensionless temperature distribution. The temperature distributions are recorded at dimensionless time of 0.0255 after the beginning of heating. The irradiated boundary is subject to a dimensionless flux of 109. The radiation-conduction parameter, N, is taken to be 0.1125. The index of refraction is chosen as n = 1.34. We assume the optical thickness to be between 0 and infinity within the semitransparent band. The temperature distributions are given for optical thicknesses of 2, 5, 10, 20 in the semitransparent band. The opaque result represents the limiting case of infinite absorption coefficient. Figure 1 shows the difference between the predicated surface temperature for the opaque and semitransparent cases. The semitransparent solid allows the penetration of heat into the solid. When heat absorption inside the slab is considered, the maximum temperature occurs within the solid not at the surface as in the opaque case. The smaller the value of the absorption coefficient allows for greater penetration within the solid. This results in a flatter temperature distribution, with maximum temperature occurring away from the surface.

Figure 2 shows the effect of the radiation-conduction parameter on temperature distribution. For a small value of N, the temperature distribution is very flat and straight. This is because heat conduction dominates the heat transfer process. For larger values of N, radiative transfer begins to affect the heat distribution. The larger is the value of N, the shorter distance in which radiation is attenuated. This causes most of heat to be stored near the front surface, leading to steeper temperature distribution.

Figure 3 shows the effect of Biot number on temperature distribution. The front and rear boundaries are subjected to forced and natural convection heat loss, respectively. The value of the forced convection heat transfer coefficient on the front boundary is imbedded in the Biot number. The larger is the Biot number, the larger is the heat loss to the ambient and the lower is the temperature in the solid. The maximum temperature tends to shift to the interior of the slab for the higher Biot number. The difference between the maximum temperature and the surface temperature also tends to increase.

Figure 4 shows the effect of index of refraction on temperature distribution. The reflectivity is determined by Snell's law. The higher is the index of refraction, the larger is the reflectivity. This means larger amount of heat is reflected away, resulting in lower temperatures in the solid.

References

Finlayson, E.U., Aung, W. and Kashiwagi, T., 1987, "Theoretical Models for Combined Radiation-Conduction in Semitransparent Solids Heated by External Radiative Flux," Proc. Second ASME/JSME Thermal Engineering Conference, Vol. 1, pp. 427-432.

Pan, Y.H., Aung, W. and Reiss, R., 1989a, "Diffusion Approximations for Interaction of Radiation and Conduction in fused Silica," Proc. ASME National Heat Transfer Conference, Vol. 106, pp. 301-308.

Pan, Y.H., Aung, W., Reiss, R., Tsou, F.K., and Gau, C., 1989b, "Rosseland Approximation with Correction Terms (RAC) for Combined Radiation and Conduction in Fused Silica," submitted to ASME Journal of Heat Transfer.

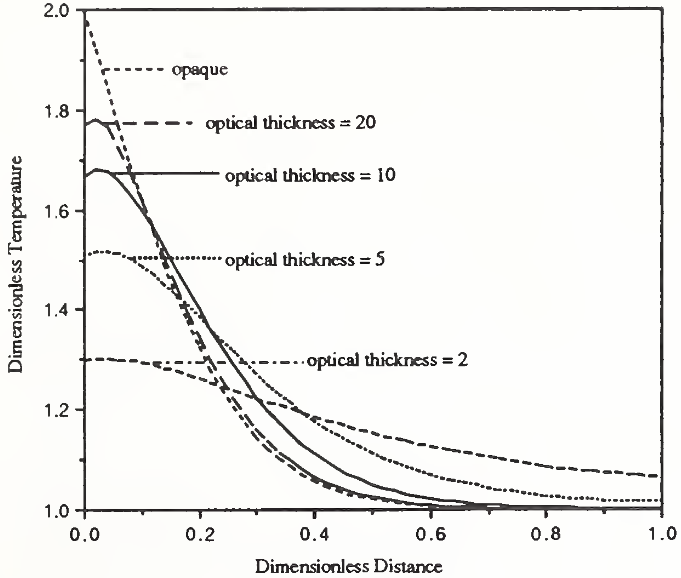


Figure 1. The effect of optical thickness on temperature distribution

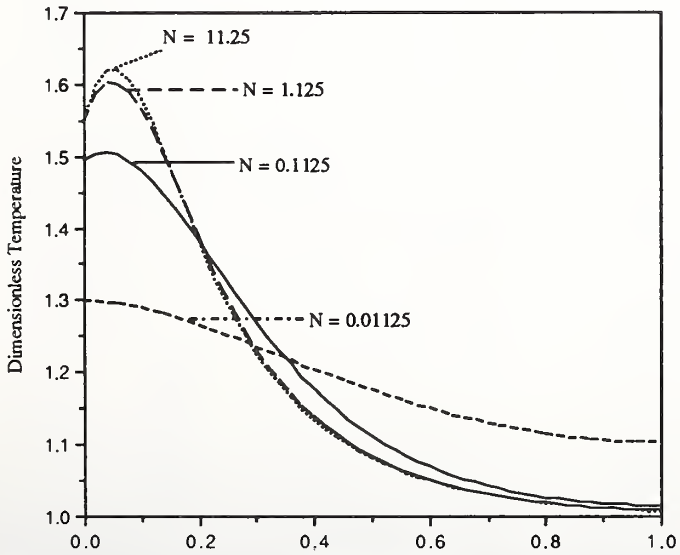


Figure 2. The effect of N (radiation/conduction parameter) on temperature distribution

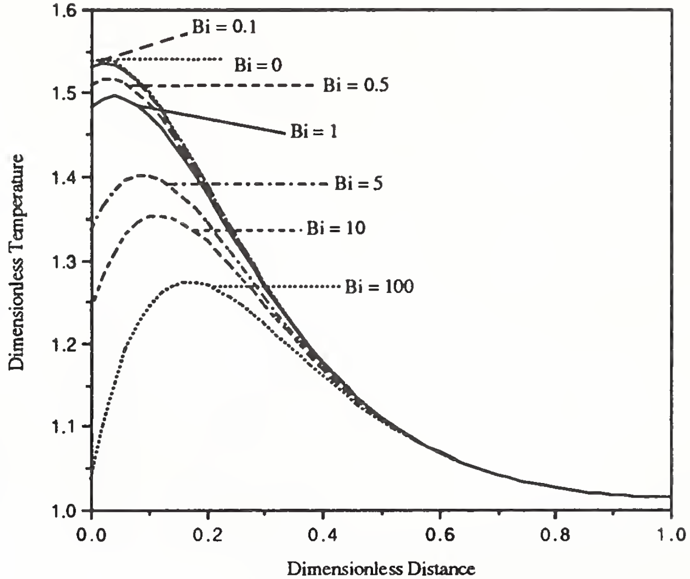


Figure 3. The effect of Biot number on temperature distribution

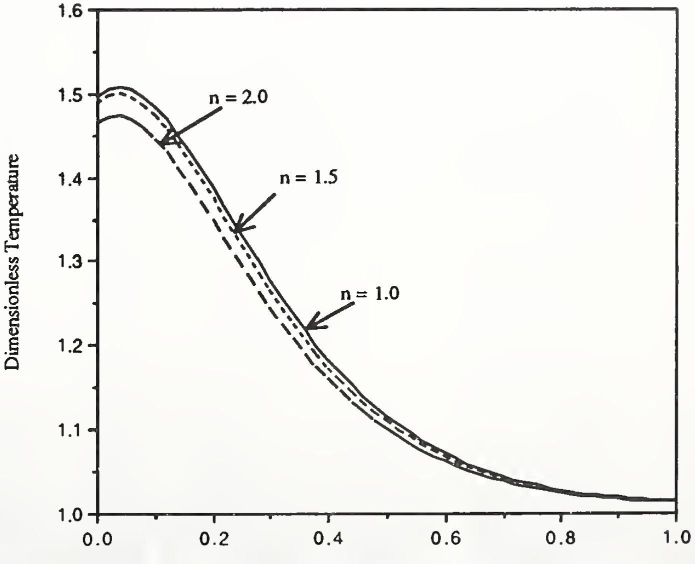


Figure 4. The effect of index of refraction on temperature distribution

E. Flame Spread

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

WALL FIRE SPREAD

Professional Personnel

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

Project Objective

To develop a method for predicting the rate and extent of fire spread on wall surfaces in a room using the fire properties of the materials involved.

Scope

This project addresses an important aspect of fire growth in enclosures leading to flashover. The upward growth rate, especially in a corner, is characteristic of the flammability of the burning wall material. Ultimately every aspect of wall fire growth will be covered, 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

The pyrolysis model described in Mitler [1] was successfully inserted into FIRST, a computer program which is an enrichment of the Harvard Computer Fire Code, Mark 5. The debugging process which was started last year was completed. A second option for the pyrolysis module was devised: given the experimental mass-loss rate $\dot{m}''(t)_{exp}$ as obtained from the Cone Calorimeter (or equivalent device), one can transform it into the mass-loss rate to be expected during actual burning, by using the transformation

$$\dot{m}''(t) = \xi(t)\dot{m}''(\tau)_{exp} \qquad (1)$$

where $$\tau \equiv \int\xi(t')dt' \qquad (2)$$

and $\xi(t)$ is the "acceleration" of the pyrolysis rate due to the net heating flux impinging on the material being greater (or smaller, as the case may be) than that to which it is exposed during the cone test.

This formulation offers an alternative to calculation from "first principles," and has the advantage of giving a first-order approximation to the results to be expected from burning <u>charring</u> solids. This transformation may also be thought of as "modeling" the Cone.

II. Spreadup model

The basic model for upward spread of the fire (i.e., of the pyrolysis front) is unchanged from what was presented last year: it is numerical, and assumes that the pyrolysis front reaches a given level when the surface temperature of the material at that level reaches a well-defined "ignition temperature" T_{ig}. The model was written up as an algorithm, and that (in turn) was programmed into the stand-alone program SPREAD. This program borrows subroutines for wall (or object) heating and for the mass-loss rate of a burning wall from FIRST.

In the second half of the year, the algorithm was documented and generalized in three ways: first, for the options (a) with and (b) without an igniting flame. Second, it was enabled to use a time-varying burner power output (as input). Third, using the transformation described in section I, the option to use these scaled values of the experimental mass-loss rate (rather than using the values calculated from the mass-loss algorithm) was added. The algorithm has been prepared for publication [2].

III. Heating Fluxes

Expressions, partly theoretical and partly empirical, were found for the convective and radiative fluxes from a wall flame to the wall from the

a. igniter alone
b. burning wall alone
c. burning wall plus igniter

This work is being documented.

IV. Experiments

A series of full-scale experiments was undertaken to validate the calculations. The results of one such experiment are shown in Fig.1. In this experiment, a one-foot-square section of the panel was ignited, but the region above it was insulated so as to prevent preheating by the igniter flame. Once ignited, both the igniter and the insulation were removed. The upward spread rate, once the insulated region heats up, is quite close to that found by Orloff *et al*.

V. Results

Fig.2 is a comparison of the experimental data from Orloff *et al* and a calculation made with SPREAD, using (approximately) the value of ρck found by using the Lateral Ignition and Flame spread Test (LIFT) apparatus and assuming that the igniter is a 2 kW line burner. As is seen, the agreement is remarkably good. In Fig.3, a comparison is given of the calculated results found when assuming 1, 2, and 4 kW burners; evidently the principal difference (as might have been expected) is at the beginning. A very interesting, important -- and puzzling --result, incidentally, is that the excellent agreement in the asymptotic rise rate of the curves in Fig.3 is found **only** when one uses the expression

$$x_f = 0.17\sqrt{\dot{Q}'} \qquad (5)$$

recently given by Markstein for the flame-tip height, rather than the usual dependence on the 2/3ds power of $\dot{Q}'$.

Reports and Publications

1. Mitler, H.E., "Algorithm for the Mass-Loss Rate of a Burning Wall", NBSIR 87-3682; National Bureau of Standards, Gaithersburg, MD, 1987, and in Fire Safety Science - Proceedings of the Second International Symposium (Eds., C.E. Grant and P.J. Pagni); Hemisphere Publishing Corp. (1988)

2. Mitler, H.E. (1989), "How to Calculate Upward Spread Rates of Wall Fires," NIST Internal Report, in review

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.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

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:
G.H. Markstein
M.A. Delichatsios
L. Orloff
H.W. Emmons

NBS 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. Such predictive models will reduce fire losses through the development of science-based techniques for rating material flammability.

Task 1. Prediction of Fire in Buildings (H.W. Emmons)
Please see a separate summary under this title.

Task 2. Models for Fire Radiation and Toxic Product Release - We are reporting significant progress towards the development of models for predicting the radiation from buoyant turbulent diffusion flames for various fuels and oxidants in terms of tabulated "fundamental" composition properties. Two approaches have been taken: (1) development of a global algebraic model for the gaseous radiation from buoyant turbulent axisymmetric flames; and 2) characterization of turbulent combustion and flame radiation by three parameters: two parameters representing the overall buoyancy flux and the buoyancy due to individual flamelets; and a new radiation parameter relating the radiant losses to the convective heat flow rate. These models utilize experimental data obtained in this study and at other laboratories. Our greater understanding of the roles of gaseous radiant emission and soot extinction provides a platform for describing wall and pool fire radiation in terms of the fuel smoke point.

The effects of soot production and extinction in turbulent flames are better understood once we describe the gaseous radiation in the absence of soot. Low sooting fuels such as H_2, CH_4, C_2H_6, etc. have smaller radiant fractions ($0.15 < \chi_r < 0.25$) since most of their flame radiation originates from gaseous products of combustion (H_2O and CO_2). More sooty fuels, such as C_2H_2, C_2H_4, etc. have larger χ_R ($0.35 < \chi_R$) due to their copious generation of soot. Our simplified global model for gaseous radiation conserves the flame mass, momentum, product species, and thermal energy for the flame taken as a whole. The only empirical inputs to this model are 1) McCaffrey's correlations of his centerline thermocouple measurements and observed flame tip heights; 2) the entrainment constant for buoyant axisymmetric turbulent flows; 3) a radiation

temperature correction factor based on Markstein's measured effective flame radiation temperature; and 4) thermophysical, chemical and radiant properties of the flame configuration. Predicted radiant fractions for typical hydrocarbon fuels with no incomplete products of combustion and no soot radiant emission are around 12%, which is close to the 15% suggested by the literature. The buoyant jet flame apparatus is being modified to supply vaporized liquid fuels such as methanol for radiation measurements on non-luminous fires. This experimental capability will allow us to check the accuracy of the predicted radiant fractions. We are also setting up instrumentation to measure the incompleteness of combustion, which is required by all our models. A draft report describing our non-luminous radiation model has been prepared.

In a parallel analysis we have developed a scaling relationship for χ_r and for flame heights obtained from scanning radiometer data (see Task 3 below). In addition to the usual hydrodynamic mixing-combustion length-scale, one has a radiative cooling length-scale which results in radiative flame heights being proportional to either $\dot{Q}'^{1/2}$ for planar flames or $\dot{Q}^{1/3}$ for axisymmetric flames in agreement with Markstein's recent measurements. An empirical correlation for luminous flames based on the fuel smoke-point, ℓ_s, but neglecting gas radiation effects, suggests that $\chi_R \sim \ell_s^{-1/4}$ and explains much of the observed dependence on ambient vitiation and oxygen enrichment. This empirical relationship was derived by arguing that χ_R is a function of the ratio of the hydrodynamic to the radiative cooling length-scale. These concepts have been extended to momentum controlled flame jets and are consistent with our previous measurements of these fires. We are currently seeking a model which explicitly accounts for both gas radiation effects and flame cooling by radiation.

Publications

1. Delichatsios, M.A., "Flame Radiation Scaling in Turbulent Jet Flames," paper for presentation at the Fall Technical Meeting, Eastern Section, The Combustion Institute, Albany, NY, October 30 - November 1, 1989.

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. Currently, five panels topped by a water-cooled heat transfer plate are used, providing an overall height of 2.2 m. Water-cooled sidewalls provide two-dimensional flame structure.

In addition to porous-wall fires, flames obtained with a slot burner, placed either adjacent to a heat transfer plate or free burning between sidewalls, and axisymmetric jet flames, are studied for comparison purposes. In recent work, a heat-transfer plate of 0.38 m width and 2.2 m height had been installed temporarily to extend the flame height and, therefore, the upper limit of heat release rate beyond previously attained values. The plate has been used both for slot-burner flames adjacent to the wall and as a background for free-burning slot burner flames and axisymmetric jet flames. Runs with this arrangement have been completed, and work with the porous-metal burner has been resumed.

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.

Four fuels of varying sooting tendency, methane, ethane, ethylene and propylene were selected for this study. One of the important results of the work concerns the radiative fraction χ_r of total heat-release rate for the various flame configurations and fuels. Values of χ_r averaged over the range of heat-release rates of about 10 to 60 kW are presented in Table 1.

Table 1. Average Radiative Fractions

		Slot Burner	
Fuel	Jet Flame	Free-Burning	Against Wall
CH_4	.200	.182	.143
C_2H_6	.240	.239	.168
C_2H_4	.372	.371	.240
C_3H_6	.445	.440	.313

The values for free-burning slot-burner flames are only slightly reduced with respect to those for jet flames, but placing the slot burner adjacent to the wall is seen to cause substantial reductions of χ_r. However, all three flame configurations show the same trend with fuel sooting tendency and thus the quantitative relationship between χ_r and fuel smoke point established previously for jet flames can certainly be applied also to free-burning slot-burner flames, and presumably can be generalized for application to wall flames. Power-law exponents relating χ_r to total heat-release rate $\dot{Q}_{tot}$, averaged over the four fuels, were 0.04 ± 0.07 for jet flames, 0.08 ± 0.04 for free-burning slot-burner flames, and 0.18 ± 0.02 for slot-burner flames adjacent to the wall.

Results of current work with the porous-metal burner are still incomplete, but indicate further reductions of χ_r relative to those obtained with the slot burner adjacent to the wall, as well as further increases of the power-law exponents.

The vertical distributions of radiant emission per unit height differed significantly for the various flame configurations. Free-burning slot-burner flames showed steeper rise and decay of radiant emission than jet flames; placing the slot burner against the wall reduced the peak radiant emission drastically and nearly doubled the height required for burnout.

The vertical distributions for jet and slot-burner flames exhibited similarity with respect to heat-release rate. For each flame configuration and fuel, the distributions for various heat-release rates could be collapsed into a single dimensionless plot by introducing a normalizing length parameter proportional to the variance of the individual distribution. The power-law exponents of the length parameter with respect to heat-release rate were about 1/3 for jet flames and about 1/2 for slot-burner flames, in contrast to the flame-height exponents derived from fluid-dynamic similarity, 2/5 for jet flames and 2/3 for slot-burner flames. Theoretical interpretations of the observed deviations from fluid-dynamic similarity are currently under study. Again, results obtained with the porous-metal wall burner are incomplete, but are being evaluated to see whether similarity relationships can be formulated for the distributions of radiant emission of these more general wall fires.

Publications

1. Markstein, G.H., "Correlations for Smoke Points and Radiant Emission of Laminar Hydrocarbon Diffusion Flames," 22nd Symposium (International) on Combustion, p. 363, The Combustion Institute, 1989.

2. 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.

Task 4. Transient Pyrolysis, Flame Radiation and Sooting Properties of Solid Materials - The objective of this task is to develop and demonstrate a practical methodology for specifying material pyrolysis properties for solid, charring and noncharring fuels. These properties include the transient pyrolysis of a material and the radiative properties of the burning pyrolysis gases.

Although significant progress has been achieved in all the areas mentioned above, we decided to outline here an important development concerning the use of time to ignition data for characterizing the thermal inertia and the minimum (critical) energy for ignition or pyrolysis.

Thermal Inertia and Minimum (Critical) Energy for Ignition or Pyrolysis - The current most common practice for interpreting ignition time data is to plot $1/\sqrt{t_{ign}}$ vs the imposed heat flux $\dot{q}''$ and force a straight line through the data, assuming in effect that a) heat transfer into the solid occurs by conduction and b) no surface heat losses, especially reradiation losses, exist. The intercept of the straight line with the heat flux axis is assumed to be the critical heat flux below which no ignition (or pyrolysis) occurs, while the slope is used to estimate the thermal inertia of the material.

Our objective in this work is to a) investigate to what extent this widely used approach accurately represents the heat up of a given material including surface reradiation losses, b) propose modifications in the current procedure for deducing the thermal inertia and the critical heat flux.

Approach-Results-Conclusions - To achieve our objectives we have followed the following procedure:

1. We solved numerically for the surface temperature history of a thermally thick conducting material including surface reradiation losses. We used a Volterra type integral equation for the surface temperature and applied a continuation method to obtain a numerical solution. The results are shown in Figure 1 where the ordinate is the dependent variable

$$\psi = \frac{T_s - T_o}{T^* - T_o} \tag{1}$$

and the abscissa is the square root of a dimensionless time

$$\tau = \frac{1}{\pi\ k\rho c}\ \frac{\dot{q}_e''^{\,2}}{(T^* - T_o)^2} \cdot t \tag{2}$$

The variables have the following meaning:

T_s : surface temperature
T_o : initial temperature

$$\dot{q}_e'' = \dot{q}'' + \varepsilon\ \sigma\ T_o^4$$

where $\dot{q}''$ is the imposed heat flux, $T^* = \left(\frac{\dot{q}''}{\varepsilon\sigma} + T_o^4\right)^{1/4}$ and the single parameter β or α in Figure 1 is:

$$\beta = 1 - \alpha = \frac{T_o}{T^*}$$ (the higher the value of β, the smaller the imposed heat flux)

$k\rho c$: is the thermal inertia of the solid.

2. We have developed excellent approximations of the numerical solution by asymptotic analysis. These are summarized in the following way here:

$$\frac{1}{\sqrt{t_{ign}}} = \frac{2}{\sqrt{\pi\ k\rho c}\ (T_p - T_o)}\ (\dot{q}'' - .64\ \dot{q}''_{cr})$$

for $\dot{q}'' \gtrsim 3\ \dot{q}''_{cr}$ (3)

$$\frac{1}{\sqrt{t_{ign}}} = \frac{\pi}{\sqrt{\pi\ k\rho c}\ (T_p - T_o)}\ (\dot{q}'' - \dot{q}''_{cr})$$

for $\dot{q}'' \lesssim (1.1)\ \dot{q}''_{cr}$ (4)

where the critical heat flux is: $\dot{q}''_{cr} = \varepsilon\ \sigma\ (T_p^4 - T_o^4)$ and T_p is the pyrolysis temperature.

3. We have shown that surface reradiation losses can indeed account for the surface temperature histories in a flammability apparatus. Figure 2 includes such experimental histories plotted in the same co-ordinates as in Figure 1. These data represent four heat fluxes: .59 W/cm^2 (β = .5); 1.2 W/cm^2 (β = .44); 3W/cm^2 (β = .36) and 6 W/cm^2 (β = .30). For the two higher heat fluxes, pyrolysis has occurred as the peak values of the ordinate in Fig. 2 imply. The agreement of the heat-up period with the theory is very good.

4. Then we have also tested eq. (3) by using time to pyrolysis data measured in our apparatus. The results are shown in Figure 3. We are also showing in the same figure what eq. (4) represents. Figure 3 illustrates to persons familiar with the problem the limitations and shortcomings of the presently used method for interpreting time to ignition data.

The present analysis and validation can provide a precise methodology for conducting time to ignition tests and for best estimating (cf with Fig. 3 and eq. (3)) the thermal inertia and the critical heat flux of a given material.

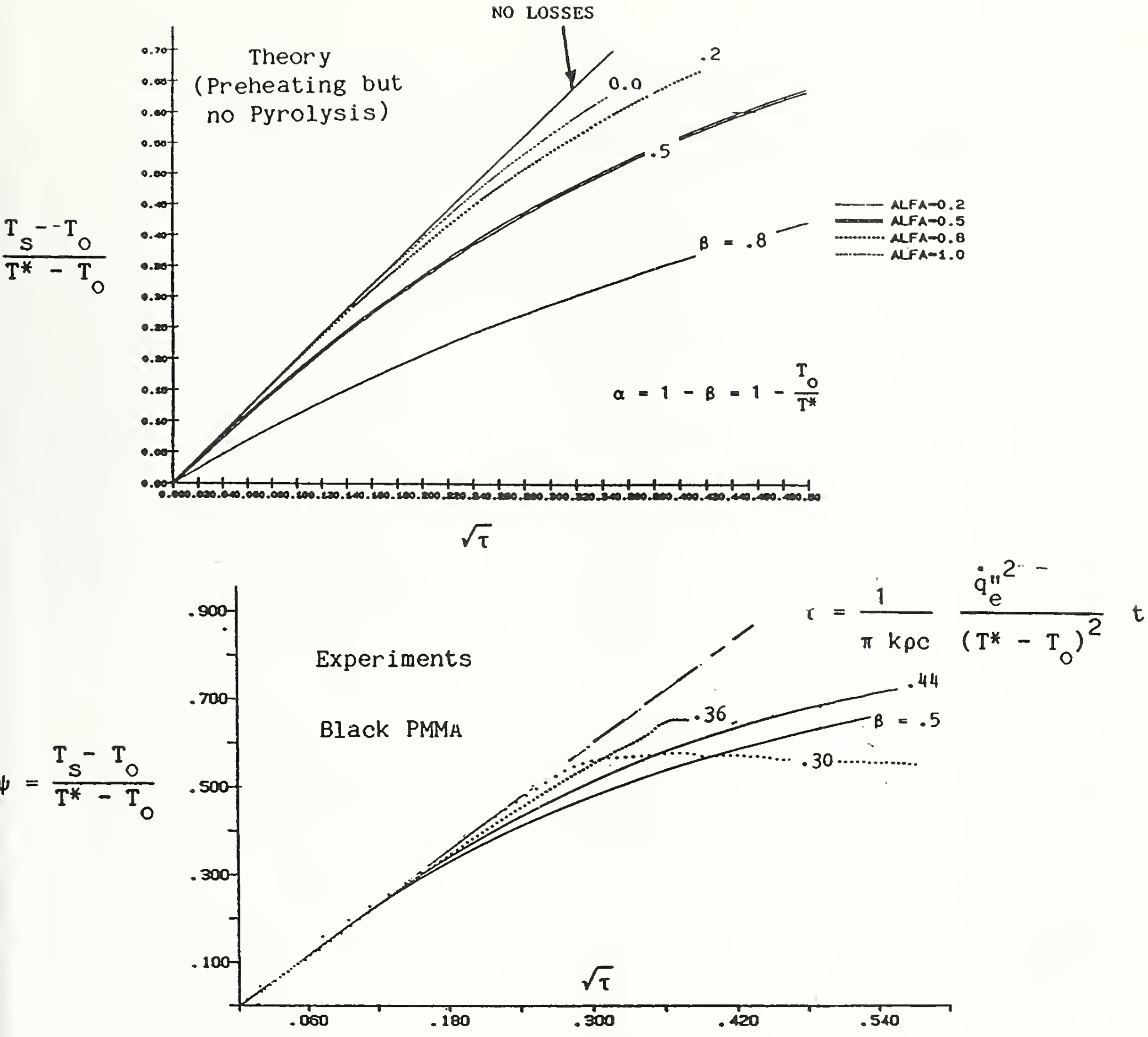


Fig. 1 and Fig. 2: Surface Temperature Histories Including Reradiation Losses

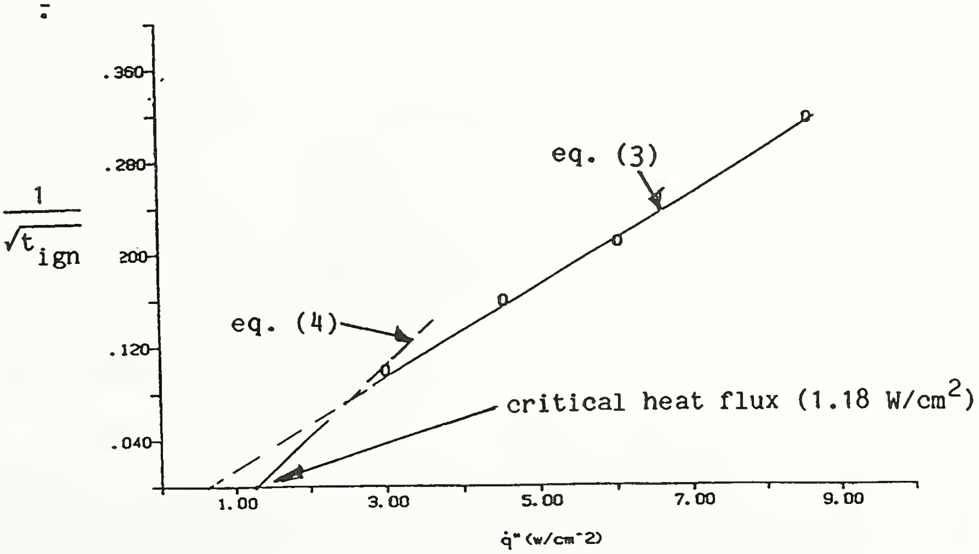


Fig. 3: Time to ignition correlation and comparison with experiments, including reradiation losses.

Center for Fire Research
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 1989

Institution:	Factory Mutual Research Corporation
Grant No:	60NANB8DO845
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

The general objective of this work is to advance the day of the availability of a fire model so comprehensive as to make a performance city fire code possible. Specific progress was made on further analysis of glass breaking, general outline of a comprehensive fire model, model heat conduction algorithm, correct use of fire test data in a fire model, effect of wind on an enclosure fire, and further analysis of ceiling jet heat transfer.

Further Analysis of Window Glass Breaking in an Enclosure Fire(1)

Pagni(2) and Keski-Rahkonen(3) showed that the temperature rise at which a window cracks is $\Delta T = \sigma_{\text{breaking}}/E\beta$. Multiple cracks are essential so that a large piece of glass falls out. Such multiple cracks always are formed. A suggestive reason (supported by beam theory) shows why crack bifurcation always occurs just beyond the cooled edge.

General Outline of a Fire Model

In connection with the work of a steering committee (Quintiere, Cooper, Zukoski, Emmons) for a proposed "Comprehensive Computer Fire Model," an outline for the needed phenomena all the way from ignition to extinguishment, collapse, escape, or death of occupants, was produced, discussed, and revised. The outline contains 204 general topics--too extensive to present here. Many of the topics are indeed general as, e.g., "Wall Fire -- simple, charring, melting, spreading up, down, sideways." The amount of scientific studies still required to make the CCFM is immense.

Model Heat Conduction Algorithm

The development of a new fire code regulation is carried out by committee consensus and prepublication inviting comments, "peer review." Each of the many phenomena in a computer fire code can be treated at many levels of approximation. How can a computer fire code be evaluated for approval for general use? The first step is to use only algorithms which have been carefully compared with all competing ideas by someone knowledgeable of the phenomena and then peer reviewed by selected small teams on each case.

As an example of what is needed, report #80,(4) presents a proposed algorithm for the calculation of the heating to ignition of a simple fuel by 1D transient heat conduction.

Correct Use of Fire Test Data in a Fire Model

Any fuel ignites and burns in a way dependent upon local air movements, radiative and convective energy feedback, and local air composition dependent upon time and the enclosure in which it is situated. No single (or small number) of fire tests can provide the fire growth and burning rate data required for general model use. It is necessary, therefore, to deduce the model constants (for each model needing the data) from the fire test results. This is done by computing the test with the model using various model constants until the model reproduces the test data to acceptable accuracy. How this can be done for FIRST is illustrated by computing the FIRST constants from the data of a furniture calorimeter test of an upholstered chair.(5,6)

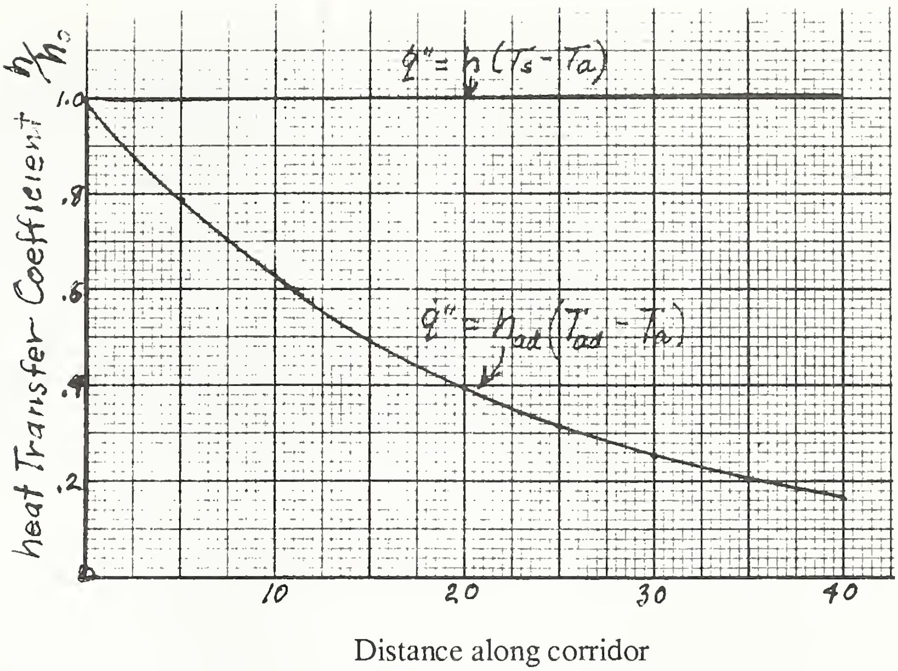
Effect of Wind on an Enclosure Fire

The pressure distribution on a structure by the wind will cause a flow throughout the interior through open doors, windows, and leaks. That flow can be calculated using appropriate flow resistance networks. When a fire occurs in that structure, additional forces by fire gas expansion and buoyancy are added. A treatment of this fire-wind interaction has been developed, but is not yet completed for publication.

Ceiling Jet Heat Transfer

Formulas and computer codes have been completed for linearized heat transfer from a transient ceiling jet with heat transfer jet to ambient, jet to ceiling, and ceiling to ambient. Test data of Chobotov(7) shows the heat transfer coefficient jet to ceiling to be nearly constant along a corridor when based upon the actual local ceiling jet temperature. The theory shows that there results a large decrease of heat transfer coefficient along the corridor when the adiabatic jet temperature, T_{ad}, is used. This occurs because the heat transfer coefficient must compensate for the fact that T_{ad} falls too slowly along the corridor.

h_0 is the heat transfer coefficient, jet to wall, at jet entrance to corridor



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4. Emmons, H., Heat Conduction in Fires, Home Fire Project Technical Report #80, p. 0-12, 1989.

8/2/89

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: The Pennsylvania State University
Grant No.: 60NANB8D0849
Grant Title: Upward Flame Spread on a Vertical Wall
Principal Investigator: A. K. Kulkarni
Department of Mechanical Engineering
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University Park, PA 16802
Other Professional Personnel: C. I. Kim, Graduate Assistant
C.-H. Kuo, Graduate Student
Scientific Officer: W. J. Parker
Technical Abstract:

Introduction: An experimental and modelling study of upward flame spread on vertical walls is being conducted. The overall objective is to develop a predictive methodology for flame propagation and growth in upward spreading configuration for vertical surfaces of practical materials. Several tests were initially made at NIST Center for Fire Research and the project was continued at Penn State. A numerical model is being developed for predicting the upward flame spread rate and the measurement of heat feedback by flame above the pyrolysis front, $\dot{q}_w''(x,t)$, is in progress.

Experiments: At NIST, experiments on wall samples of several different materials were conducted and the data were analyzed in terms of the upward spread of the flame tip, upward spread of the pyrolysis front, and the rate of heat release as a function of time. Also, comparison of data was made with an approximate model developed earlier. Details of the setup and procedures can be found in reference 1. Some of the results are presented in a summary form in Figure 1. Data and predictions of energy release rate per unit width for various materials clearly show the relative fire growth potential for the materials in upward flame spread orientation, which is a very common way for fire growth in the initial stage. The PMMA fire is clearly much more hazardous than the textile fires in this situation. Such results are necessary for predicting fire growth and for defining material flammability in upward flame spreading situations.

Although the predictions appear to generally represent the experimentally observed performance of materials, the model needs improvement. In the previous model, the heat feedback, $\dot{q}_w''$, was assumed to be a fixed number (25kW/m^2) for $x_p < x < x_f$ and zero for $x > x_f$. In order to improve the estimation of $\dot{q}_w''$, an experimental apparatus has been constructed which will measure $\dot{q}_w''(x,t)$ for wall samples of various materials and test are currently in progress. The heat feedback data will be suitably reduced and correlated for use in the upward flame spread models. Details of experiments are included in our second quarter progress report.

Mathematical Model: The present model differs from the previous model in four major aspects: (i) The heating of the surface above pyrolysis front is calculated using a more accurate heat conduction model, rather than the approach of employing a fixed, inert heating time constant, (ii) the heat feedback distribution above the flame tip (i.e. for $x > x_f$) is allowed to decay gradually instead of assuming it to be zero, (iii) the surface temperature is permitted to decrease gradually even beyond $x > x_f$, rather than assuming it to be ambient because the hot plume gases from the fire preheat the surface above $x > x_f$, and (iv) heat feedback distribution between $x_p < x < x_f$ is allowed to vary based on experimentally obtained, curve-fitted data. It is assumed that the ignition temperature does not vary with location; there is no heat conduction in the solid in x-direction; and the material is inert during the heating process.

The surface temperature of a semi-infinite slab (T_s), initially at the temperature of T_o subjected to the external flux of $\dot{q}''_w(x,t)$ is given by,

$$T_s(x,t) = T_o + \frac{1}{\sqrt{\pi k \rho c}} \int_0^t \frac{\dot{q}''_w(x,t')\,dt'}{\sqrt{t-t'}} \tag{1}$$

where $\dot{q}''_w(x,t)$ is obtained from curve-fitting experimental data and it can be written in the form,

$$\dot{q}''_w(x,t) = \dot{q}''_{wo}\; g\{\, x_b(t), x_p(t), x_f(t), x \,\} \tag{2}$$

where $\dot{q}''_{wo}$ is a "fire property" of the wall material and g is a generalized function of burnout edge (x_b), pyrolysis height (x_p), and flame tip height (x_f).

The flame tip height is obtained from an available correlation,

$$x_f(t) - x_b(t) = K \left[\dot{Q}'(t) + h_c \int_{x_b(t)}^{x_p(t)} \dot{m}''\,dx \right]^n \tag{3}$$

where $\dot{Q}'$ is the igniter strength (kW/m), h_c is the heat of combustion of the fuel, K and n are experimentally obtained constants, and $\dot{m}''$ and x_b are described as,

$$\begin{aligned} \dot{m}''(\lambda) &= a_4\lambda^4 + a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 \;;\; \text{if } \lambda < t_b \\ \dot{m}''(\lambda) &= 0 \;;\; \text{if } \lambda > t_b \end{aligned} \tag{4}$$

$$x_b(t) = x_p(t - t_b) \tag{5}$$

where λ is a local time which is the time after the surface reaches the ignition temperature, t_b is the burnout time which is the time period from the instant of ignition to the end of pyrolysis at a given location. $\dot{m}''(\lambda)$ is treated as a material "fire property" which is independent of the location and it is obtained in separate, small scale experiments (cf. ref. 1).

The above set of equations is solved with a numerical procedure that involves finite difference method and numerical integration.

Results: Depending upon the igniter strength, the height of the initially ignited portion of the sample, x_{po} , (which has a surface temperature of T_{ig}) is determined. The surface temperature above the initial pyrolysis height x_{po} is assumed to be exponentially decaying (Fig. 2). The functional form of $\dot{q}''_w(x,t)$ is such that the forward heat flux is constant up to the flame tip height then exponentially decays. This is generally consistent with previous experimental results. With these conditions, numerical computations are performed for various wall materials. Fig. 3 shows flame tip height prediction for 1/2" thick particle board. When compared to the experimental results of Kulkarni [1], the computations overpredict the data. However, considering the fact that the estimation of x_f in the experiments was based on the highly visible and continuous flame tip, the actual x_f might have been higher and thus closer to the prediction. Fig. 4 shows the pyrolysis height prediction for particle board and masonite. Experimental results for pyrolysis height in this time domain were not available for comparison, but x_p measured at $t \cong 300$s for masonite was 110cm which is close to the prediction.

The current heat feedback measurement experiments are needed to quantify the behavior of practical materials, and to subsequently define the "fire properties" needed for modelling purposes. The upward flame spread prediction procedure, and its experimental verification, has tremendous importance and potential for use in predicting fire growth and for ranking materials based on their flammability.

Reports and Papers

1. Kulkarni, A. K. "Upward Flame Spread on Vertical Walls," Final Report on Grant No. 60NANB4D0037 submitted to Center for Fire Research, National Institute of Standards and Technology, 1989.

2. Kulkarni, A. K. and Fischer, S. J. "Upward flame Spread on Vertical Walls: Model and Experiments," to be presented at the III International Seminar on Flame Structure, Alma-Ata, USSR, September 1989.

3. Kulkarni, A. K. and Fischer, S. J. "Upward flame Spread on Vertical Walls: An Approximate But Complete Model and Experiments," Accepted for presentation at the 1989 ASME Winter Annual Meeting, San Francisco, CA, December 1989.

4. Kim, C. I. and Kulkarni, A. K. "A Numerical Model for Upward Flame Spread," Submitted to Eastern Section of the Combustion Institute Meeting, 1989.

Other Related Papers on NIST Grant

5. Kulkarni, A. K. and Chou, S. L. "Turbulent Natural Convection Flow on a Heated Vertical Wall Immersed in a Stratified Atmosphere," Journal of Heat Transfer 3, pp 378-384, 1989.

6. Hwang, J. J. and Kulkarni, A. K. "An Experimental Study of Vertical Wall Fire in a Stratified Atmosphere," Experimental Thermal and Fluid Science 2, pp 216-223, 1989.

7. Kulkarni, A. K. and Kim, C. I. "Heat Loss to the Interior of a Free Burning Vertical PMMA Slab and Its Influence on Heat of Pyrolysis," Heat Transfer Phenomena in Radiation, Combustion and Fires, 1989 NHTC, HTD vol. 106, pp359-365, 1989.

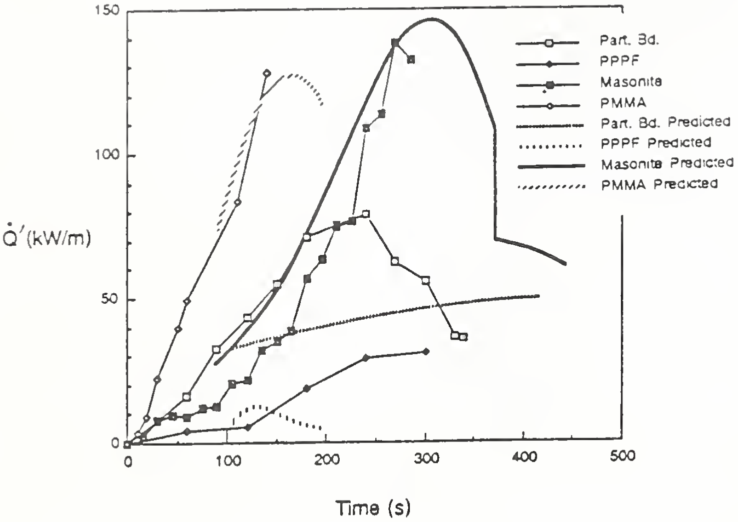

Fig. 1 Measured and Predicted Values of Energy Release Rate for Various Materials as a Function of Time.

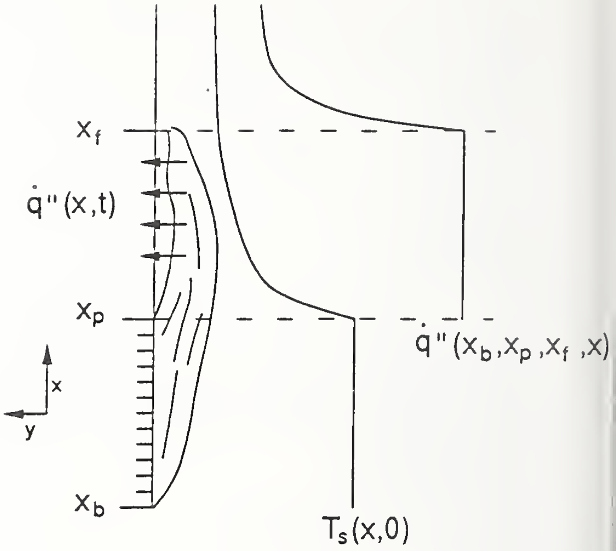

Fig. 2 Schematic of Upward Spreading Wall Fire, Forward Heat Flux and Initial Surface Temperature.

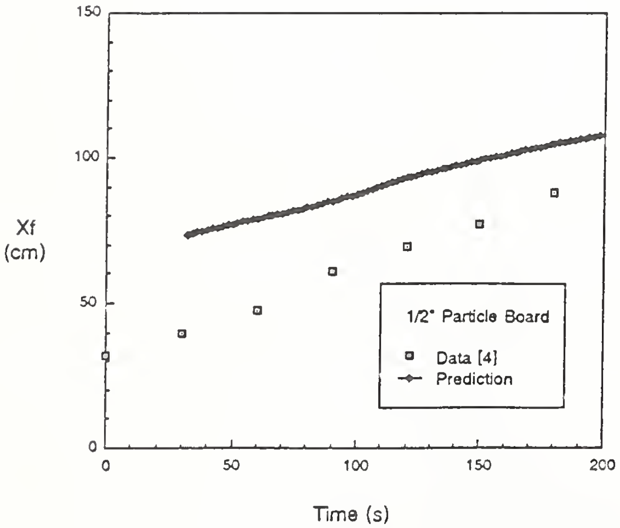

Fig. 3 Flame Height Prediction and Comparison with Data [1] for 1/2" Thick Particle Board

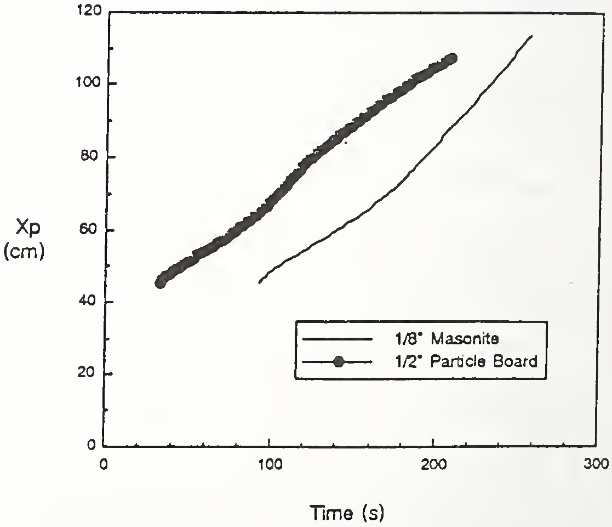

Fig. 4 Pyrolysis Height Predictions for 1/2" Thick Particle Board and 1/8" Thick Masonite.

F. Toxic Potency

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

TOXIC POTENCY MEASUREMENT

Professional Personnel

Vytenis Babrauskas, Group Leader
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Nancy Eller, Guest Worker, University of Pittsburgh

Project Objective

To develop models and methods to predict and measure the combustion products that evolve from burning materials and to predict the impact of those products on living organisms.

Scope

1. Develop a proper small-scale combustion apparatus and the analytical tools for generation, identification, and quantitation of toxic agents in fire atmospheres.
2. Develop general validation procedures for verifying that a bench-scale toxic potency test correctly represents full-scale fire behavior.
3. Develop a simplified gas model to predict the toxicity of complex gas mixtures found in fire atmospheres.
4. Develop a bioanalytical screening test to determine whether the combustion products from materials are extremely toxic (*i.e.*, low concentrations produce toxic effect) or unusually toxic (*i.e.*, the toxicity of the combined major fire gases is not sufficient to account for the observed toxicity). This test is also designed to minimize the use of animals.
5. Determine the best physiologically-based pharmacokinetic model for predicting the rate of absorption and equilibrium levels of carboxyhemoglobin (COHb) in rats and humans during exposure to carbon monoxide (CO).

Technical Accomplishments

A proper small-scale generator of combustion products is being developed in order to better correlate the toxic potency of smoke from small-scale test procedures with that from large-scale "real" fires. This year, the criteria for an optimal small-scale toxicity test were formulated, a number of practical alternatives examined, and a straw-man candidate test method selected. The method is a variation on the radiant heat toxicity test apparatus developed at the Southwest Research Institute. SwRI is building the new apparatus and is testing a series of representative materials - Douglas fir, rigid polyurethane foam, flexible polyurethane foam and PTFE.

The validation task was a special 1-year project intended to develop the needed validation methodology. Only a limited amount of actual testing or validation work was included. The full-scale configuration considered was a room/corridor/room geometry, with two room walls being lined with the test material. Ignition was with a crib of the same material as being tested. Two materials were tested in this configuration: Douglas fir, and rigid polyurethane foam. The bench-scale tests examined were the cup furnace toxicity test and the new radiant heat method being developed in conjunction with SwRI (discussed above).

FTIR analysis is considered the state-of-the-art approach for the continuous identification and quantitation of the multiple combustion products in fires. The feasibility of using this technique was demonstrated this year by the examination of gases from a series of materials burned in the Cone Calorimeter and a fluidized-bed incinerator. Such a continuous monitoring device for toxicants in fire gases will provide analytical data which will complement animal exposure studies in assessing toxic potency of fire gases.

The Center for Fire Research has been developing a simplified gas model (known as the N-Gas Model) to predict the toxicity of the complex gas mixtures found in fire atmospheres. One of the advantages of this model is the reduction in the cost of and the dependence on animal testing without sacrificing test accuracy. Research on the N-Gas model has progressed from the determination of the toxicity of individual gases - CO, CO_2, HCN, and reduced O_2 - in Fischer 344 rats exposed for 30 minutes and observed for at least 14 days to the development of a four-gas model based on the combined toxicological results of these four gases. Other exposure times ranging from 1 to 60 minutes for single gases and 5 to 60 minutes for two gas combinations - CO plus HCN and CO plus CO_2 - have also been examined. The additivity and synergistic effects observed from the 30-minute animal exposures were observed at the other times. The toxicity of the combined three and four gases were also examined for 30 minute exposures and the additivity and synergism observed previously were still applicable. The current N-gas model appears to explain the deaths observed at the 30-minute LC_{50} values from most materials' thermal decomposition products. Some materials need further examination.

Based on these results, equation (1) was derived to predict the combined toxicities of these four gases:

$$\frac{m[CO]}{[CO_2] - b} + \frac{[HCN]}{d} + \frac{21 - [O_2]}{21 - LC_{50}\ O_2} \approx 1 \qquad (1)$$

where the values in brackets are the atmospheric concentrations of the gases in ppm (CO, CO_2, HCN) or percent (O_2); m and b are the slope and y intercept of the CO/CO_2 interaction curve; and [HCN] and d are the atmospheric test and the lethal concentrations of HCN, respectively. The value of d will vary depending on whether it is the within-exposure deaths or the within plus post-exposure deaths that are of concern. Based on all the data to date in which some percent of the animals died (not 0 or 100%), the mean value of equation 1 is 1.1 with 95% confidence limits ranging from 0.9 to 1.3. In other words, at the mean value of 1.1, 50% of the exposed animals would be predicted to die; whereas, below 0.9 or above 1.3, none or all of the animals would be expected to die from these exposures, respectively.

This year, research was initiated to add a fifth gas - NO_2 - to this model. NO_2 is considered a significant toxic combustion product because of its potential evolution both from nitrogen-fixation and nitrogen-containing materials. With the addition of this fifth gas, the N-Gas model will more closely predict the toxicity of complex fire gas mixtures. The toxicity of NO_2 with and without CO_2 was examined and a synergistic interaction was discovered. In Fischer 344 male rats, the LC_{50} (30 minute exposure plus 14 day post-exposure observation period) for NO_2 was 200 ppm (with 95% confidence limits ranging from 190-210 ppm); the LC_{50} for CO_2 was 47%[1] (with 95% confidence limits of 43 to 51%); whereas, the LC_{50} for NO_2 in the presence of 5% CO_2 was 90 ppm (with 95% confidence limits ranging from 70-120 ppm). Exposure to NO_2 increased the methemoglobin (MetHb) levels in the arterial blood. At the end of the 30 minute exposures, the MetHb levels were 2 - 3 times higher in the animals exposed to the combination of NO_2 (200 ppm) and CO_2 (5%) than in those exposed to NO_2 only. Deaths from NO_2 were all post-exposure and occurred earlier in the presence of NO_2 plus 5% CO_2 than in the absence of the CO_2. The time of death was concentration-dependent when both gases were present. At death, evidence of hemorrhage and extensive edema was observed in the lungs. The mean lung wet weight/body weight ratio from rats exposed to 200 ppm NO_2 with and without 5% CO_2 was 3-4 times that of non-exposed rats. More edema was noted with NO_2 and CO_2 than with NO_2 alone.

Work was begun on the determination of the best available physiologically-based pharmacokinetic model for predicting the rate of absorption of CO and formation of COHb and equilibrium levels in both rats and humans. It was found that the Coburn, Forster, Kane (CFK) model only works for low levels of atmospheric CO, i.e., up to 600 ppm for both rats and humans. A modified CFK model seems to work well for all steady-state CO concentrations. This work will enable more accurate human safety predictions.

Funding from Other Agencies/Institutions

In addition to CFR Priority Project funding, the above research was partially supported with funds from The Society of Plastics, Inc.

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Nyden, M.R. and Chittur, K., Component spectrum reconstruction from partially characterized mixtures. **Applied Spect. 43**, 123-128 (1989).

Levin, B.C. and Gann, R.G., Toxic potency of fire smoke: its measurement and use. Proceedings of American Chemical Society Symposium on Fire and Polymers, Dallas, TX, April, 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). [U.S.] Natl. Inst. of Standards and Technology (1989).

Levin, B.C. The N-Gas Model Screening Test for Assessing the Acute Inhalation Lethality of Smoke, Appendix A of Report by E. Braun entitled Implementation of

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[1] 1% is equal to 10,000 ppm.

N-Gas Model Screening Test for Assessing the Acute Inhalation Lethality of Smoke. NIST Report to the Navy (1989).

Levin, B.C., Paabo, M., Gurman, J.L., Clark, H.M., and Yoklavich, M.F., Further Studies of the Toxicological Effects of Different Time Exposures to the Individual and Combined Fire Gases: Carbon Monoxide, Hydrogen Cyanide, Carbon Dioxide, and Reduced Oxygen, pp. 249-252 in **Polyurethane '88**, Proceedings of the 31st Society of Plastics Meeting, Philadelphia, PA, October, 1988, Technomic Publishing Company, Inc., Lancaster, PA.

Levin, B.C., Gurman, J.L., Paabo, M., Baier, L., and Holt, T., Toxicological Effects of Different Time Exposures to the Fire Gases: Carbon Monoxide or Hydrogen Cyanide or to Carbon Monoxide Combined with Hydrogen Cyanide or Carbon Dioxide, pp. 240-248 in **Polyurethane '88**, Proceedings of the 31st Society of Plastics Meeting, Philadelphia, PA, October, 1988, Technomic Publishing Company, Inc., Lancaster, PA.

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 (Accepted for publication, **J. of Forensic Sciences**).

Related Grants

1. Southwest Research Institute, PI - Walter Switzer and Alex Wenzel, Analysis of Hazards to Life Safety in Fires.
2. Southwest Research Institute, PI - Arthur Grand, Development of a Strategy for Evaluating the Potential Toxic Hazard of Items in Fires using the SwRI Radiant Combustion/Exposure System.
3. University of Pittsburgh, PI - Yves Alarie, Toxicity of Plastic Combustion Products.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY FY89

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

Principal Investigator:
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Other Professional Personnel:
Dr. Arthur F. Grand
Staff Scientist
Dr. Gordon E. Hartzell (Retired)
Principal Investigator, Oct 88–Apr 89

NIST 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. Predicting the combined toxic effects of these mixtures is one of the most difficult problems in combustion toxicology. Basic toxicological data are needed to develop models to address this problem in order to relate small-scale results to large-scale, improve testing protocols, and reduce the number of animals required for testing. Both the n-gas model (1) and the FED model (2) are under development but require additional data and verification. Our approach consists of conducting animal exposures to controlled levels, both individually and in combination, of known combustion gas toxicants. 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 developed lethality and associated toxicological data for the following: 1) hydrogen bromide (HBr), 2) binary combinations of hydrogen cyanide (HCN) and hydrogen chloride (HCl) and 3) tertiary mixtures containing carbon monoxide (CO), HCN and HCl.

Hydrogen Bromide:

Hydrogen bromide (HBr) has been identified as a gas of potential toxicological importance in fires because certain fire retardants contain bromine and consequently are capable of releasing HBr when thermally degraded. To initiate the data base for incorporation of HBr into the n-gas model, an LC_{50} (lethal concentration 50%) determination was accomplished (Table 1). The LC_{50} estimate obtained for a 30-minute exposure and 14-day survival period was 3360 ppm, with associated 95-percent confidence limits of 2,300 to 4,300 ppm.

Multiple Gas Exposures:

HCN and HCl:

LC_{50} values for combinations of HCN and HCl were developed, with HCN as the independent variable. The HCl levels selected were 600, 1,000, and 1,900 ppm. The LC_{50} values calculated for HCN at each HCl level are as follows:

A statistical comparison of the LC_{50} values demonstrated a significant difference between the values at both 1,000 and 1,900 ppm HCl combined with HCN, compared to HCN alone. This is indicative of an interactive effect between these gases.

CO, HCl and HCN Combinations:

Combustion atmospheres commonly contain more than two toxicants and it is important to be able to model multiple components. In a pilot study, experiments were conducted with a combination of CO, HCl and HCN (Table 3). Various ratios of the three gases, calculated by the n-gas and FED models to result in 1.0 (equivalent to 50% lethality), were tested. Two of the experiments resulted in 50% mortality, as expected from the calculation. In the first test, all deaths occurred post exposure, a pattern of lethality associated with HCl. However, the HCl level of 1,200 ppm would not be expected to result in 50% lethality by itself. In the second test, all deaths occurred during the exposure period. The contribution of HCl to lethality in this test is unclear since the FED summation of HCN and CO values was equal to 0.98 of an LC_{50}. The summation of the FED values for the third test equalled 1.07, but no lethalities occurred. This is not according to expectation since the FED summation of similiar concentrations of HCl and HCN in the binary combination studies resulted in lethalities. Additional tests are needed for this combination of gases to determine if this result is significant, since the addition of HCl can greatly increase the variability of the dose-response relationship.

In summary, some evidence was presented that HCl and HCN can apparently interact toxicologically in an additive manner so as to affect lethality in rats, despite different target sites. This is a similiar result to that found for CO and HCl combinations (3). Further work is needed to determine the variance associated with the addition of fractional parts of LC_{50} values, so that error limits can be defined and the degree of confidence in the predictions improved.

TABLE 1
DATA SUMMARY
HYDROGEN BROMIDE (HBr)
RAT, 30-MINUTE EXPOSURE

AVERAGE HBr (ppm)	EXPOSURE NUMBER DEAD	POSTEXPOSURE NUMBER DEAD n=6			TOTAL NUMBER DEAD
		DAY 0	DAYS 1-4	DAYS 5-14	
1710	0	0	0	1	1
2780	0	0	1	0	1
4200	2	0	0	1	3
4280	1	0	0	5	6
5380	0	0	0	4	4
6380	2	0	4	--	6

HBr LC50 = 3360 (2300-4300)

Table 2

Nominal HCl ppm	Fraction LC$_{50}$	LC$_{50}$ HCN ppm	Fraction LC$_{50}$	Σ FED Lethality
0	0.00	212	1.00	1.00
600	0.16	219	1.03	1.19
1000	0.26	112*	0.53	0.79
1900	0.50	70*	0.33	0.83

* = significant difference ($p < 0.05$)

TABLE 3
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		
HCL HCN CO	1200 75 2140	0.31 0.35 0.33	0	0	0	3	3	1.00
HCL HCN CO	720 125 2530	0.19 0.59 0.39	3**	0	0	0	3	1.17
HCL HCN CO	1870 70 1610	0.49 0.33 0.25	0	0	0	0	0	1.07

* Based on the following LC50 values: CO=6410, HCl=3810, HCN=212

** Mean %COHb=70.7 s.d. 1.5

References:

1. Levin, B. C., M. Paabo, J. L. Gurman and S. E. Harris, "Effects of Exposure to Single or Multiple Combinations of the Predominant Toxic Gases and Low Oxygen Atmospheres Produced in Fires," Fundamental and Applied Toxicology, 9, pp. 236-250 (1987).

2. Hartzell, G. E., D. N. Priest and W. G. Switzer. "Modeling of Toxicological Effects of Fire Gases: II. Mathematical Modeling of Intoxication of Rats by Carbon Monoxide and Hydrogen Cyanide," J. Fire Sciences, 3, 115-128 (March/April 1985).

3. Hartzell, G. E., A. F. Grand, and W. G. Switzer. "Modeling of Toxicological Effects of Fire Gases: VI. Further Studies on the Toxicity of Smoke Containing Hydrogen Chloride," J. Fire Sciences, 2, pp. 368-391 (November/December 1987).

Reports and Papers:

1. Hartzell, G. E., A. F. Grand and W. G. Switzer, "Modeling of Toxicological effects of Fire Gases: VII. Studies on Evaluation of Animal Models in Combustion Toxicology," J. Fire Sciences, 6, pp. 411-429, 1988.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY FY89

Institution: Southwest Research Institute

Grant No.: 60NANB9D0943

Grant Title: "Development of a Strategy for Evaluating the Potential Toxic Hazard of Items in Fires Using the Southwest Research Institute Radiant Combustion/Exposure System"

Principal Investigator:
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Other Professional Personnel: Walter G. Switzer

NIST Scientific Officer: Dr. Vytenis Babrauskas

Technical Abstract:

A new laboratory apparatus and test method have been under development, under the auspices of the National Institute of Building Sciences (NIBS) and conducted at Southwest Research Institute, for evaluating the "potential toxic hazard" of actual products when involved in fires. The apparatus (shown in Figure 1) utilizes the principle of radiant heat combustion of the specimen, along with collection of all of the smoke produced for exposure of the test animals, and is based on the radiant furnace modification (1) to the NBS smoke toxicity test apparatus (2). Three critical fire parameters may be determined in this test method; they are 1) time to ignition, 2) rate of smoke evolution, and 3) toxic potency of the smoke. Under the NIBS program, these were combined in a single, measured test variable called "irradiation time" (IT).

The original objective of this program was to develop data, using the new radiant combustion apparatus, for the development of a method of estimating toxic hazard by a mathematical combination of the same parameters used to determine the IT in the current NIBS protocol. However, during the course of the program, it became evident that the oxygen concentration in the combustion chamber had an effect on the evolution of carbon monoxide (particularly in the case of the wood specimens). Therefore, the focus of the study was redirected in an attempt to develop more data on the CO/O_2 relationship.

The four products examined in this program were 1) Douglas fir board (DF), cut down to a thickness of approximately 1.3 cm (1/2 in.); 2) non-fire retarded flexible polyurethane foam (FPU), used as received in 5-cm (2-in.) thickness; 3) rigid polyurethane foam (RPU), used as received in 2.5-cm (1-in.) thickness; and 4) polytetrafluoroethylene (PTFE), supplied as a sheet 0.3-cm (1/8-in.) thick.

Times to ignition of full-size specimens under the influence of the tungsten-quartz radiant lamps were determined for blackened vs. unblackened specimens. These data are listed in Table 1.

TABLE 1.
TIMES TO IGNITION (SECONDS) FOR
7.6-CM X 12.7-CM SPECIMENS AT 50 KW/M^2

	Unblackened	Blackened
DF	55	13
FPU	15-20	5
RPU	21	4
PTFE	no ignition	no ignition

Blackening the surface of the DF, FPU and RPU specimens caused shorter times to ignition under the 50 kW/m^2 radiant heat flux from the tungsten-quartz lamps. Any differences in the resulting mass loss rates were not obvious. Under these test and specimen conditions, the PTFE did not ignite.

The effect of oxygen concentration on CO evolution in this apparatus was briefly studied. Figure 2 illustrates the relationship observed for carbon monoxide yields (g CO/g mass loss) as a function of the approximate equilibrium oxygen concentration for up to 15 minutes for the tests performed on Douglas fir. Evolution of CO from these specimens appears to have been affected by the oxygen concentration, with higher CO yields generally observed for lower oxygen concentrations.

Carbon monoxide evolution from the FPU and RPU specimens did not show the same pattern with changing oxygen concentrations. One FPU test run produced less CO with higher O_2 than another run; however, a third run did not follow the same pattern. For the RPU specimens, it appears that higher O_2 levels corresponded to more CO evolution, rather than the other way around.

Insufficient data were obtained to actually calculate LC_{50}'s for these specimens; however, the range of lethal smoke concentrations (i.e., the range within which lethalities were observed) are presented in Table 2.

TABLE 2.
RANGE OF SMOKE AND GAS CONCENTRATIONS
WITHIN WHICH LETHALITIES WERE OBSERVED

	Smoke Concentration (mg/L)	CO Ct (ppm-min)	HCN Ct (ppm-min)
DF	100-217	52,000-120,700	---
FPU	>62	>36,400	>1,670
RPU	19-33	42,600-84,400	1,490-2,980

It is somewhat difficult to compare the lethal smoke concentrations obtained for these materials until data on these same materials under a different test protocol are available. For the Douglas fir, however, the range of smoke concentrations leading to lethality (100 mg/L, at which no deaths were observed, up to 217 mg/L, at which five deaths were observed during the 30-minute exposure and 14-day postexposure periods) seems to be distinctly higher than that generally observed for such a material under the conditions of the cup furnace. This is explainable by the fact that much higher concentrations of CO_2 were observed in these tests (7 to 13 percent) compared to the cup furnace (generally much less than 5 percent), suggesting that more efficient combustion occurred in this device compared to the cup furnace.

The specimens of PTFE did not ignite under the conditions tested. We have in the past been able to ignite PTFE specimens in this apparatus under a radiant heat flux of 50 kW/m^2. It is unknown at this time why these specimens failed to ignite.

In summary, this very brief study has illustrated that this device is capable of being used for research studies on the toxic effects of smoke. However, specimen considerations such as surface color and experimental conditions such as oxygen concentration would appear to have an influence on the outcome of the test procedure. Consideration has been given to a method for incorporating these data into a mathematical formula for estimating a "toxic hazard parameter."

References:

1. Alexeeff, G. V., and S. C. Packham, "Use of a Radiant Furnace Fire Model to Evaluate Acute Toxicity of Smoke," J. Fire Sciences, Vol. 2, July/August 1984, pp. 306-320.

2. Levin, B. C., A. J. Fowell, M. M. Birky, M. Paabo, A. Stale, and D. Malek, "Further Development of a Test Method for the Assessment of the Acute Inhalation Toxicity of Combustion Products," National Bureau of Standards (U.S.), NBSIR82-2532 (1982).

Reports and Papers:

1. Grand, A. F., Development of a Laboratory Radiant Combustion Apparatus for Smoke Toxicity and Smoke Corrosivity Studies, Presentation to the 11th Joint Meeting of the UJNR Panel on Fire Research and Safety, Berkeley, CA, October 19-24, 1989.

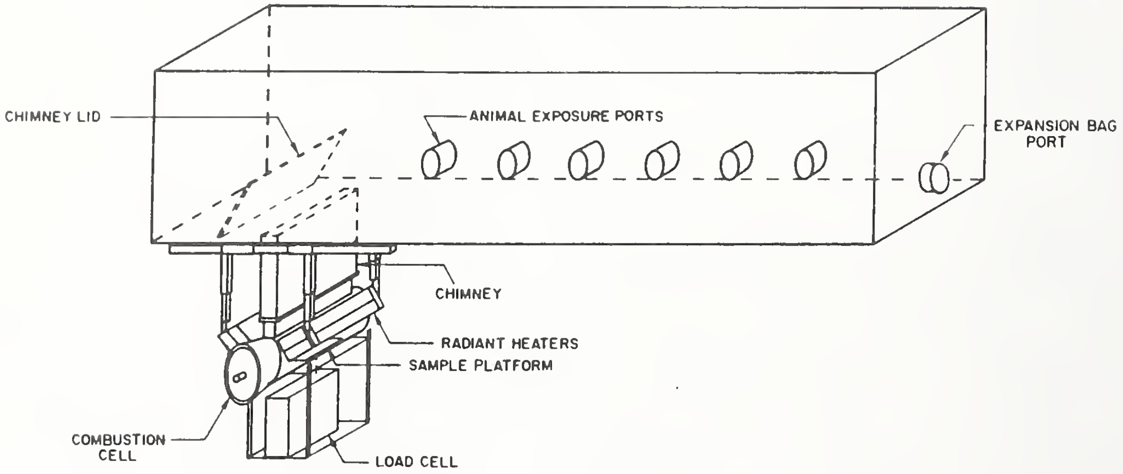

Figure 1. Schematic drawing of radiant combustion/exposure apparatus

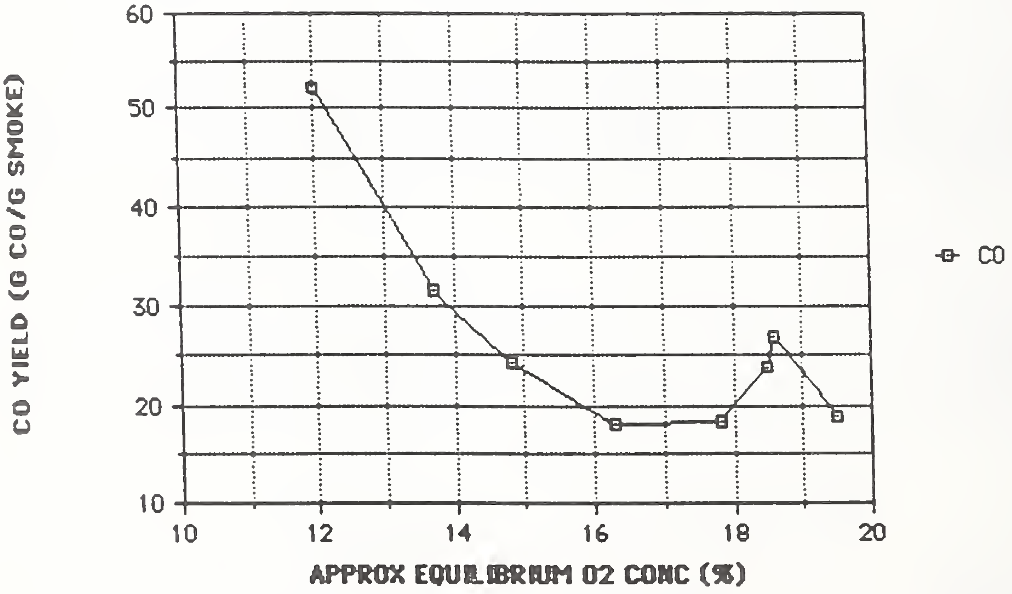

Figure 2. NIST - CO as a function of O_2

CENTER FOR FIRE RESEARCH

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: University of Pittsburgh

Grant No.: 60NANB8D0813

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)

NBS Scientific Officer: Dr. Barbara C. Levin, Ph.D.

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:

A. Combustion Module:

The cone heater used by NIST for the cone calorimeter used to measure heat release was selected for the energy source to initiate burning (flaming) and to maintain burning at a constant rate. The NIST cone heater has been enclosed within a hood (cone hood, 112 L volume) which also contains a load cell on which the specimen to be studied is placed. The irradiance levels were selected at 21, 35 and 50 kW/m^2. Once the irradiance level is set, the specimen is placed under the cone heater, the door of the hood is closed and the hood is ventilated at known airflow rates from 15 to 60 L/min. The lowest ventilation rate is just sufficient to sustain continuous flaming while the higher rates will result in more efficient combustion (i.e. low CO yield) for all 3 irradiance levels given above.

B. Toxicity Module:

The exhaust from the cone hood is directed toward the exposure system previously used for the University of Pittsburgh toxicity protocol. This exposure system has been modified to accommodate exposure of 16 mice.

C. Analytical Module:

Chemical analysis of the exhaust from the exposure chamber is made on a continuous basis for O_2, CO and CO_2. For nitrogen containing specimens hydrogen cyanide is also measured.

D. Data Collection and Calculation Module:

A computer collects the digitized values of the analog voltage output of the O_2, CO or CO_2 analyzers and the load cell. From these the mass loss rate is calculated. From the value entered for the ventilation rate of the cone hood the O_2 consumed and CO and CO_2 produced are calculated. The time to ignition (sustained flaming) is entered manually. Flame height above the specimen is also entered manually every minute. From the O_2 consumed, the heat release is calculated. These are quite simmilar to the calculations made with the NIST cone calorimeter except for flame height entries. For toxicity (lethality) the values collected for O_2 and CO are used to calculate carboxy-hemoglobin levels (for mice and humans) during burning of the specimens. This is done using the Coburn-Forster-Kane equation as modified by Tyuma et al., Jap. J. Physiol. 31, 131-143, 1981.

E. Specimen:

The only specimen extensively used so far has been Douglas fir, clear vertical grain, grade No. 1. Each specimen tested was 38 mm thick and cut to 110 mm X 110 mm. The average mass of all specimens tested was 255 g ± 43.5 (n = 104) with the lightest specimen being 180 g and the heaviest 330 g. All specimens were equilibrated at 45-55 RH and 20-22°C. The specimens were placed in the metal holder provided by NIST to obviate side effects and insure that a constant surface area (100 mm X 100 mm, 0.01 m^2) was exposed to the irradiance level selected. Each experiment consisted in having a specimen under a given irradiance level and ventilation rate for a period of 30 min.

II. Results:

A total of 104 experiments with Douglas fir have been completed with the above UPITT/NIST system. The protocol was designed so that the data could be analyzed by regression analysis to determine the influence of i) irradiance levels ii) ventilation and iii) specimen density on mass loss rate, oxygen consumption and CO_2 and CO production. Our results can be summarized as follows:

a) time to ignition: the time to ignition decreased with irradiance level; very variable at 21 kW/m^2 with much less variability at 35 and 50 kW/m^2; not greatly influenced by ventilation or specimen density.

b) flame height: proportional to irradiance level and not influenced in a major way by ventilation or specimen density.

c) mass loss: proportional to irradiance level; slightly influenced by ventilation, but not by specimen density.

d) oxygen consumption: proportional to irradiance level; slightly influenced by ventilation but not by specimen density.

e) carbon dioxide production: same as for oxygen consumption.

f) carbon monoxide production: at all three irradiance levels there was a sharp increase in CO production which was dependent upon the ventilation rate. At 21 and 35 kW/m^2 CO levels were below lethal levels if the ventilation rates were above 22.5 L/min. At 50 kW/m^2 CO levels were below lethal levels if the ventilation rates were above 17.5 L/min. The influence of the ventilation rate can also be observed by calculating a ratio, rm, as follows:

rm = A/B where:

A = $\dot{m}$ air (g/min from ventilation rate)/rg

rg = rg (wood) taken to be 5.7 g air/g specimen

B = Mass loss of the specimen ($\dot{m}$, g/min)

We find a sharp increase in CO to above lethal levels when rm was 3 or below with irradiance levels of 21 kW/m^2. At 35 kW/m^2 this sharp increase in CO occurred with rm below 1.7 while at 50 kW/m^2 it occurred at an rm value of 1.1.

Conclusions:

We find that the cone heater is easy to operate and when used with the cone hood/exposure apparatus an entire system can be operated to obtain reproducible results for given irradiance levels and ventilation rates. That the mass loss rate increased with irradiance level was expected, however the ventilation rate had little influence on this variable. Rather, the influence of the ventilation rate was on the efficiency of combustion. Therefore we can conclude that within the irradiance levels tested smoke produced by flaming Douglas fir can be of very low toxicity or definitely lethal depending upon the ventilation rate. From the CO produced and O_2 depletion, COHb levels can be predicted for mice used as experimental animals in this system as well as for humans. Experiments with animals will be undertaken to examine how close the measured values will be with the predicted values.

Reports and Papers:

1. D.E. Malek and Y. Alarie, "Ergometer Within a Whole Body Plethysmograph to Evaluate Performance of Guinea Pigs Under Toxic Atmospheres," Toxicol. Appl. Pharmacol. in press.

G. Furniture Flammability

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

FURNITURE FLAMMABILITY

Professional Personnel

W. Parker, Project Leader
T. Ohlemiller, Chemical Engineer
J. Quintiere, Division Chief
K. Villa, Textile Technologist
K. Tu, Mechanical Engineer

Project Objective

To provide a technical basis for evaluating the Bulletin 133 room fire test and for making recommendations with regard to modifications that might improve its utility as a fire test method for upholstered furniture.

Scope

An improved ignition source with greater reproducibility will be checked out in the room fire tests to be conducted at the California Bureau of Home Furnishings (CBHF). The use of instrumentation for measuring the heat release rate in the Bulletin 133 test will be demonstrated. The burning characteristics of chairs in the furniture calorimeter will be compared with those in the Bulletin 133 room test. The impact of changing the room dimensions from those of the Bulletin 133 room to those of the proposed ASTM room on the test results will be examined. Recommendations will be made with regard to the modification and use of the Bulletin 133 test for a room fire test of upholstered furniture. A long range plan will be developed for the use of bench scale tests to predict the fire hazard of upholstered furniture.

Technical Accomplishments

I. Analysis of the Hazard

It was determined that the major fire hazard of upholstered furniture is its total heat release rate. The attainment of flashover in a room is related to the total heat release rate of all the items burning in the room. The spread of fire from one item to another depends on the thermal radiation levels produced by the first item which in turn is proportional to its total heat release rate. Excessive levels of CO and temperature rise in the lower part of the room or in the rooms beyond the room of fire origin typically occur after flashover is reached.

II. Heat release rate Instrumentation

A new collection hood and exhaust system capable of being used for the measurement of the total rates of heat, carbon monoxide and smoke production during the test is being installed in the California Bulletin 133 Room at CBHF.

III. Ignition Source

1. Critical Assessment of the California Bulletin 133 Ignition Source

This ignition source consists of five crumpled sheets of newsprint placed at the seat/back juncture of a chair to be tested. The newsprint is covered with a sheet metal/wire mesh box which permits flames to impinge on the seat and back surfaces of the chair as well as, potentially, on the inner surface of the chair side arms. This is a strong ignition source that poses a severe test of the ignition resistance of the chair. Its main weak point comes from the use of crumpled paper whose behavior is difficult to make reproducible. The issue of reproducibility was examined in three ways. First, the degree of flame extension out the sides of the box was measured by videotaping a series of nominally identical tests. Second, the variability of the two-dimensional, time-dependent heat flux pattern which the source imposes on the seat back was measured by means of an infrared imaging radiometer. Third the quantitative test-to-test variation in heat flux incident on six fixed points on the seat back was measured. In all of these measurements the level of reproducibility of this ignition source was such that it was deemed desirable to replace it in subsequent in-house testing of furniture flammability.

2. Development of an Alternative Furniture Ignition Source

It was decided that a gas flame with a controlled flow rate and fixed duration of application could provide a simple and reproducible alternative to the newsprint source. However, it was also deemed desirable that this alternative source yield flammability behavior comparable to the CB 133 source. The first alternative source was based on the T-burner being utilized by S. Ames of the British Fire Research Station. Tests with propane showed that it could yield comparable peak heat fluxes to those seen from the CB 133 source. Tests with mock-up chairs using fabric/cushioning combinations thought to be marginal in ignitibility and, therefore, sensitive to ignitor conditions gave equal ignition behavior from the two sources. However the area ignited by the two sources was not very comparable with the result that the ensuing rate of heat release curves differed appreciably. We have designed a variation of the Ames ignitor that should overcome this shortcoming; it is to be tested in the near future.

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

SMOLDERING COMBUSTION OF FURNITURE COMPONENTS

Professional Personnel

T. J. Ohlemiller, Project Leader
S. Dolan, Chemist

Project Objectives

To further our fundamental understanding of smoldering combustion phenomena while, at the same time, providing input data for hazard analysis models.

Project Scope

Smoldering combustion is responsible for a large fraction of residential fire deaths and it appears that CO poisoning is a major underlying cause. We have thus undertaken a program to characterize the emissions from this mode of combustion for some common residential fuels. At the same time, we are exploring the smoldering behavior of these fuels between the extinction and flaming limits in order to obtain insights into the controlling factors.

Technical Accomplishments

The initial work has focused on the smoldering of solid wood since this dovetails with prior work for DOE. Experiments have been completed in which samples of red oak and white pine were made to undergo self-sustained smolder under conditions of controlled air supply. Achievement of self-sustained smolder over solid wood requires a configuration which limits the heat loss rate from the oxidizing char surface; propagation along the interior surface of a U-shaped channel was used here. Results have been obtained for the case in which the smolder zone propagates in the same direction as the air flow along the channel (termed forward smolder), for the opposite case (termed reverse smolder) and for the more general mixed case of simultaneous forward and reverse smolder. The range of air flow rates for which stable propagation is possible in the current configuration is rather narrow -- about 8 to 20 cm/sec referred to the initial channel cross section. Transition to flaming occurs with higher flow rates and extinction occurs with lower flow rates. In the range of stable smolder, CO comprises 3 to 4 mole % of the exhaust gases evolved from the combustion chamber and 10 to 20 weight % of the evolved mass from the wood. Other products have also been characterized and compared with those evolved from the same woods in other modes of gasification. In addition we have obtained estimates of the rate of heat release from this smolder situation on the basis of oxygen consumption. Analysis of temperature profiles in the wood during smolder propagation leads to the inference that radiation along the channel axis is a major heat transfer mode driving the propagation. Current work is focused on the development of a two-dimensional smolder spread model.

Reports and Publications

Ohlemiller, T. and Shaub, W., "Products of Wood Smolder and Their Relation to Wood-Burning Stoves", National Bureau of Standards NBSIR 88-3767, May, 1988

Ohlemiller, T., "Effects of Some Physical Factors on Smoldering Combustion of Wood-Based Materials", presented at American Chemical Society Symposium on Fire and Polymers, Dallas, Texas, April, 1989; manuscript in preparation.

Related Grant

"Chemical Factors Influencing Ignition and Combustion in Lignocellulosics", G. Richards, U. of Montana

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: University of Montana

Grant Number: 60NANB8D0822

Grant Title: Chemical Factors Influencing Ignition and Combustion in Lignocellulosics

Principal Investigator: Professor Geoffrey N. Richards
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Other Professional Personnel: Dr. F.-Y. Hshieh, Postdoctoral Research Associate until October 31, 1988
Mr. L.A. Edye, Research Associate, from May 10, 1989

NBS Scientific Officer: Dr. Thomas Ohlemiller

Technical Abstract:

Fires, especially domestic fires, very often involve smoldering combustion of "cellulosic" materials such as insulation and timber. Such materials should more properly be described as lignocellulosics because they contain three major components, viz. cellulose, hemicellulose and lignin. It is probable that in combustion these three components interact. In this project the latter two components will be isolated in the exact form in which they occur in wood (cellulose has previously been extensively studied). Special attention will be paid to influences of metal ions, which occur especially in the hemicellulose component of wood and can be controlled by simple procedures to dramatically influence ignition and combustion behavior of lignocellulosics.

As a preliminary to the study of individual wood constitutents the effect of exposure of lignocellulosics to moderate temperatures for long periods has been studied in relation to subsequent ignition and combustion behavior. These studies relate to situations where "cellulosic" insulation or timbers are exposed to heat sources such as flues, steam pipes, light bulbs, etc.

Samples of solid cottonwood in the form of discs have been heated at 250°C in both air and nitrogen, up to 12 hours, and in air at 150°C up to 30 days. The preheated samples were then further heated in air at 5°C per min^{-1} to unpiloted ignition. Despite major chemical changes during the various preheating treatments, the ignition temperatures were not significantly affected, except for a slight decrease (11°C) after 5 days at 150°C in air.

The isolation of hemicellulose from cottonwood by non-degradative methods has been completed. The hemicellulose obtained has been shown to be chemically unchanged from its original structure in the wood. Methods for removal and

control of cations in the hemicellulose are being developed in preparation for ignition and combustion studies. Non-degradative isolation of lignin from cottonwood (milled wood lignin) is underway.

There has been a hiatus in this project of about six months during the period under consideration because of a delay in finding a suitable replacement for Dr. Hshieh.

Reports and Papers

1. W.F. DeGroot, W.-P. Pan, M.D. Rahman and G.N. Richards, "First Chemical Events in Pyrolysis of Wood," J. Anal. and Appl. Pyrol., 13 (1988) 221-231.

2. M.G. Essig and G.N. Richards, "1,5-Anhydro-β-L-arabinofuranose from Pyrolysis of Plant Cell Wall Materials (Biomass)," Carbohydr. Res., 181 (1988) 189-196.

3. M. Essig, T. Lowary, G.N. Richards and E. Schenck, "Influences of "Neutral" Salts on Thermochemical Conversion of Cellulose and of Sucrose," Proceedings from the International Biomass Conversion Conference, Phoenix, 1988.

4. F.-Y. Hshieh and G.N. Richards, "Factors Influencing Chemisorption and Ignition of Wood Chars," Combustion and Flame, 76 (1989) 37-47.

5. W.F. DeGroot, T.H. Osterheld and G.N. Richards, "The Influence of Natural and Added Catalysts on the Gasification of Wood Chars," Proceedings from the International Biomass Conversion Conference, Phoenix, 1988.

6. W.F. DeGroot, M.P. Kannan and G.N. Richards and O. Theander, "Gasification of Agricultural Residues (Biomass); Influence of Inorganic Constituents," J. Agric. Food Chem., in press.

7. F.-Y. Hshieh and G.N. Richards, "Factors Influencing Oxygen Chemisorption and Ignition of Chars from Newsprint," Comb. and Flame, 76 (1989) 49-56.

8. W.F. DeGroot, "Methylchloride as a Gaseous Tracer for Wood Burning", Environmental Science and Tech., 23(3) (1989) 252.

9. W.F. DeGroot and G.N. Richards, "Relative Rates of Carbon Gasification in Oxygen, Steam and Carbon Dioxide", Carbon, 27(2) (1989) 247-252.

10. M.G. Essig, G.N. Richards and E.M. Schenck, "Mechanisms of Formation of the Major Volatile Products from the Pyrolysis of Cellulose," Applied Polymer Symposia, (1989) 841-862.

11. H.-X. Qiu and G.N. Richards, "Attempted Removal of Metal Ions and Subsequent Vacuum Pyrolysis of Barks from Five Species of Softwood", J. Wood Chem. and Tech., in press.

12. W.P. Pan and G.N. Richards, "Influence of Metal Ions on Volatile Products of Pyrolysis of Wood," J. Anal. and Appl. Pyrol., in press.

13. F.-Y. Hshieh and G.N. Richards, "Effect of Preheating of Wood on Ignition Temperature of Wood Chars," Combust. Flame, in press.

H. Building Fire Modeling and Smoke Transport

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

CONSOLIDATED COMPARTMENT FIRE MODEL

Professional Personnel

Leonard Y. Cooper, Head, Building Fire Modeling Group and Project Leader
John H. Klote, Mechanical Engineer
Glenn P. Forney, Computer Scientist
William Davis, Physicist
Daniel Alvord, Computer Specialist
Jean Bailey, Guest Researcher (Naval Research Laboratory)
Duy Q. Duong, Guest Researcher (National Building Tech. Center, Australia)
Ulrich Max, Guest Researcher (Kassel University, Federal Republic of Germany)
Tokiyoshi Yamada, Guest Researcher (Fire Research Institute, Japan)

Program Objectives

To develop a comprehensive fire model computer code to simulate all physical and chemical aspects of fire in complex structures.

Scope

The work of the project has focused mainly on the development of the Consolidated Compartment Fire Model (CCFM) computer code which consolidates past progress in zone-type compartment fire modeling, and which allows readily for integration of advances with the greatest possible flexibility. The project now focuses on the development of mathematical submodels of the separate compartment fire phenomena to be simulated. In this, concise algorithms and associated modular computer subroutines are developed which are readily usable in zone-type compartment fire model computer codes.

Technical Accomplishments

This year the CCFM development effort led to the completion of the first-stage product, CCFM.VENTS, which is now in review. CCFM.VENTS is a well-documented, user-friendly, prototype, multi-room compartment fire model computer code. It involves a generic CCFM model formulation and code structure. Although it was developed and tested on the NIST mainframe CYBER computer, the code runs also at comparable speeds on personal-computer hardware. Features of CCFM.VENTS include: simulations of concentrations of oxygen and an unspecified number of other products of combustion, as required; robust numerics; unforced vent flows under both low- and high-cross-vent pressure difference conditions; forced ventilation via simple fan/duct systems; stack effect; and wind effects. Finally, the code uses the simplest possible, point-source-plume, smoke-filling fire physics in the rooms-of-fire-origin and a very simple heat transfer calculation there and in other spaces.

An executable version of CCFM.VENTS has been used successfully to simulate fire phenomena under different conditions and in a variety of different types of facility, e.g., fires in multi-room and multi-story facilities with stack effect, wind conditions, and forced ventilation.

Documentation of CCFM.VENTS, which is now in review, is in four parts:

> The Consolidated Compartment Fire Model (CCFM) Computer Code Application CCFM.VENTS - Part I: Physical Basis;
>
> The Consolidated Compartment Fire Model (CCFM) Computer Code Application CCFM.VENTS - Part II: Software Reference Guide;
>
> The Consolidated Compartment Fire Model (CCFM) Computer Code Application CCFM.VENTS - Part III: Catalog of Algorithms and Subroutines; and
>
> The Consolidated Compartment Fire Model (CCFM) Computer Code Application CCFM.VENTS - Part IV: User Guide.

Throughout the course of the year, progress has been made on developing new and improved submodel algorithms and subroutines. An example of this is the development of a uniformly valid theory and an algorithm for computing flow through horizontal ceiling/floor vents. Once validated or refined appropriately through use of the results of experimental programs that have been initiated, use of this algorithm will fill a significant gap that existed in the modeling of certain significant top-/bottom-vented compartment fire scenarios. As they become available, newly developed submodels will be added to available zone-type fire models.

Funding from Other Agencies/Institutions

In addition to CFR Priority Project funding the above activities were carried out with support from the following sponsors:

Sponsor: Department of the Navy, Naval Sea Systems Command
Title: Evaluation of Smoke Control on Navy Ships

Sponsor: Department of the Navy, Naval Research Laboratory
Title: Fire and Smoke Spread in Ships

Reports and Publications

"Comparisons of NBS/Harvard VI Simulations and Full-Scale, Multi-room Fire Test Data," J.A. Rockett, M. Morita, and L.Y. Cooper, Fire Safety Science - Proceedings of the Second International Symposium, pp. 481-490, T. Wakumatsu et al, Eds., International Association of Fire Safety Science, Tokyo, June 13-17, 1988, Hemisphere Publishing Co., New York, 1989; also: "Comparisons of NBS/Harvard VI Simulations and Data From All Runs of a Full-Scale, Multi-room Fire Test Program," J.A. Rockett, M. Morita, and L.Y. Cooper, to appear in Fire Safety Journal.

"Ceiling Jet-Driven Wall Flows in Compartment Fires," Cooper, L.Y., Combustion Science and Technology, Vol. 62, pp. 285-296, 1988.

"A Note on Calculating Flows Through Vertical Vents in Zone Fire Models Under Conditions of Arbitrary Cross-Vent Pressure Difference," Cooper, L.Y., Combustion Science and Technology, 64, 1-3, pp. 43-50, 1989.

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"Enclosed Buoyant Convection in a Two-Layer Stratified Fluid," Rehm, R.G., Lozier, D.W., Baum, H.R., and Cooper, L.Y., Proceedings of the 1988 Annual Technical Meeting of the Eastern Section of the Combustion Institute, Clearwater FL, Dec. 5-7, 1988.

"Model of a Simple Fan-Resistance Ventilation System and Its Application to Fire Modeling," Klote, J.H. and Cooper, L.Y., NISTIR 89-4141, National Institute of Standards and Technology (formerly National Bureau of Standards), Gaithersburg MD, 1989.

"Negatively Buoyant Wall Flows Generated in Enclosure Fires, Jaluria, Y, and Cooper, L.Y.," invited paper to appear in Progress in Energy and Combustion Science.

"Calculation of the Flow Through a Horizontal Ceiling/Floor Vent," Cooper, L.Y., NISTIR 89-4052, National Institute of Standards and Technology (formerly National Bureau of Standards), Gaithersburg MD, March 1989; also "An Algorithm for Flow Through Ceiling/Floor Vents," Cooper, L.Y., Proceedings of the 1989 Fall Technical Meeting of Eastern Section of the Combustion Institute, Oct. 30 - Nov. 1, 1989, Albany, NY.

"Burning Characteristics of Combat Ship Compartments and Vertical Fire Spread," Gross, D., and Davis, W.D., NISTIR 88-3897, National Institute of Standards and Technology (formerly National Bureau of Standards), Gaithersburg MD, 1988.

"Impact of Stack Effect on the Flow Field in a Compartment in a High Rise Building," Jones, W.W., and Klote J.H., Proceedings of the 1988 Annual Technical Meeting of the Eastern Section of the Combustion Institute, Clearwater FL, Dec. 5-7, 1988.

"Considerations of Stack Effect in Building Fires," Klote, J.H., NISTIR 89-4035, National Institute of Standards and Technology (formerly National Bureau of Standards), Gaithersburg MD 1989.

"Full Scale Smoke Control Fire Tests in the Plaza Hotel Building," Klote, J.H., ASHRAE Journal, Vol. 31, No. 4, pp. 28-32, April 1989.

Related Grants

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

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

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

Numerical Analysis Support for Compartment Fire Modeling Code Development, W.F. Moss, Clemson University.

Prediction of Fire Dynamics, R. Alpert, Factory Mutual Research Corporation.

CENTER FOR FIRE RESEARCH
NATIONAL BUREAU OF STANDARDS
FY 89

INSTITUTION:	California Institute of Technology
GRANT NO.:	NBS5 60NANB600638
GRANT TITLE:	Experimental Study of Environment and Heat Transfer in a Room Fire
Principal Investigator:	Professor Edward E. Zukoski Jet Propulsion Center (301–46) California Institute of Technology Pasadena, CA 91125
Other Professional Personnel:	Professor Toshi Kubota Richard Chan, PhD Candidate James Morehart, PhD Candidate
NBS Scientific Officer:	Dr. Leonard Y. Cooper

Technical Abstract:

Introduction. Smoke which is produced by a fire spreading through a building can act to aid in the spread of the flame by the transport of hot and perhaps combustible gas, and can be harmful to occupants because of its temperature and toxicity or because its opacity hinders the rapid movement of the occupants through the building. Under certain circumstances, the combustion of the fuel produced in the fire can occur under conditions in which the concentration of oxygen in the ambient gas is far below normal and a fuel rich mixture can be produced which will burn later in an adjacent space and aid in the spread of the fire. We are interested in developing models for the production and movement of smoke in complex structures and have been studying several fluid dynamic processes which will be described below. These processes are difficult to describe analytically because the flows are turbulent and are strongly influenced by turbulent mixing between streams in which buoyancy forces are predominant and because the chemical processes in turbulent-buoyant flames are not understood completely.

Gravity Currents. The flow of hot gas in a gravity current in hallways or across very wide rooms allows for very rapid transport of gas which may be toxic and which may also be combustible. Our aim is to understand this transport process and, in particular, the influence of heat transfer between the current and the ceiling on the current and on the subsequent development of the ceiling layer in the hallway or room. Gravity currents in hallways which are horizontal and inclined with respect to the horizontal are being investigated.

Two types of apparatus are being used: first is a salt-water/water facility which is a 2.4 meter long channel with a 15 cm square cross section. This is being used to investigate the dependence of the gravity current parameters on the Reynolds number and the inclination angle, and to determine the nature of the return flow which develops after the gravity current has impinged on a vertical wall closing the downstream end of the channel. Work in this facility is nearing completion and some of the results are summarized in the following paragraphs which concern the speed of the head of the initial current, its depth and the velocity profiles in the current itself.

The parameters used to describe the flow are: g', defined as $(\Delta\rho/\rho)g$, and Q where $\Delta\rho$ is the difference of the fluid densities, ρ is the ambient fluid density, g is the gravitational acceleration and Q is the input volumetric flow rate per unit width of the duct. The measured head speed normalized by $(g'Q)^{1/3}$ is nearly constant along the duct except near the end wall, for Reynolds numbers, Re, which are greater than 1500. Here, Re is Q divided by the kinematic viscosity. For Re lower than 500, it has been observed that the head speed decreases after some distance from the source. The nondimensional head speed observed in the present investigation is about 0.9 over a range of Re from 1000 to 5000.

As the current moves down the hall, the head height, defined as the depth of the current immediately behind the front, at first increases for a short time, and then remains constant throughout the remainder of the test. However, we observed that the dimensionless head height, the head height divided by the reference length, $(Q^2/g')^{1/3}$, decreases from 1.8 to 1.5 when Re increases from 1000 to 4000.

At a fixed spatial position, the layer thickness is only about 40 % of the head height immediately after the passage of the head, but it gradually increases with time until the return wave arrives after the head impinges on the end wall. The increase is due to the development of the boundary layer between the current and the wall and its increase can be approximated by a mathematical expression, $A + B\sqrt{t - C}$, where t is time and A, B and C are constants. A represents the initial layer depth before the boundary layer develops, and B controls the thickness growth with time, and C is related to the time the current reaches the position in question. We observed that A at a fixed spatial position does not change significantly for Re ranging from 1000 to 4000, but the value of A decreases as the distance from the source of the current increases. Its value, when nondimensionalized by the reference length, drops from 0.8 at 50 *cm* downstream from the source to 0.7 at 150 *cm* downstream. On the other hand, the dimensionless value of B increases from 2.0 for Re about 1500 to 2.8 for Re about 3300. We are still developing scaling rules for these parameters.

Velocity profiles in the salt-water layer, obtained by the hydrogen bubble method, at 100 cm downstream of the source is shown in Fig. 1 for the region between the wall and the top of the layer. Note that the layer thickness increases with time, while the maximum velocity decreases with time. The profiles at time 5.90 sec and at 6.10 sec after the head passage show significant difference, indicating that the flow is not very steady right after the head passed, but the stability increases as time passes. These nondimensional velocities are about 120% of the front velocity which is 0.9 for this example.

The volumetric flow rate in the current was obtained by integrating the velocity profiles up to the interface. Typical time histories of Q are shown in Fig. 2, for two cases of similar experimental conditions. The computed flow rate increases from 15 cm^2/s at time 2 *sec* after the head passage to 22 cm^2/s at time 9 *sec* after the head passage, and then levels off. The dashed line is the input flow rate, 23.8 cm^2/s and the difference between the input flow rate and the value computed from the measured velocity at 40 *in* downstream is caused by the layer growth with time at all fixed spatial position. Fast growth requires more of the input fluid, and thus a lower flow rate in the layer for early times. As the growth rate decreases with increasing time, the computed volumr flux approaches the input flow rate.

We are attempting to use correlations of this type to develop a general model for the flow in gravity currents of the type of interest in fire situations.

The second apparatus is an air facility 8.6 m long and 0.5 m square. This apparatus and the experimental results obtained in it are described in detail in the papers by Chobotov et al. Experiments in this apparatus are being used to study currents which initially occupy between 20 to 30% of the depth of the channel and the reverse flow produced when the current impinges on the closed end of the hall.

COMBUSTION IN TWO LAYERS. During the past year we continued our investigation of combustion in the two layer configuration in which the base of a diffusion flame is immersed in an unvitiated atmosphere and the upper part is immersed in strongly vitiated air. We have found that when the equivalence ratio for the gases which form the vitiated layer is much grater than one, the mass fraction of oxygen remaining in the vitiated gas varied from 1 to 5% as the hood configuration was changed. The experiments suggest that combustion in the bulk of the gas or on the surfaces of the hood might be responsible for this change and thus that the gas temperature was a key variable.

To investigate the effects of the upper layer temperature on the species produced, with all other conditions held constant, the 1.83 *m* square by 1.22 *m* deep, bare–metal hood was insulated on the outside in several phases. Each phase consisted of the addition of high–temperature fibergalss (increasing coverage of the hood's surface area or building up multiple layers), and experiments with otherwise fixed conditions were conducted between each phase. Gas temperatures increased from 242 °C (bare metal) to 385 °C (fully insulated), while the mass fraction of oxygen ranged from .036 to .011, respectively (see Figure 3). This reduction in the oxygen measurements was compensated by balanced increases in CO, CO_2, and H_2O. The data points which extend beyond the curves on Figure 3 were reported by Toner for similiar experiments. These results indicate that upper layer temperature will only have a weak effect on species production in this two layer configuration.

Also of concern was the issue of how well–stirred the product layer was in these experiments, i.e. did the chemistry or temperature measurements depend on the position probed within the hood? Experiments were performed without air addition using a 75 kW natural gas fire stabilized on a 19 cm diameter burner with an unvitiated air entrainment height of 10 cm. The probed position was varied to include seven positions at four elevations. Temperature and species mass fractions profiles are shown in Figure 4 with open symbols. The data show uniform species concentrations, even though a vertical temperature gradient exists. Although the temperatures at each elevation were nearly uniform, measurements at the lowest positions probed were 25% lower than those at the highest elevations. These results are in keeping with those of previous work at Caltech which was carried out in the 1.2 *m* cubic hood.

A second set of experiments was performed which maintained identical conditions, except with air addition. There was concern that samples withdrawn from positions nearest to the air addition network might show artifically exaggerated entrainment rates due to incomplete mixing, even though the nearest was still 144 injector diameters from the closest injection port. Indeed, the solid points in Figure 4 indicate that species concentrations were nearly independent of elevation and that the temperature gradient was similar to that found in the previous case.

These tests show that the distribution of all species within the hood is uniform and hence is not an issue in the interpretation of our experimental results.

Further experiments with this apparatus will be used to investigate the product species formed in fires using propylene and ethylene as fuel.

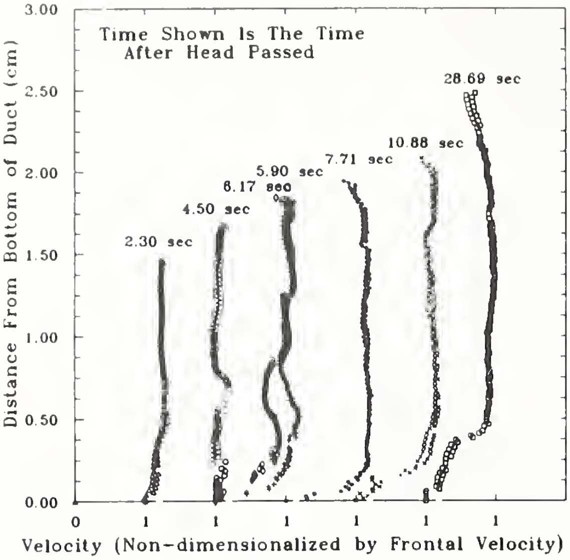


Figure 1: Velocity Profile At 40 Inches Downstream

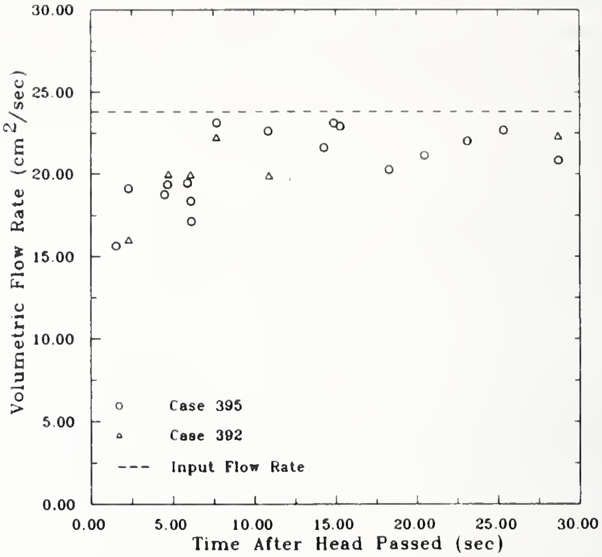


Figure 2: Time History Of Volumetric Flow Rate At 40 Inches Downstream

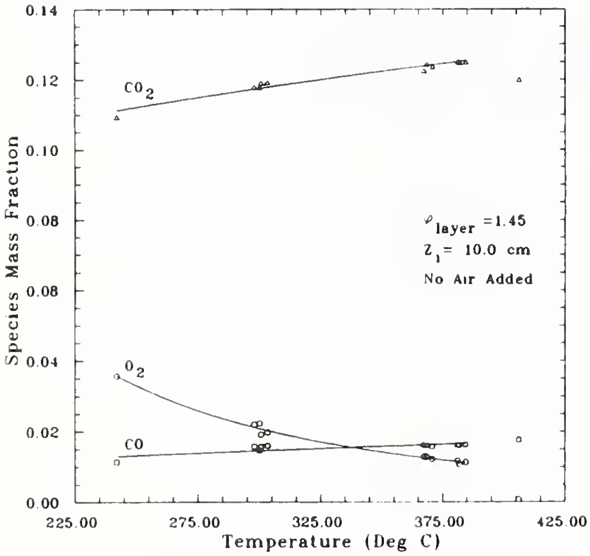


Figure 3: Chemistry Measurements As A Function Of Temperature

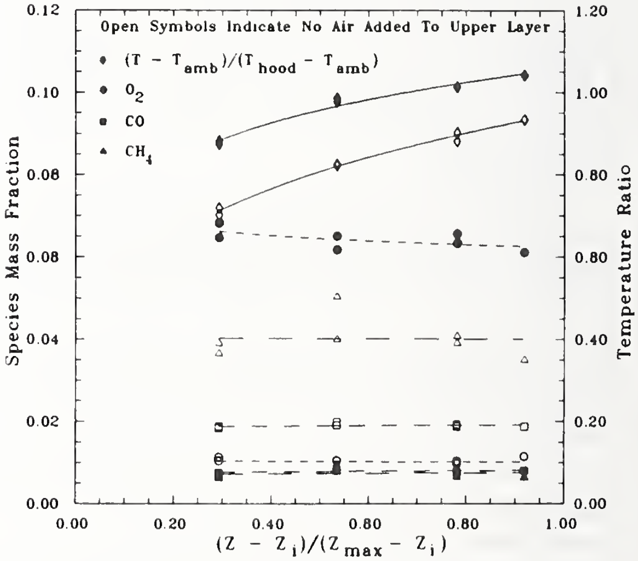


Figure 4: Concentration and Temperature Ratio Profiles As A Function Of Elevation

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution:	Rutgers, The State University of New Jersey New Brunswick, New Jersey
Grant No.:	60NANB7D0743
Grant Title:	Penetration of and Transport Due to Negatively Buoyant Flows Generated in Enclosure Fires
Principal Investigator:	Professor Yogesh Jaluria Department of Mechanical and Aerospace Engineering Rutgers, The State University of New Jersey New Brunswick, NJ 08903 Telephone: (201) 932-3652
Other Professional Personnel:	A. Abib (Ph.D. Student) Q. Tan (M.S. Student) R. Ungar (M.S. Student)
NIST Scientific Officer:	Dr. Leonard Y. Cooper

Technical Abstract:

Introduction. The overall objective of this research effort is to develop models for incorporating the transport due to negatively buoyant and penetrative flows, arising in enclosure fires, in the zone model analysis of the changing environment in a room with a fire. The flows under consideration include the wall flows generated by the downward turning of the fire-plume-driven ceiling jet and the flows resulting from the temperature difference between the wall and the adjacent environment. These flows arise in an essentially uniform medium at the onset of the fire and in a stably stratified medium at later stages, following the establishment of the hot upper layer overlying the relatively cooler lower layer.

Wall Flows. A substantial amount of work has been done on wall jets and buoyancy-induced wall flows arising in uniform and stably stratified media. Detailed experimental results have been obtained on the penetration, entrainment and heat transfer associated with these flows. The results obtained have been presented in terms of correlating equations which can be employed to provide the appropriate inputs for the analytical modeling of enclosure fires [1-3]. A few typical room fire situations have been considered and the experimental results applied to these in order to demonstrate the importance of the negatively buoyant and penetrative flows in enclosure fires and the validity of this approach [4]. A recent review presents the results for the various circumstances considered and application of these results to actual fire situations [5]. The numerical modeling of the relevant enclosure flows has also been investigated [6].

Ceiling Jets. Much of the recent effort has focused on the ceiling jet and its downward turning at the corners of an enclosure. Employing a jet of heated air discharged adjacent to a well-instrumented horizontal, isothermal, surface, which forms a corner with a similarly instrument vertical surface, the heat transfer to the horizontal and vertical surfaces, the downward penetration of the flow and the entrainment into the flow are measured. Figure 1

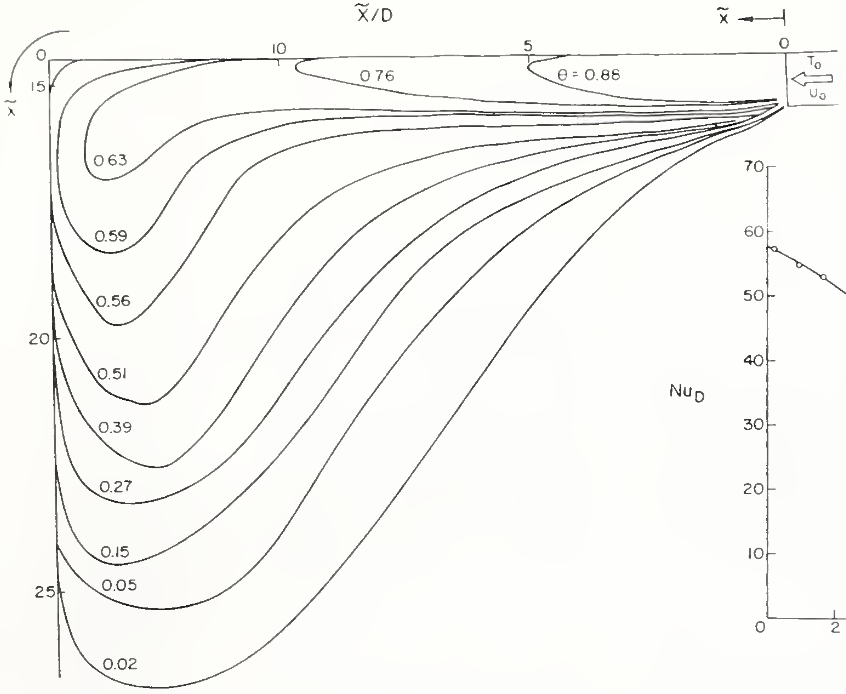


Fig. 1. Measured thermal field at Ri = 0.042.

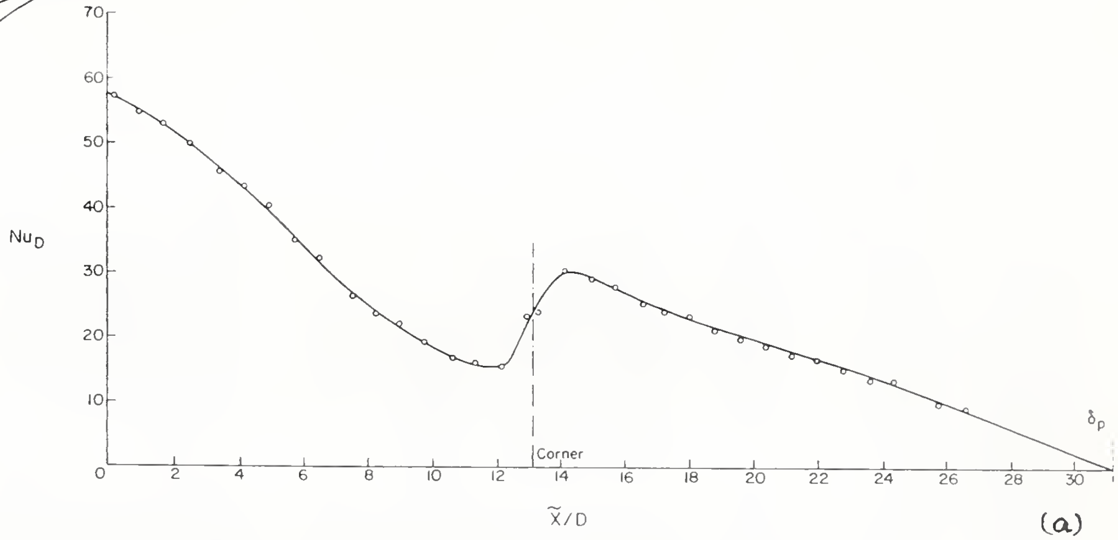
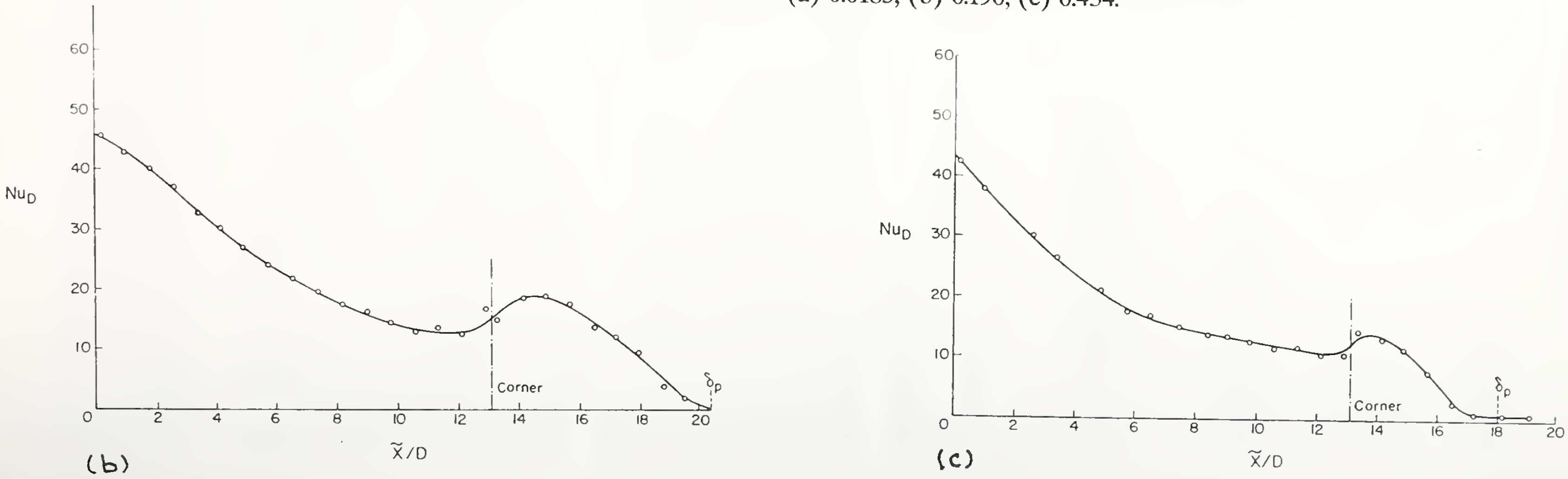


Fig. 2. Variation of the local Nusselt number Nu_D with distance $\tilde{x}$ at Ri values of (a) 0.0185; (b) 0.190, (c) 0.434.



shows the isotherms obtained by interpolation of the temperature data in the flow region for a typical ceiling jet flow circumstance. The downward penetration distance δ_p is obtained by determining the vertical distance to which thermal effects penetrate, as outlined in earlier papers. The heat transfer rate is also measured and presented as a local Nusselt number $Nu_D = hD/k$, where h is the local heat transfer coefficient, D the height of the jet discharge slot and k the fluid thermal conductivity. Figure 2 shows Nu_D as a function of the distance $\tilde{x}$ (see Fig. 1) from the discharge point. The heat transfer rate decreases with $\tilde{x}$, due to increasing boundary layer thickness, up to the corner. A minimum arises due to stagnation near the corner and a further decrease occurs beyond the reattachment point on the vertical wall. Correlating equations were derived for the average Nusselt number $\overline{Nu}_D$ and the penetration depth δ_p. These are given as

$$(\overline{Nu}_D)_{ceiling} = 19.12\ Ri^{-0.15}, \qquad (\overline{Nu}_D)_{wall} = 6.67\ Ri^{-0.25}$$

$$(\overline{Nu}_D)_{ceiling + wall} = 16.95\ Ri^{-0.09}, \qquad \frac{\delta_p}{D} = 3.51\ Ri^{-0.41}$$

where Ri is the Richardson number based on inlet conditions. The variation of the penetration depth with Ri is shown in Figure 3. Here, $Ri = g\beta(T_0-T_\infty)D/U_0^2$, where g is the gravitational acceleration, β the coefficient of volumetric expansion, T_0 the discharge temperature, U_0 the discharge velocity and T_∞ the ambient temperature. The corresponding results for a vertically discharged wall jet are also shown from Refs. [1-3]. Clearly, the penetration is larger for the vertical wall jet at a given Ri. This is largely due to the shear at the ceiling and entrainment into the flow that reduce the flow velocity available to the negatively buoyant wall jet at the corner. Several other such results are obtained for this flow circumstance [7]. These trends agree with results in the literature.

The ceiling jet may impinge on the vertical wall at an oblique orientation, i.e., different from normal impingement. Figures 4 and 5 show some of the results obtained for this flow. Clearly, the penetration distance δ_p and the Nusselt number Nu_D vary with the transverse location on the wall and the inclination. Two transverse locations are chosen, one close to the far end of the plate and one at the near end, with respect to the jet discharge. Thus, the flow travels the largest distance before turning downward in the former case and the shortest distance in the latter. The results are also compared with those for normal impingement.

Further work has been done on these flows and on comparing the results obtained with those for a wall jet in a uniform environment. The results obtained for various circumstances in this project have been compared and the resulting correlations derived in order to determine, in a consistent manner, what results are to be employed at what stage of a growing enclosure fire. These correlations are also being applied to a wide range of room fires to obtain the resulting effect on the transport processes that arise.

Reports and Papers

1. K. Kapoor and Y. Jaluria, "Heat Transfer from a Negatively Buoyant Wall Jet," Int. J. Heat Mass Transfer, 32, 697, 1989.

2. K. Kapoor and Y. Jaluria, "An Experimental Study of the Generation and Characteristics of a Two-Layer Thermally Stable Environment," Int. Comm. Heat Mass Transfer, 15, 751, 1988.

3. Y. Jaluria, "Natural Convection Wall Flows," SFPE Handbook, Sec. 1, Ch. 7, 1988.

4. Y. Jaluria and K. Kapoor, "Importance of Wall Flows at the Early Stages of Fire Growth in the Mathematical Modeling of Enclosure Fires," Combust. Sci. Tech., 59, 355, 1988.

5. Y. Jaluria and L.Y. Cooper, "Negatively Buoyant Wall Flows Generated in Enclosure Fires," Prog. Energy Combust. Sci., 1989, to appear.

6. A. Abib and Y. Jaluria, "Numerical Simulation of the Buoyancy-Induced Flow in a Partially Open Enclosure," Num. Heat Transfer, 14, 235, 1988.

7. Y. Jaluria and K. Kapoor, "Thermal Transport in Ceiling Jet Driven Wall Flows in Enclosure Fires," submitted, 1989.

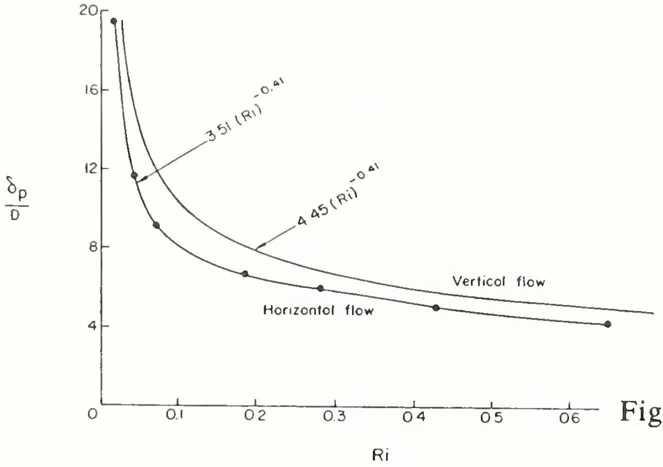


Fig. 3. Penetration depth δ_p as a function of Ri for a vertical wall jet and a downward turning horizontal ceiling jet flow.

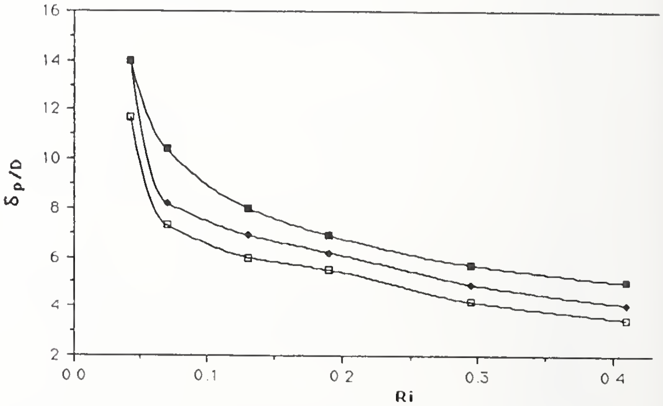


Fig. 4. Penetration depth δ_p as a function of Ri for the downward turning ceiling jet flow for normal and oblique impingement with the vertical wall turned through 30° from the normal position. ■ , normal impingement; ◆, oblique impingement, transverse location farthest from jet discharge; □ , oblique impingement, transverse location closest to jet discharge.

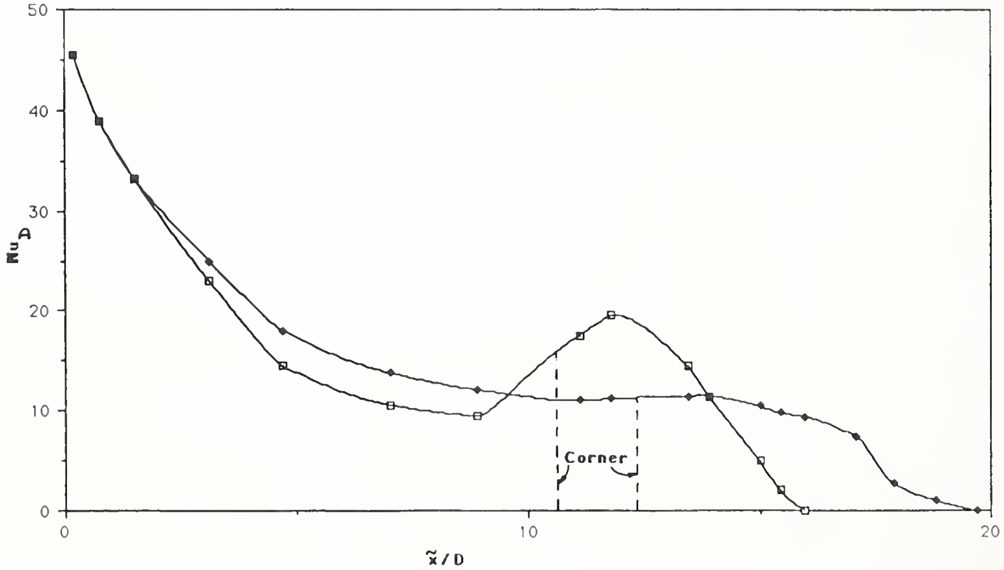


Fig. 5. Variation of the local Nusselt number Nu_D with distance $\tilde{x}$ at Ri = 0.19.
◆ , transverse location farthest from jet discharge;
□, transverse location closest to jet discharge.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: Clemson University

Grant No.: 60NANB8D0857

Grant Title: Numerical Analysis Support for Compartment Fire Modeling Code Development

Principal Investigator: Professor William F. Moss

Other Professional Personnel: Karen Dunlap (M.S. Candidate)

NBS Scientific Officer: Dr. Glenn P. Forney

Technical Abstract:

The primary purpose of this grant was to provide numerical analysis support for compartment fire modeling and in particular, to improve the performance of an already existing code called CCFM.VENTS. The code CCFM.VENTS is based on past advancements in compartment fire modeling. This computer code simulates the conditions which develop during the course of a fire in a building with multiple rooms and floors. Numerically, the simulation is done by applying an ordinary differential equation solver to a system of ordinary differential equations with at least four equations per room. Since these equations are either unstable or stiff over much of the simulation, they are difficult to solve. The dependent variables solved for in each room were (in October 1988) pressure at the floor, smoke layer height, smoke layer density, air layer density, and combustion product concentrations. All other physical variables are computed from these. Rooms can be interconnected by doors and leaks, and rooms can be connected to the outside by doors, windows or leaks. Doors, windows, and leaks are referred to as vents. The mass and energy flow through a vent is governed by a modification of Bernoulli's Law.

The tasks for the first year of this grant (8-15-88 to 8-14-89) were to (1) assist in the preparation of a users' guide, (2) improve the efficiency of the numerics, (3) improve transportability, and (4) improve the users' interface. The following work was completed.

Task 3:

CCFM.VENTS was ported to a Macintosh II and SAVE (Fortran 77) statements were added to provide static memory allocation where needed.

Task 1:

An outline of a users' guide was prepared which included a tutorial carrying the user, step by step, through a two room example.

Task 4:

A list of suggested changes to the users' interface was prepared. For the most part, these have been incorporated into the current version of CCFM.VENTS.

Task 2:

Most of the effort in the first year has been devoted to investigating the numerics of

CCFM.VENTS. Two changes to this code were proposed.

First change:

After a careful study of the physics, an alternative set of dependent variables for each room was proposed: pressure at the floor, smoke layer height, smoke layer mass, air layer mass, and combustion product masses. There are several technical reasons for replacing density by mass. One is that there is less chance for cancellation error in computing the right hand side of the differential equations. A second is that the upper layer density is generally indeterminate at the beginning of the simulation, but the upper layer mass is zero. Indeterminate initial density must be circumvented by a start up heuristic which causes a slow start up.

Second change:

An equivalent, but simpler method for computing mass and energy flows through vents was proposed.

Development of a Research Code:

These two proposed changes were incorporated into a research code CCFM.MOSS. It was the purpose of this code to provide independent verification of CCFM.VENTS and to allow for easy investigation of equation formulations, ordinary differential equation solvers, precision requirements, slow code start up, and vent algorithms. In addition to incorporating the above changes, this research code contains several improvements: (1) a check in CCFM.VENTS for discontinuity in the right hand side of the differential equations has been eliminated as unnecessary, (2) a polynomial approximation has been constructed to allow for more efficient evaluation of a high pressure vent coefficient, (3) and a linearization was applied to Bernoulli's Law near zero pressure difference to make the vent algorithm handle a wider range of cases.

Comparison of CCFM.VENTS and CCFM.MOSS showed that (1) CCFM.VENTS contained a division by 3 error causing it to report incorrect floor pressures, (2) CCFM.MOSS ran about eight times faster than CCFM.VENTS, (3) demonstrated that double precision is required in this computation, and (4) showed that the ordinary differential equations being solved are unstable and stiff.

The October 1989 version of CCFM.VENTS differs from the October 1988 version in the following ways. The mass formulation of the differential equations has been adopted and the start up heuristic deleted. A check for discontinuity in the right hand side of the differential equations has been deleted as unnecessary. A linearization has been added to Bernoulli's Law near zero pressure difference to make the vent algorithm handle a wider range of cases. An increase in speed of at least a factor of four has been realized.

Presentations:

This work was presented at the CFR Grantees Conference, Gaithersburg, February 1989. Two presentations were made at the Annual Meeting of the Society for Industrial and Applied Mathematics, San Diego, July 1989. The titles were "Some Numerical Characteristics of Zone Fire Models" and Stiff Equations Arising in Fire Modeling."

Renewal:

During this grant period, a grant renewal was prepared. The title is "Incorporating (Existing Models of) Convective and Radiative Heat Transfer into the Code CCFM.VENTS."

In chronological order of completion the proposed effort will focus on four tasks. Task 1: Modification of the principal investigator's research code CCFM.MOSS to produce a one room code to test the numerics of modeling convective heat transfer between the hot upper layer and the lower ceiling surface and between the upper ceiling surface and the outside, and to test the numerics of modeling 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. Task 2: Study the efficiency and accuracy of two methods for approximating radiative and convective heat transfer. Task 3: Extend the convective heat transfer to walls and floors and the radiative heat transfer to layers. Task 4: Assist CFR personnel with the development of appropriate data structures for description buildings with multiple rooms.

Reports and Papers:

1. W. F. Moss, G. P. Forney, and L. Y. Cooper, "Numerical Characteristics of Zone Fire Modeling," in preparation.

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

SMOKE TRANSPORT

Professional Personnel

John H. Klote, Project Leader
Leonard Y. Cooper, Head, Building Fire Modeling Group
Kevin Greenaugh, Engineer

Project Objective

Develop physical and mathematical models to predict the motion of smoke in buildings due to all significant mechanisms.

Scope

This program studies the motion of smoke in buildings due to any driving force such as stack effect, wind effect, forced ventilation systems, and expansion and buoyancy of fire gases. Studies are by full scale and scale model experiments with initial emphasis on smoke movement in shafts and smoke control in buildings. The information generated by this effort is intended to lead to the development of mathematical models suitable for incorporation in existing fire models.

Technical Accomplishments

I. Full-Scale Experiments

Full-scale experiments were conducted to study zoned smoke control and smoke movement in stairwells. The objective of the smoke control effort was to evaluate the current approach to zoned smoke control systems. Accordingly, the smoke control system was designed using the calculational methods of the NBS Handbook "Design of Smoke Control System for Buildings," and it was designed to produce the levels of pressurization recommended by the National Fire Protection Association (NFPA). A zoned smoke control system is a system that uses pressurization produced by fans to restrict smoke flow to the zone of fire origin. The benefit of these systems is that other zones in the building remain essentially "smoke free" reducing property loss and hazard to life. No zoned smoke control system has been tested under real fire conditions either by a research effort or an accidental fire. However, fire experiments of smoke control systems for stairwells and elevators have been conducted.

The experiments were conducted in the Plaza Hotel building in Washington DC near the U.S. Capitol Building. The Architect of the Capitol obtained official approval of the U.S. Senate Committee on Rules and Administration for CFR to use the Plaza Hotel Building for this project. The Plaza Hotel building was built around the turn of the century and was scheduled for demolition after this research project. The building is a masonry structure consisting of two wings, one three stories and the other seven stories tall. Partitions were built separating the wings so that the experiments could be conducted in the tall wing with instrumentation and data acquisition in the shorter wing. To measure temperatures, pressure differences, gas concentrations, smoke obscuration, wind speed and wind direction, over 2½ miles of wire were installed between the instruments and a data acquisition system.

Fires consisting of 200 to 600 lbs of wood were set on the second floor of the Plaza Hotel, and the resulting second floor temperatures exceeded 1000 °F (540 °C). The walls, floors and ceilings of the fire areas were covered with calcium silicate board to minimize structural damage to the building.

During the fires for which the smoke control system was not operating, there was extensive smoke movement into the stairwell and to other floors especially the seventh floor. When the smoke control system was operating, the stairwell and floors away from the fire remained essentially "smoke free." These results demonstrated that zoned smoke control systems can achieve their objective. The experimental data is being analyzed to evaluate the underlying assumptions of zoned smoke control, and a detailed report will be published in the near future. The understanding gained from this project will lead to systems of improved reliability and cost effectiveness.

Video cameras were located in the stairwell on floors 2, 4 and 7. During fires without smoke control, the smoke observed at these locations seemed to indicate that the flow was similar to plug flow. This is very different from the zone approach currently used in fire models, and smoke flow in shafts was the subject of the scale model effort discussed below.

II. Reduced-Scale Experiments

A 1/8 scale model of a seven story building was constructed of calcium silicate board with several glass walls and with a forced air heating system. The model has a stairwell and an elevator shaft. The stairwell had an opening between the runs of stairs as did the stairwell at the Plaza Hotel. The glass walls were included to allow visualization of the smoke flow on the floors and up the shafts. The heating system was included to allow study of stack effect, and some tests with the heating system were conducted measuring temperatures in the model.

Visualization experiments were conducted of smoke movement in the stairwell. Smoke was produced by a chemical smoke generator to simulate a fire on the second floor of the model. Smoke was observed on the second floor and flowing into and up the stairwell. The highly turbulent nature of the flow was apparent. It seems that the upward flow can be generalized into two types. The first being a plug flow going up under the runs of stairs and turning 180° at each landing. The second is flow through the opening between the runs of stairs forming "vortex ring" like patterns. The second flow type moved up faster, but the quantity of smoke thus transported was relatively small. Study is needed to understand these flows and develop a realistic model of shaft smoke flow.

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I. Fire Hazard Assessment

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

FIRE HAZARD ASSESSMENT

Professional Personnel

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Emil Braun, Physicist

Project Objective

The objective is to develop methods for the quantitative assessment of fire hazard and support implementation of these methods by the fire protection community.

Scope

The project is intended to produce a fundamental capability to analyze the hazards associated with a specified fire scenario. This capability will be provided in the form of a fully-supported software package for MS-DOS 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.

Technical Accomplishments

1. General release of HAZARD I

The Center for Fire Research at the National Institute of Standards and Technology has released a method for quantifying the hazards to occupants of buildings from fires, and the relative contribution of specific products (e.g., furniture, wire insulation) to those hazards. The HAZARD I method, the culmination of six years of development, is the first such comprehensive application of fire modeling in the world. HAZARD I combines expert judgment and calculations to estimate the consequences of a specified fire. The procedures, outlined in figure 2, involve four steps: 1) defining the context, 2)

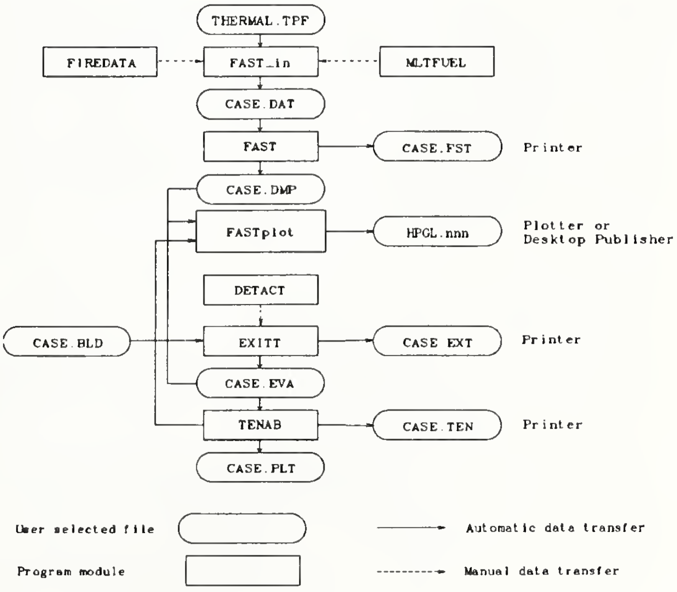

Figure 1 HAZARD I software.

1. DEFINE CONTEXT OF PRODUCT USE:

   - What is the problem to be resolved?
   - What is the scope or context of product use? - occupancy type(s), building design(s), contents, occupants.
   - Who are the key decision-makers?
   - What criteria will they use to accept/reject the product?

2. DEFINE FIRE SCENARIO(S) OF CONCERN: (A scenario is a specified fire in a prescribed building with well characterized contents and occupants.)

   - Examine relevant fire incident experience with same/similar products,
   - Identify the likely role/involvement of the product in fire,
   - Which fire scenarios do the decision-makers feel are . . .
     - most common/likely?
     - most challenging?

3. CALCULATE HAZARDS/OUTCOMES: for each of the scenarios identified above using the technical reference guide and software provided.

   - The major software subroutines are . . .
     - "FAST_in" - scenario specification (building, contents, occupants, fire)
     - "FAST" - fire and smoke transport calculations
     - "EXITT" - prediction of occupant decisions and actions
     - "TENAB" - calculation of outcomes, i.e., impacts on occupants

4. EVALUATE CONSEQUENCES:

   - Examine outcomes for each of the relevant fire scenarios selected in step 2 relative to the decision criteria.
   - Establish confidence in the predicted results using sensitivity analysis, expert judgment and, when needed, complementary small or large scale tests.
   - Delimit the range of applicability of the results based on the above.

Figure 2. Hazard analysis procedure.

defining the scenario, 3) calculating the hazard, and 4) evaluating the consequences. Steps 1, 2, and 4 are largely judgmental and depend on the expertise of the user. Step 3, which involves use of the extensive computer software, requires considerable expertise in fire safety practice. The heart of HAZARD I is a sequence of computer software procedures which calculates the development of hazardous conditions over time, calculates the time needed by building occupants to escape under those conditions, and estimates the resulting loss of life based on assumed occupant behavior and tenability criteria.

This first version can model up to six rooms on multiple floors of a building, but data against which its results have been compared are only available for structures of the general dimensions of single-family homes. The method guides the user to identify the fire problems of concern and then to specify representative fire scenarios. The user then employs a computer software package to predict the outcome of each of the identified scenarios in considerable detail. The software predicts: (1) the temperature, smoke, and fire gas concentrations in each room of the building; (2) the behavior and movement of the building occupants as they interact with the fire, the building, and each other; and (3) the impact of exposure of each occupant to the fire-generated environment. These impacts are presented as a prediction of successful escape, physical incapacitation or death along with the time, location, and cause. By accounting for the interactions of a large array of factors on the result of a given fire situation, the method enables the user to analyze the impact of changes in the fire performance of products, building design and arrangement, or the inherent capabilities of occupants on the likely outcome of fires. With such information it should be possible to provide better, more cost-effective strategies for reducing fire losses. A far more detailed guide to the theory and use of the method is available.

Both the National Fire Protection Association and the National Technical Information Service are distributing and promoting HAZARD I. Training programs tailored to a variety of audiences have been held or are being planned.

HAZARD I can be used to examine a variety of options. Table 1, culled from more than 450 pages of results, shows a matrix of fire types and variables. Three different cases of conditions affecting occupant response to eight example fire scenarios were formulated as follows:

- working smoke detectors were present,
- no smoke detectors were present, and
- an immobile occupant was positioned in each room.

The effect of smoke detectors can be seen by comparing the predicted response of occupants in the cases with smoke detectors (column 1) and without smoke detectors (column 2). It can be seen that the major effect of smoke detectors is predicted to be earlier evacuation based on an earlier warning of the occupants to the presence of the fire. An effect on fatalities can also be observed. Without smoke detectors, the occupants become aware of the fire at a much later time and are trapped on the second floor.

As an indicator of the effects of assumptions in the scenario descriptions (for example, fire growth or occupant placement), consider the last case of an occupant trapped in each of the six rooms in the houses (column 3). Deaths occur in all cases, with some deaths occurring in as little as 2 minutes from the start of the fire. In almost all examples, the first person to die is the one located in the room of fire origin. Obviously the assumed rate of fire growth is very important. In some scenarios, occupants remain safe in their room for the duration of the fire. This may be the result of the fire itself never growing large (e.g., the trash fire in the townhouse), or because occupants are protected by closed doors (e.g., scenarios in the two-story house).

While HAZARD I can be used for many such "what if" comparisons, the user must take into account the limitations of the methodology. For example, since fire growth is based upon a user defined input, the effects of structural involvement and ultimate failure are difficult to predict. Thus, occupants who remain behind closed doors may "survive" the fire while those who investigate or attempt to escape may become disabled and die. Thus, observed effects may be real or may be artifacts of the assumptions made in the analysis. Further, in HAZARD I, occupant response to a given fire is deterministic. In real fire situations, the responses of different people will vary for similar fire exposures.

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Related Grants

"Mathematical Modeling of Furniture Fires," M. A. Dietenberger, University of Dayton Research Institute.

"Graphical Presentation and Numerical Analysis of Fire Data for Model Validation," J. P. Jarvis and M. Kostreva, Clemson University.

"Development of an Instructional Program for Practicing Engineers: HAZARD I," J. Barnett, Worcester Polytechnic Institute.

Table 1
HAZARD I - Example Cases

Fire Scenarios[1]	Flashover	(1) With Smoke Detectors Escape Time[2]	(1) With Smoke Detectors Number of Fatalities[3]	(2) Without Smoke Detectors Escape Time[2]	(2) Without Smoke Detectors Number of Fatalities[3]	(3) Immobile Occupant in each room Time to Fatalities[4]	(3) Immobile Occupant in each room Number of Fatalities[3]
RANCH HOUSE							
1. Smoldering Sofa in L.R	No	20 min	0/1	21 min	0/1	44-49 min	6/6
2 Grease Fire in Kitchen	3 min	1 min	0/5	1-2 min	0/5	2-8 min	6/6
3. Bed Fire in MBR	No	1 min	0/5	2->15 min	0/5	2->15 min[5]	5/6
TOWNHOUSE							
4. Trash in Closet	No	1 min	0/3	6 min	0/3	2->15 min	1/6
5. Christmas Tree & Chair in L.R	No	6 min	2/4	--[6]	4/4	7->40 min	5/6
TWO-STORY "COLONIAL"							
6 Couch & Paneling in L.R., B.R. Doors Closed	4 min	3 min	0/4	15 min	0/4	4->25 min	5/6
7. Couch with L.R. and B.R. Doors Closed	4 min	3 min	0/4	25 min	0/4	4->25 min	5/6
8. Trash, Drapes, Desk in Office/B.R	14 min	6 min	0/4	7 min	0/4	7->33 min	4/6

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[1] For examples with and without smoke detectors, all occupants are assumed capable of escape and make no "mistakes".

[2] Time needed for all escaping occupants to get out of building. Occupants who arrive at windows are considered to have escaped the building.

[3] Number of fatalities / number of occupants in building.

[4] Times over which fatalities occur.

[5] The greater than sign (>) indicates times which are at least greater than the total time of the simulation.

[6] All occupants are trapped inside the building and die within 37 minutes.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: University of Dayton Research Institute

Grant No.: 60NANB8D0862

Grant Title: Mathematical Modeling of Furniture Fires

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NIST Scientific Officer: Dr. Vytenis Babrauskas

Technical Abstract:

This contract supports the development of FAST/FFM (formerly HEMFAST) computer program. The 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 the current project are (1) to develop full documentation of the model, (2) demonstrate model capabilities, (3) develop better algorithms for scaling the bench scale data, and (4) develop new formulae and methodologies of using the flame spread data.

Documentation The technical reference guide include a description of model equations, the program structure, and a user's guide. The recent release of the FAST version 18 technical reference guide from CFR was useful in our documentation efforts. Our FAST/FFM technical reference guide start with a brief explanation of the interface between FAST and FFM. The furniture fire model (FFM) model equations are described and explained after that. References to particular subroutines in the code that implement these equations are provided. The section on the program structure contain primarily the program tree and the logic flowcharts for each FFM subroutine. The remaining sections are essentially the user's guide in which the input/output is explained and a sample computer run is provided.

Fire Scenarios The second version of HEMFAST was exercised on the State of Ohio's CRAY computer to demonstrate variations in the mockups on the

predictability of the fire growth simulations. The first series of simulations involved varying the number of cushions on the mockup. The HEMFAST code has the capability of representing of up to four cushions on a furniture. In each case the ignition was at the same spot on the seat cushion. The predicted furniture burnrate for each case are shown in Fig. 1. It is noted the peak burnrate is enhanced with the vertical cushions. The next fire scenario simulated was the wall fire spread from a point source as shown in Fig. 2. The corresponding burnrate history is shown in Fig. 3.

The most recently released version of HEMFAST was made operational on NIST computers in August 1988. The CFR personnel have since found a new application for the model; the wall fire spread on a wallpaper/gypsum board from a point source. In the process the input/output of the model was rearranged and the FFM modules were adapted to a higher version of FAST. We also were involved in this conversion process and our new version of FAST/FFM will also reflect these changes.

New FFM algorithms In developing the new version of FAST/FFM the mockup algorithm was revised to permit construction of multiple combustible objects in a room. The modularity of the code was such that only one subroutine needed extensive revision. The other new algorithm developed was the automatical calibration of the scaling constants used in scaling the heat and mass release rates from the cone calorimeter. The objective was to provide less dependence on the user's judgement for calibrating the scaling constants through a interactive graphical procedure.

Ignition and flame spread modeling The recent improvement in the mathematical modeling of ignition and flame spread resulted in new formulae for application to FFM. Consequently, this application 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 new formulae to a furniture fire spread. Note that this approach differs significantly from the approach described in the document for the LIFT apparatus. This is because 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.

Conclusion The FAST/FFM model has developed to the point where use is being found in statistical studies with HAZARD. Sufficient documentation has been developed so that the CFR personnel can make intelligent use of the model. However, the model has not yet developed to the point where the user's judgement is not needed to calibrate certain model constants.

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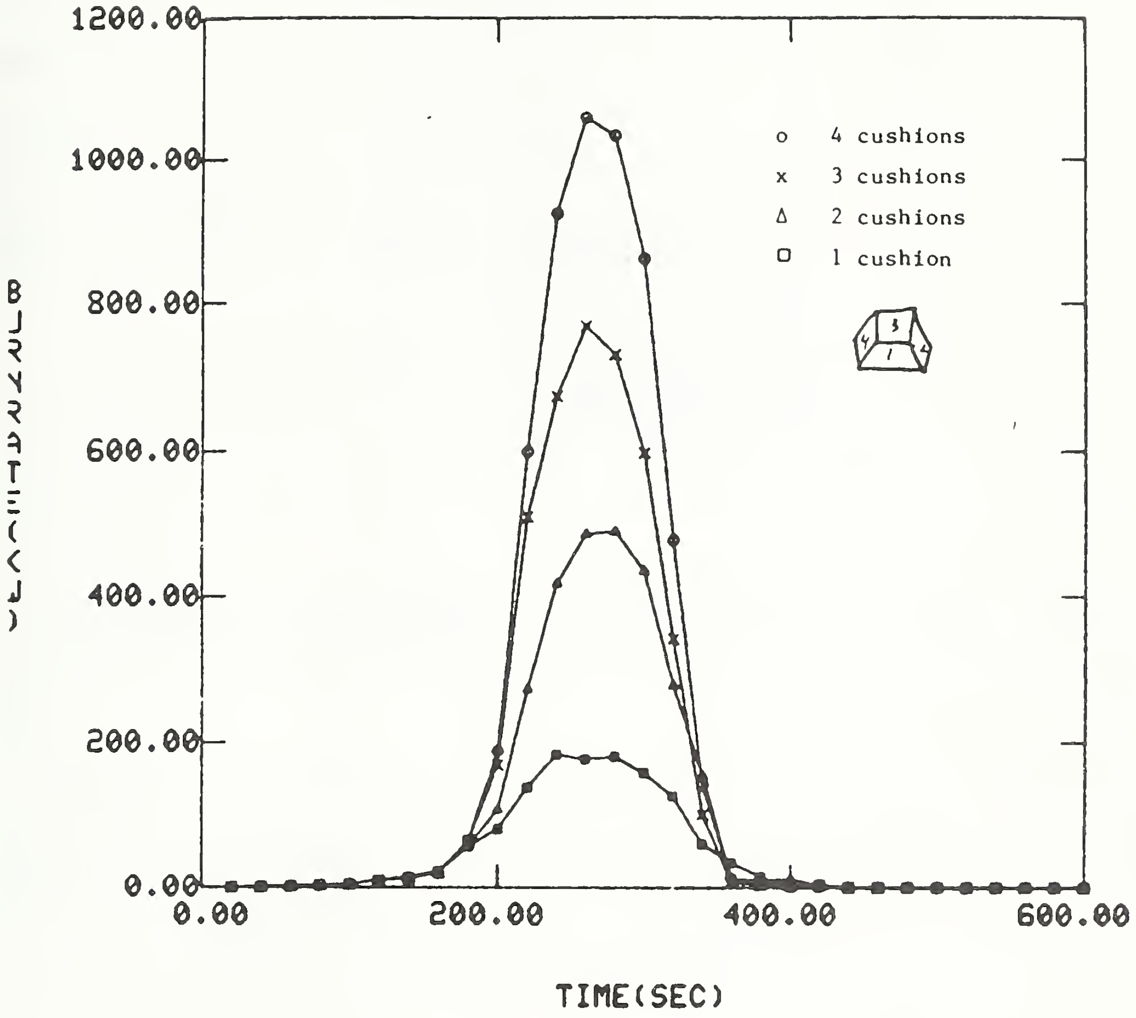

Figure 1. Comparison of HEMFAST predicted burnrate for varying number of cushions.

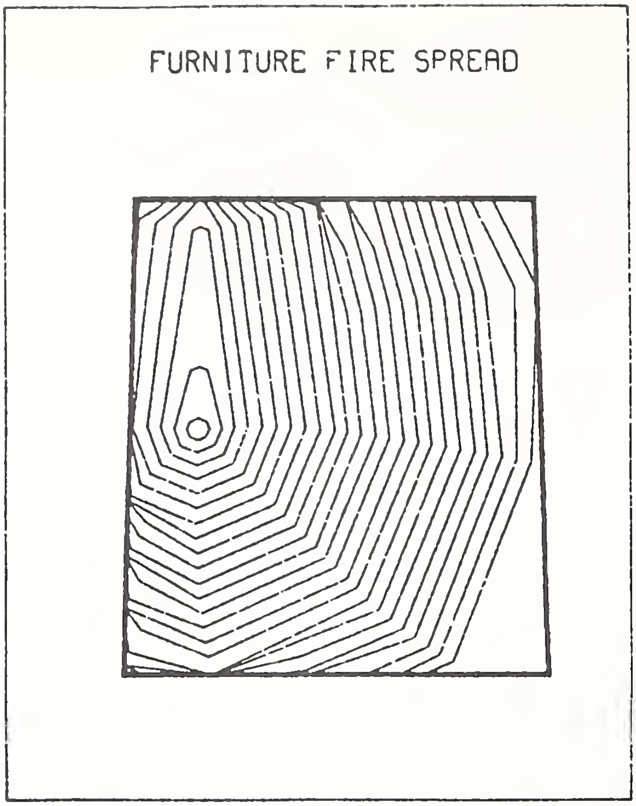

Figure 2. Predicted flame spread at 20 second intervals on a vertical cushion (heavy olefin fabric/fire retarded polyurethane foam or HO/FRPU) from a point source with HEMFAST.

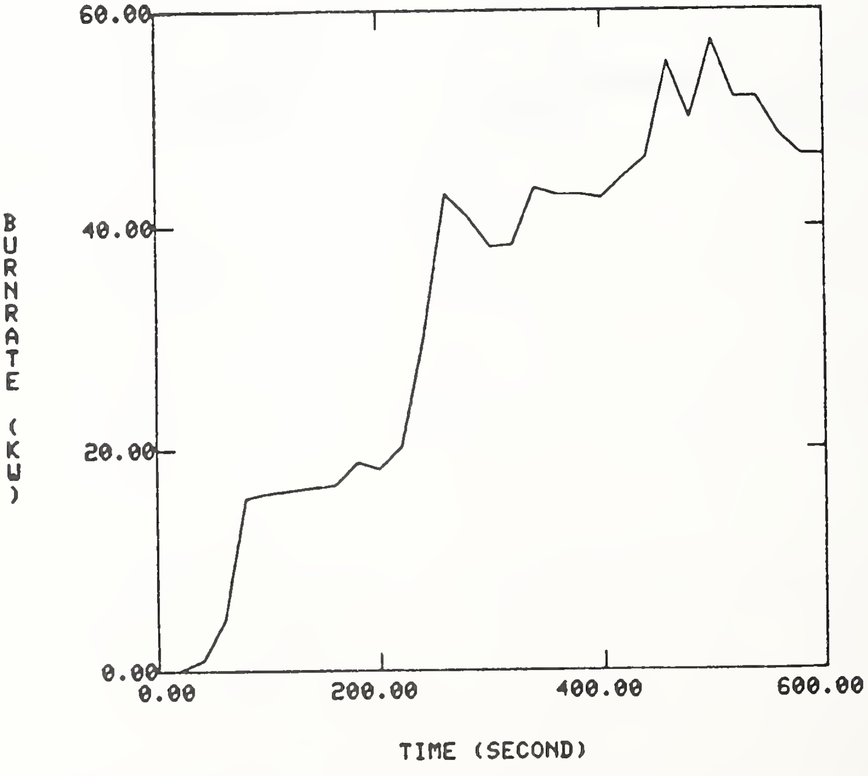

Figure 3. Predicted heat release rate from a vertical cushion (HO/FRPU) as a function of time.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution:	Clemson University
Grant No:	60NANB6D0627
Grant Title:	Graphical Presentation and Numerical Analysis of Fire Data for Model Validation
Principal Investigator:	Michael M. Kostreva, Professor Department of Mathematical Sciences Clemson University 0-104 Martin Hall Clemson, SC 29634-1907 Telephone: (803) 656-2616
Other Professional Personnel:	Malgorzata Wiecek, Assistant Professor Cheryl L. Forney, Research Associate
NBS Scientific Officer:	Richard Peacock

Technical Abstract:

Research supporting mathematical modeling and the validation of mathematical models of fires in residential buildings is being performed in this project. Techniques include model simplification for efficient model validation and multiple objective decision analysis related to the HAZARD I model of CFR.

Introduction:

The phenomena of human beings interacting with fires in buildings is very complex. It involves physics, chemistry, as well as sophisticated decision making. Obviously, because of the great costs involved in actual fires, it is important to understand and analyze this phenomena, to model it mathematically and to continue to try to refine these models to improve our understanding. This improved understanding can lead us to superior health policy and safety planning in the future.

In support of those researchers at CFR who build math models, this research project made contributions to a methodology for model simplification in preparation for validation.

Reduction to Core Parameters:

From its earliest beginnings, the specification of mathematical models of fire in buildings has been concerned with approximation and selection of parameters (Hottel, 1961). This is because the environment being modelled is not simple, and hence one cannot provide all of the details of reality and still have hope of solving the model.

Two important steps of any application of mathematical models are model validation and interpretation. In order to perform these steps in a systematic and economical manner, it is essential that the mathematical model undergo a simplification process known as dimensional analysis, and that the minimum number of dimensionless parameters be found. Once these parameters, which we have denoted as core parameters (Kostreva, 1989), are known, the organization of the validation and the interpretation of the model follow. Many additional experiments have to be performed in model validation if model validation is attempted without first determining the core parameters. Also these experiments will not justify additional confidence in the model. The reason for this is that the same experiments will be repeated, simply in another parametric description. To see this, suppose two parameters, say a and b, occur in an unsimplified but dimensionless form of a model, always as the product $a \cdot b$. Then experiments which double the parameter a while halving the parameter b will produce the same result as the base case. Since validation, including very expensive laboratory work, forms a part of fire modeling, it becomes increasingly important to find the core parameters and validate models using core parameters.

To illustrate this procedure with models familiar to fire researchers let us consider the following. The ASET model of Cooper (1982) and Cooper and Stroup (1985), is a single room zone fire model. In his derivation of ASET, Cooper performed dimensional analysis and simplified the ASET model from twelve raw physical parameters to four dimensionless parameters. However, we asked: is four the smallest number of parameters needed to specify ASET ? Are other models of interest in fire research currently formulated in terms of core parameters? Is there a general algorithm for obtaining core parameters? Some progress has been made in answering these questions. Consider the model

$$\underline{x}' = \underline{f}(\underline{x}, t, \underline{\alpha}), \quad \underline{x}(0, \underline{\alpha}) = \underline{x}_0 \text{ and } \underline{\alpha} \in R^m, \underline{x} \in R^n.$$

Cooper's model for available safe egress time (ASET) takes this form where $\underline{x} = (x_1, x_2)'$

and x_1 = dimensionless interface position while x_2 = upper layer temperature.

Cooper's original formulation has <u>four</u> dimensionless parameters, namely:

$\alpha_1 = \zeta_0 = H/L_c$, $\alpha_2 = \delta = \Delta/L_c$, $\alpha_3 = c_1 = (1-\lambda_c)Q_0 t_c / (\rho_a C_p T_a A L_c)$, and

$\alpha_4 = c_2 = (0.21 t_c / A)\{(1-\lambda_r) Q_0 g L_c^2 / (\rho_a C_p T_a)\}^{1/3}$

Applying additional information and some mathematical transformations, we reduced the ASET model to <u>two core parameters</u>:

$$\tilde{\alpha}_1 = \frac{\Delta}{\Delta+H}$$

$$\tilde{\alpha}_2 = \frac{0.210}{(1-\lambda_c)} \left[\frac{(1-\lambda_r)\, g(\Delta+H)^5 \rho_a^2 C_p^2 T_a^2}{(\dot{Q}_0)^2} \right]^{1/3}$$

From this reduction one learns that the explicit dependence on A and on t_c in Cooper's formulation is not necessary. The area A and the characteristic time t_c do not appear in the core parameters. From the analysis, one learns how to scale time in a manner natural to the ASET model, and that the model depends on area only through the λ_c and λ_r parameters.

Following our previous research (Jarvis, Kostreva and Forney, 1987), we studied techniques for reducing the number of dimensionless parameters in mathematical models in an effort to obtain a general methodology for reduction to core parameters. Such a methodology would prove valuable to all mathematical modelers, especially those engaged in fire modeling. Research to date, including conversations with experienced mathematical modelers, indicates that such a methodology does not exist at present, and that the need for such a methodology is recognized. Even though a complete methodology, capable of reducing any model to the core parameters, has not been found, techniques which tend to reduce the number of dimensionless parameters have been studied and collected. Analyses, including subjecting the model to programs in a symbolic manipulation language (MAPLE 4.2 for the Macintosh) have been performed. A collection of techniques from other related mathematical models are being formed and classified in preparation for the design of a general algorithm for reduction to core parameters. Representation of the problem of dimensional analysis and reduction to core parameters as another, well defined mathematical model with its own distinct structure may also lead us to discover the desired general algorithm.

In July 1989, CFR published HAZARD I under the auspices of the National Fire Protection Agency. Mathematical models of fires in residential buildings together with decision making models of the occupants are included in HAZARD I. Our research has led us to consider some potentially valuable enhancements to the basic models.

Multiple Objective Analysis for HAZARD I:

During the current year the research activity has been focused on incorporating multiple objective analysis into the HAZARD I methodology in order to develop a better representation of the human/fire hazard interactions. The main idea is to view a residential building as a network in which to each link is assigned two (or more) objectives (attributes), and an occupant as human subject who looks for a "best" evacuation path. Thus, it is assumed that the evacuation process is multiple objective in nature and the human decision makers reacting to fire make decisions in presence of conflicting criteria (eg. minimum evacuation distance versus maximum path accessibility).

The first stage of the analysis includes introducing two attributes: evacuation time and distance, their mathematical formulation and availability through HAZARD I. Then, for a given type of a residential house (a ranch house or 2-story house) and its specified group of occupants the evacuation facilities in different fire locations are analyzed. Thus, we face a bi-criteria decision situation: a few available evacuation paths to be chosen by an individual. The number of paths strongly depends on the network density (number of nodes and links between them) which in this case results not only from the type of the house, but also from the current location of the individual, his/her physical abilities, etc. The set of accessible paths includes the set of nondominated (Pareto) paths. All paths are available to the decision maker in terms of both criteria values. A nondominated path is of a special nature: its criteria values cannot be improved simultaneously. An improvement of one value must cause a deterioration of the other value. Solving a multiple objective optimization problem means now to find nondominated paths accessible from a current individual's location. Figure 1 shows accessible paths A, B, C, D, and E, among which paths A and B are nondominated.

Assuming a simple house design (a ranch house) it seems reasonable to integrate evacuation time and distance, that in an emergency become identical to the occupant. When fire is in progress decision making is a very quick action based on personal feelings (fear, haste, uncertainty) and judgements ("this path is safe", or "investigate fire", or "help a disabled occupant", or "rescue a baby", etc.), that all result from individual age, sex, physical ability, current location, etc. Thus, time as an "objective" and quantitative criterion is in conflict with the "subjective" and qualitative criterion, that is given as the compound personal utility (or disutility).

Figure 2 shows a possible decision situation an occupant can face, where the criteria taken under consideration are time and personal disutility. Both criteria are to be minimized. There are four possible destinations for the occupant from his/her current location: window 1 (path A) or door in the dining-room (path E), both leading to the yard, window 2 (path B) or door in the living-room (path C), both leading to the drive-way. There is also path D, that goes through the kitchen and leads to the door in the dining-room and eventually to the drive-way. Paths A and B have the same evacuation time but B has lower personal disutility than A, since the drive-way could be a less safe destination than the yard (hard concrete vs. soft grass). Path C dominates paths D and E, (the individual decides that path C has better access and shorter time than path E, and although path C has the same disutulity as path D, it is shorter). Thus, the occupant has two nondominated paths, B and C, and chooses, for example, path C as the optimal , so he/she decides to move towards the living-room.

While the individual travels along an arc of the optimal path, he/she arrives at the next intermediate node that is a new decision point, at which the multiple objective analysis takes place again. Hence, the optimal evacuation path is generated 'dynamically'. Each link is found by solving a two-objective optimization problem with the criteria given by the updated occupant's disutility and time needed to reach the destination node.

The major tasks at this stage of the research are:
- formulate the personal disutility objective for given types of residential houses,
- develop a method to search for an optimal path,
- develop an algorithmic procedure that would simulate the multiple objective decision making during the evacuation process,
- develop guidelines on how the multiple objective model is matched to different types of problem and user aptitudes within HAZARD I and its generalizations.

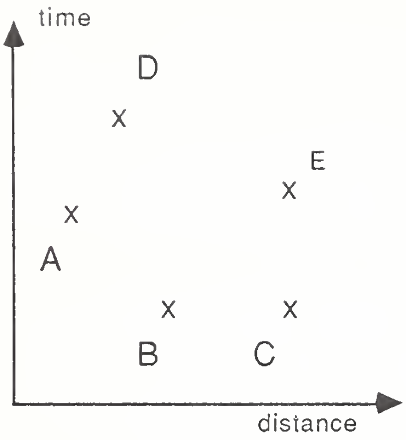

Fig.1

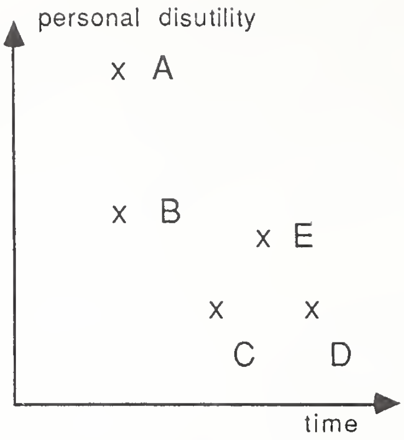

Fig.2

The introduction of multiple objective optimization approach to decision making in the HAZARD I model (and later generalizations) will allow for a more comprehensive and realistic study of the occupants' reactions to the residential dwelling fire. Inclusion of attributes in addition to distance together with personal disutility will provide a more sophisticated model of decision making, and hence more will be learned from the application of the HAZARD models.

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3. Cooper, L.Y. and Stroup, D.W., "ASET - A Computer Program for Calculating Available Safe Egress Time", Fire Safety Journal 9, 29-45 (1985).
4. Jarvis, J.P., Kostreva, M.M. and Forney, C.L., "Tools for Validation and Analysis of Fire Models", Combined Proceedings, 20th Fall Technical Meeting of the Eastern Section of the Combustion Institute & Annual Conference of the Center for Fire Research, November 1987.

Reports and Papers:

1. Kostreva, M.M., Ordoyne, T.J. and Wiecek, M., "Multiple Objective Optimization with Polynomial Objectives and Constraints", submitted for publication.
2. Kostreva, M.M. and Wiecek, M., "Linear Complementarity Problems and Multiple Objective Programming", submitted for publication.
3. Mirchandani, P.B. and Wiecek, M., "Routing with Nonlinear Multiattribute Cost Function", submitted for publication.
4. Kostreva, M.M., "The Core Parameters of Parameterized Nonlinear Equation Systems", Third SIAM Conference on Optimization, Society for Industrial and Applied Mathematics, April 3-5, 1989, Boston.
5. Kostreva, M. M., Ordoyne, T. and Wiecek, M.,"Multiple Objective Programming with Polynomial Objectives and Constraints," presented at CORS/TIMS/ORSA Joint National Meeting, Vancouver, May 1989.
6. Mirchandani, P.B. and Wiecek, M., "Optimization in a Discrete Feasible Space - Application to a Routing Problem", presented at Optimization Days, Montreal, May 1989.
7. Mirchandani, P.B. and Wiecek, M., "Routing with Nonlinear Multiattribute Cost Functions", presented at CORS/TIMS/ORSA Joint National Meeting, Vancouver, May 1989.

Center for Fire Research
National Institute of Standards and Technology
FY 89

Institution: Worcester Polytechnic Institute

Grant No.: 60NANB9D0949

Grant Title: Development of an Instructional Program for Practicing Engineers: HAZARD I

Principal Investigator:
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NIST Scientific Officer: Richard Bukowski

Technical Abstract:

With formal announcement of the release of HAZARD I, a prototype hazard assessment method and software, NIST has provided a new generation of hazard analysis capabilities to the fire protection engineering community. This release presents major educational challenges to practicing engineers who have not in the past used fire modeling or formal hazard analysis methodologies.

In response to these educational challenges, the Center for Firesafety Studies at Worcester Polytechnic Institute has developed a prototype short course for practicing engineers to prepare them to use the HAZARD I methodology. The five day short course introduces the HAZARD I methodology and the software to practicing engineers.

Two pilot courses, training a total of thirty students, have been offered on the WPI campus, using computer laboratory facilities. In order to train engineers to be effective and efficient users of HAZARD I, the course includes an overview of the hazard analysis, the scientific basis of the models, the limitations and accuracy of the models, determination of the required model inputs, and use of the programs. During the course the students use each component of the package while conducting a hazard analysis on a sample building.

The role of HAZARD I is to facilitate the systematic evaluations of hazards presented in a building. The components of such an analysis include problem definition, scenario selection, model input determination, hazard calculations, sensitivity analysis, and consequence analysis. These aspects of the process are covered through a combination of lectures, laboratory demonstrations, and small group laboratory work. The week long course schedule is included as Figure 1.

The technical basis of the programs included in HAZARD I are reviewed in the light of the state-of-the-art. This provides the student with a knowledge of what the programs are capable of performing, what input data is required for the models, and how to establish these inputs. Limitations of the models are fully discussed.

Determination of inputs to the models is a major task, requiring significant engineering insight and technical knowledge. A significant portion of the course addresses scenario development, building descriptions, determination of the rate of heat release(and other fire specifications), determination of occupants and occupant paths, and detector characteristics.

Analysis of the model results is stressed throughout the course. Students evaluate sample outputs prepared by the instructors as well as their own work.

The use of the actual programs contained in HAZARD I is explored through computer laboratory sessions, using computer demonstrations as well as student project work. During the course students prepare input sets for all the programs, run each program, evaluate the outputs, and design and carry out a limited sensitivity analysis. Each student is provided with an AT&T 6286 WGS PC with 40 MB hard drives and VGA color monitor. Printers and plotters are provided for student use.

Evaluation of the course's effectiveness as measured in the pilot course offerings is currently underway. This includes a study of the entry and exit questionaires completed by the students and the students' coursework(input and output files).

Preliminary results show the great promise of such a course in assisting engineers in the effective use of fire models. Course offerings by WPI around the country are planned.

HAZARD I SHORT COURSE SCHEDULE

Rev. 8/10/89

Monday	Tuesday	Wednesday	Thursday	Friday
	830-920 FAST(2) Combustion CLB	830-920 FAST(7) Running FAST JRB	830-920 TENAB(2) CLB	830-920 EXAMPLE (Lab) JRB
	925-1015 Project Discussion(1) (Lab) JRB	925-1015 Project(3) FAST Input (Lab)	925-1015 TENAB-use (Lab) CLB	925-1015 Project(8) Work Session (Lab)
	1015-1035 BREAK	1015-1035 BREAK	1015-1035 BREAK	1015-1035 BREAK
1035-1125 Introduction to the Short Course CLB	1035-1125 FAST(3) Fluid Flows CLB	1035-1125 FASTPLOT (Lab) JRB	1035-1125 EXITT(1) CLB	1035-1125 Project(9) Work Session (Lab)
1130-1220 The Hazard Analysis Process CLB	1130-1220 FAST(4) Model Inputs JRB	1130-1220 FAST(8) Review CLB	1130-1220 Project(5) Model Refinement (Lab)	1130-1220 Project(10) Project Presentations (Lab)
1220-120 LUNCH	1220-120 LUNCH	1220-120 LUNCH	1220-120 LUNCH	1220-120 LUNCH
120-210 Overview of Hazard I CLB	120-210 FAST(5) Heat Transfer CLB	120-210 DETACT CLB	120-210 EXITT-use (Lab) input file generation JRB	120-210 Project(10) Project Presentations
215-305 Introduction to Hazard I & Its Components CLB	215-305 FAST.IN (Lab) JRB	215-305 DETACT-use (Lab) CLB	215-305 Project(6) EXITT (Lab)	215-305 Project Review & Course Evaluation
305-320 BREAK	305-320 BREAK	305-320 BREAK	305-320 BREAK	
325-415 Introduction to the Hazard I Software(Lab) JRB	325-415 Project(2) FAST Input (Lab)	325-415 TENAB(1) CLB	325-415 EXITT(2) CLB	
420-510 FAST(1) Phenomonology CLB	420-510 FAST(6) Fire Scenarios, RHR CLB	420-510 Project(4) Running FAST (Lab)	420-510 Project(7) TENAB (Lab)	

J. Engineering Analysis System and Fire Reconstruction

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

ENGINEERING ANALYSIS SYSTEM & FIRE RECONSTRUCTION

Professional Personnel

Harold E. Nelson, Project Leader
Robert Levine, Senior Scientist
C. 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, a fire hazard assessment tool for building design and evaluation has been developed. This methodology is based on a simple filling model (ASET) enhanced to estimate door flows, heat losses, sprinkler response, and other factors. It is currently operational and in peer review.

FIREFORM has been expanded to include features related to the development of files describing free burn rates of fuel arrays. Most other additional features incorporated into FIREFORM relate to user friendliness.

2. Fire Reconstruction

The report on the fire in the First Interstate Bank Building and an article covering the same material have been published. This fire destroyed the 12th through 15th floors of this high rise building. The analysis traced the spread of the fire across the furnishings, the response of the smoke detectors, the development of flashover conditions, the floor to floor fire spread, and the spread of smoke through the building.

An investigation is underway on the five fatality fire in the Peachtree - 25th Building in Atlanta.

Funding from Other Agencies/Institutions

In addition to CFR Priority Project funding, the above activities were carried out with significant support from the General Services Administration. This support is continuing with some enhancement from agencies within the Department of Health and Human Services and the Department of Education.

Reports and Publications

Nelson, Harold E., Engineering Analysis of Fire Development in the Hospice of Southern Michigan, December 15, 1985 Proceedings, International Association for Fire Safety Science, Proceedings, 2nd International Symposium, Tokyo, Japan, June 13-17, 1988.

Nelson, Harold E., Science in Action--An Engineering View of the Fire at the First Interstate Bank Building, Fire Journal, v83, no. 4, pp28-32,34, July/August 1989.

Nelson, Harold E., NISTIR 89-4061, Engineering View of the Fire of May 4, 1988 in the First Interstate Bank Building, Los Angeles, California, 33pp, March 1989.

K. Suppression

CENTER FOR FIRE RESEARCH
PRIORITY AND OTHER AGENCY PROJECT - 1989

FIRE SUPPRESSION

Funding Agency: U.S. Fire Administration
U.S. General Services Administration
Swedish Fire Research Board

Professional Staff: David Evans, Project Leader
Dan Madrzykowski, Mechanical Engineer
Randy Lawson, Physical Scientist
Doug Walton, Fire Protection Engineer

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. Comparative Effectiveness of Water with Compressed Air Foam

This study investigates the feasibility of a residential, self-contained, compressed air foam (CAF) sprinkler system and CAF's extinguishment effectiveness on Class A fires. Two types of fire tests were conducted: sprinklered compartment fire suppression tests and fire extinguishment effectiveness tests. The CAF and water were compared on a mass flow rate basis in both of the test series. In the sprinklered compartment fire suppression tests, the CAF exhibited the same effectiveness as water in suppressing the fire. The fire extinguishment tests utilized wood cribs, excelsior and polyurethane foam as fuels. The CAF demonstrated an advantage over water when extinguishing the fires involving porous Class A fuels due to its ability to cling to the fuel. This characteristic enables the CAF to have an increased smothering capability relative to water. Cost comparisons were made between a self-contained residential sprinkler system, which utilizes water and a proposed residential CAF unit. For this application, CAF does not increase the performance of water enough to justify the additional expense of a CAF system.

This limited series of tests has shown that in a sprinklered compartment with a developing wood crib fuel fire, there is not a significant difference in the fire suppression capabilities of CAF compared to those of water on a mass basis. In the fire extinguishment tests, it was demonstrated that CAF does not have superior heat absorbing properties relative to water, but it does have better physical characteristics for smothering a fire. However, smothering efficiency would not necessarily reduce the amount of water required to suppress a fire in a residential fire situation.

New hardware would need to be developed for CAF sprinkler systems before they could be made commercially available. The cost of existing hardware required for a CAF sprinkler system is almost double the cost of a water sprinkler system. The examined self-contained CAF residential sprinkler system does not appear to be more efficient than a self-contained water sprinkler system with respect to fire suppression performance or economy.

2. Suppression of Post-Flashover Compartment Fires Using Manually Applied Water Sprays

A series of four full scale fire tests were conducted to examine the effect of fire fighting efforts on flashed over room fires. One objective of these tests was to generate data for evaluation of computer models of the fire suppression process. The tests were conducted in a simulation of a significant portion of a room and corridor. The burn room was a 2.44 m cube, and it was connected to a 12.8 m long, 2.44 m wide, and 2.44 m high corridor. Prior to initiation of the fire suppression efforts, the opening between the burn room and corridor was closed. Water sprays from various fire fighting hose nozzles were used to suppress the fires. Gas temperatures, wall surface temperatures and concentrations of oxygen, carbon dioxide, and carbon monoxide were measured in the burn room. Specialized aspirated and shielded thermocouples were used to minimize the effects of the water sprays on gas temperature measurements.

Peak heat release rates of between 2.5 and 3 MW were obtained and the heat release rate remained at or above 1.5 MW for eight minutes. From the heat release rate data, it can readily be seen that "flashover" occurred very quickly (within about two minutes after ignition). After "flashover" and for the duration of the test (until extinguishment), there was no measurable oxygen remaining in the gases leaving the burn room. This indicates that for a majority of the time prior to initiation of the fire suppression efforts, the fire in the compartment was ventilation limited. The gas temperatures measured in the burn room indicate that after flashover the gas temperature is almost constant throughout the room. This indicates that the compartment gas is "well-stirred" as required by the Fire Demand Model (Pietrzak, L. M., Johnson, G. A., and J. Ball, "A Physically Based Fire Suppression Computer Simulation for Post-Flashover Compartment Fires", Mission Research Corporation, Santa Barbara, California; June 1984.)

Each fire was extinguished in a manner designed to simulate the action of fire fighters. The effects of these extinguishment activities were monitored through the measurement of gas and wall surface temperatures and gas concentrations in the burn room. The data generated during this test series is intended to be used for validation of models of the fire suppression process. Based on calculations done using the Fire Demand Model, three flow rates were selected for use in suppressing the fires. The first (37.8 ℓ/min) should have just been able to control the fire. The second (18.9 ℓ/min) should not have controlled the fire while the last (87 ℓ/min) should have definitely extinguished the fire. As determined by visual observation of the tests, this objective was accomplished.

Related Grants:

Extinguishment of Combustible Porous Solids by Water Droplets, A. Atreya and I. Wichman, Michigan State University.

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

A Study of the Suppression and Extinction of Fires by Water Sprays, W. Yuen and W. Lick, University of California.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

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: M. Abu-Zaid (Ph.D student - graduated)
Peter Caffrey (Ph.D candidate)

NBS Scientific Officer: Dr. David D. Evans

TECHNICAL ABSTRACT:

The objective of this project is to extend our work on cooling of inert isothermal porous ceramic solids by water droplet evaporation to real combustible materials. FY 89 was a transition year in which Mr. Abu-Zaid who worked on cooling of isothermal porous ceramic solids graduated and Mr. Caffrey started working on extinguishment of combustible porous solids.

From our work on isothermal porous ceramic solids we were able to demonstrate that large differences exist between porous and non-porous materials due to in depth absorption of water. The volume of droplet influence is significantly larger for the porous solid and the evaporation time is correspondingly shorter. Thus, compared with non-porous solids, a more frequent but spatially sparse distribution of water droplets is required for porous solids. From the transient measurements of surface and in depth temperatures and the droplet diameter on the solid surface, instantaneous average evaporative heat flux and the evaporation rate were determined. It was found that the average evaporative heat flux is higher for smaller droplets. The theoretical and experimental contact temperatures were found to be in excellent agreement up to the boiling point of water. It then becomes roughly constant at a value slightly greater than the boiling point.

The next phase of this project i.e. study of combustible porous solids is just beginning. Here our objective is to quantify the rate of suppression as measured by the decrease in the energy release rate from the porous solid during a fire due to water application and eventually the time to extinction. A novel apparatus is being constructed for this purpose.

Study of Cooling of Porous Ceramic Solids and Piloted Ignition of Moist Wood:

This experimental study quantifies the cooling of hot porous and non-porous isothermal ceramic solids by water droplet evaporation. These solids were used to simulate low-thermal-diffusivity combustible building materials and were instrumented by several surface and in-depth thermocouples. Temperature measurements in the solid were used to quantify the heat transfer during droplet evaporation, the volume of influence and the recovery time of the solid. These measurements enabled determining the most efficient size of the water droplet, the frequency of droplet application and their distribution on the surface in order to maintain the surface temperature below the piloted ignition temperature. This work has been submitted for publication in the ASME J of Heat Transfer (Ref. [1]) and a portion of this work was presented in the Eastern Section of the Combustion Institute (Ref. [2]).

The second part of this study was directed toward the evaluation of the effect of adsorbed moisture on piloted ignition and thermal decomposition of wood in air. Both these phenomena were studied as a function of sample moisture content and externally applied radiation. Simultaneous measurements of weight loss rate; surface and in-depth temperatures; O_2 depletion and production of CO_2, CO, total hydrocarbons and water were made. As expected, the presence of moisture delayed the decomposition process, diluted the decomposition products and increased the time to ignition. The surface temperature and the evolved mass flux at ignition also increased with increase in moisture content. A single equation was derived to correlate all the ignition data. This correlation accounts for the moisture-dependent thermal properties and the heat loss from the sample surface. This work is currently being written for publication. Preliminary results were published in the Central Section of the Combustion Institute (Ref. [3]).

In the third part of this study two models for piloted ignition were developed. The first model published in the ASME J of Heat Transfer (Ref.[4]) is an approximate analytical model which addresses the combined gas and the solid phase problem, while the second model focuses only on the gas phase problem. The transient boundary layer equations in the second model are numerically solved. The second model is submitted for publication in Combustion and Flame (Ref. [5]).

Study of Extinguishment of Combustible Porous Solids:

This study has just begun. An apparatus for introducing water droplets over burning samples of wood is being constructed. Meanwhile exploratory experiments are being conducted to observe the effect of water droplets on burning solids. Attempts were also made to study the cooling of a porous ceramic by droplet evaporation in the presence of a flat plate boundary layer diffusion flame. The existing combustion wind tunnel was used for this purpose and special ceramic solids instrumented with thermocouples were constructed. The 30" test section of the wind tunnel was filled with five 6" x 3" ceramic solids. Each solid was instrumented with surface and in-depth thermocouples. A methane burner was used to provide a diffusion flame in the boundary layer above the solid surface. The gas-phase temperatures directly above the location of the solid-phase thermocouples were also measured. From these measurements, the convective and the radiative component and the total heat transfer were determined via an inverse heat transfer calculation. However, attempts at reproducibly introducing the water droplets exactly on top of the thermocouples inside the solid were not successful. Thus, meaningful data in the presence of water droplets was not obtained. A sample of these measurements is shown in Figure 1.

Reports and Papers:

1. Abu-Zaid, M. and Atreya, A., "Transient Cooling of Hot Porous and Non-porous Ceramic Solids by Droplet Evaporation," Accepted for publication in *ASME J. of Heat Transfer*, 1989.
2. Abu-Zaid, M. and Atreya, A., "Heat Transfer during Evaporation of a Water Droplet on a Heated Non-porous Ceramic Solid," Proceedings of the *Eastern Section of the Combustion Institute*, 1988.
3. Atreya, A. and Abu-Zaid, M., "The Effect of Adsorbed Water on Piloted Ignition," Proceedings of the *Central Section of the Combustion Institute*, 1989.
4. Atreya, A. and Wichman, I. S., "Heat and Mass Transfer During Piloted Ignition of Cellulosic Solids," *ASME J. of Heat Transfer*, V.111, p.719, 1989.
5. Tzeng, L. S., Atreya, A., and Wichman, I. S., "A One-Dimensional Model of Piloted Ignition," Accepted for Publication in *Combustion and Flame*, 1989.
6. 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.

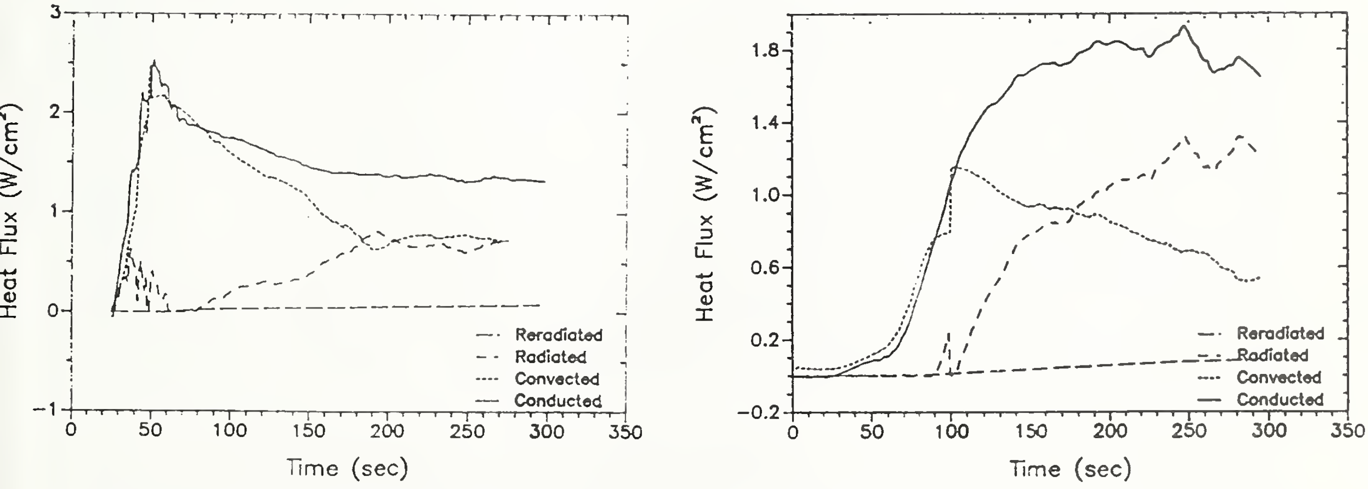

Figure a Heat Fluxes History at x = 7.5 cm at U = 1.7 m/sec,P3M14

Figure b Heat Fluxes History at x = 20.0 cm at U = 1.7 m/sec,P3M14

FIGURE 1 HEAT FLUX HISTORIES AT DIFFERENT LOCATIONS DOWNSTREAM OF THE METHANE BURNER.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

Institution: University of Maryland, College Park

Grant No.: COMM 70NANB8H0840

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

Principal Investigator:
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Mechanical Engineering Department
University of Maryland
College Park, MD 20742
tel. (301) 454-4994

Other Professional Personnel: Farzad Kavoosi, Graduate Research Assistant
Michael Klassen, Graduate Research Assistant

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. Preliminary results of a new theoretical model are presented and a successful infrared thermographic technique, which describe the solid surface temperature behavior during the droplet evaporation, is illustrated.

Theoretical Studies A Boundary Element Method (BEM) is developed to describe the transient thermal behavior of the solid, the same method is applied to the liquid droplet. Surface integrals were developed in the spherical coordinates, as dictated by the geometry of the liquid region which is approximated to a spherical segment, using the original choice of the Green's functions . The resulting formulations are described in diMarzo (1989). These integrals are complex because a) both the Green's function and its gradient are non-zero on this spherical segment surface; b) the liquid region is bounded by the spherical segment and by the solid-liquid interface; c) the formulation of all possible inter-surface relations in a combined spherical/cylindrical coordinate system is cumbersome; d) the evaluation of these integral at the initial time brings about an additional mathematical challenge. Therefore, a decision was made to abandon the BEM applied to the liquid region and to opt for a hybrid technique: BEM for the solid and Control Volume Method (CVM) for the liquid region.

The CVM, using geometry-fitted cell arrangement, is proposed to handle the liquid region. In particular, the cell generation is aimed at following the shrinkage/collapse pattern of the droplet. In addition, the radial grid is devised to define spherical segments with decreasing curvature towards the axis of symmetry. Finally, image points are introduced in the nodalization process to better describe the boundary conditions.

The solid-liquid interface is imbedded in the problem solution by matching temperatures and fluxes. In a first attempt to obtain converging solution for the solid liquid coupled problem, the interfacial temperature is computed by a shooting technique: with an initial guess for the interface temperature, the liquid domain is solved and the interface flux is calculated accordingly. This flux is then fed into the BEM solid-solver which will return with the interface temperature for the CVM liquid solver. Typically, it takes between two to five iterations to achieve convergence for each time step. Figure 1 illustrates typical results of this technique.

To eliminate the need for such shooting technique, a matrix technique is currently being developed where the top portion of the matrix holds the coefficients resulting from the CVM the liquid region, and the bottom portion consists of the corresponding weight coefficients for the solid as described by the BEM. The interfacial temperature and flux values are the communication links between the two domains. The unknown vector comprises temperatures in the liquid domain, the interfacial fluxes and temperatures and the solid surface temperatures. The right hand side contains the known quantities vector.

Experiments An infrared thermographic technique is developed to obtain the transient solid surface temperatures surrounding the droplet during vaporization. This technique is particularly appealing because it is non-intrusive, detailing the surface response to the droplet without affecting the evaporation process. Surface recovery can also be monitored using this thermographic method.

The technique utilizes image processing to obtain the temperature profile of the solid surface surrounding an evaporating droplet. This technique can not be utilized to obtain temperature information beneath the droplet since the droplet is transparent. The infrared thermographic image provides the temperature distribution along a line through the droplet center. This visual information is processed in order to eliminate noise and unwanted information. The resulting image is available as a file containing screen coordinates of the various data points. This file is then converted in a temperature versus location data set. An exponential curve-fit is used to fit the temperature profile of the solid surface during dropwise evaporation to yield the final information in spread-sheet format suitable for comparison with the analytical results.

Figure 2 shows typical transient temperature distributions. This figure shows that contact temperature is held at the droplet edge during most of the evaporation. This finding differs from the observations of Abu-Zaid (1989) who found temperatures under the droplet well above the contact temperature for most of the evaporative process. When the droplet thickness diminishes greatly, the temperature of the solid surface surrounding the droplet begins the rise (70s < t < 100s). After the evaporation is complete (t ≃ 100s), the solid surface temperature slowly recovers its orginal value.

Figure 3 shows the radius of influence of droplet cooling versus evaporation time. Data for droplets of 10 μl are not reported; they are scattered between three and seven normalized radii and do not provide any significant trend information. Two distinct linear regressions are performed on the evaporative data and on the boiling data reported in the figure. The resulting trend indicates that a maximum radius of influence of about seven characterizes the evaporative process while, for the boiling case, the radius of influence is a strong function of the evaporation time. This is reasonable because the low conductivity of Macor constrains the surface area affected to a small region around the droplet with a very intense localized cooling for the rapid boiling process. While a less intense, more spread-out effect is observed for the slower evaporative transient.

The data obtained on the cooling effect induced on aluminum (diMarzo 1986) and on Macor (diMarzo, 1987) is used in concert with new data obtained on a quartz surface to characterize the induced cooling of a hot surface by an evaporating droplet. In particular, the role of the droplet size and shape is investigated for the various high and low conductivity surfaces. The evaporation process on quartz is similar to those found in the earlier work on Macor and aluminum. The evaporation time for the droplets on the quartz surface are consistently greater than for the droplets on the Macor surface, even though the quartz surface is of a slightly higher thermal conductivity. The shape parameter β_0 is greater for the quartz surface (1.53 for quartz and 1.43 for the Macor). All the evaporation time versus initial solid surface temperature curves are reduced by plotting evaporation time versus contact temperature. This transformation correlates the data along the horizontal axis. A suitable parameter to correlate the data in terms of evaporation time cannot be found at this time due to the numerous parameters affecting the solid-liquid interactions: high/low thermal conductivity, shape parameter, evaporation/boiling process, etc.. The newly developed theoretical model will be used to gain in depth understanding of the relative importance of these various governing parameters.

Acknowledgements The authors are indebted to Dr. Howard Baum of CFR-NIST for his guidance on the development of the boundary element method 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:

M. Abu-Zaid, A. Atreya, "Effect of Water on Piloted Ignition of Cellulosic Materials", NIST-GCR-89-561 (1989)

M. di Marzo, A. K. Trehan, "Transient Cooling of a Hot Surface by Droplets Evaporation", NBS-GCR-86-516 (1986)

M. di Marzo, Z. Y. Wang, W. H. Meng, "Transient Cooling of a Hot Surface by Droplets Evaporation, NBS-GCR-87-534 (1987)

Reports and Papers:

M. di Marzo, F. Kavoosi, M. Klassen, "Transient Cooling of a Hot Surface by Droplets Evaporation", NIST-GCR-89-559 (1989)

M. di Marzo, D. D. Evans, "Evaporation of a Water Droplet Deposited on a Hot High Conductivity Solid Surface", *Transactions of ASME Journal of Heat Transfer*, Vol. 111, No. 1, pp. 210-213 (1989)

F. Kavoosi, M. di Marzo, H. R. Baum, D. D. Evans, "An Application of Boundary Element Methods to a Transient Axisymmetric Heat Conduction Problem", *Proceedings of the 26th AIChE/ASME/ANS National Heat Transfer Conference*, HTD Vol. 110, pp. 79-85 (1989)

FIGURE ONE

Computed transient temperature distribution in Macor. Initial solid surface temperature 110 °C, initial droplet volume 40 μl.

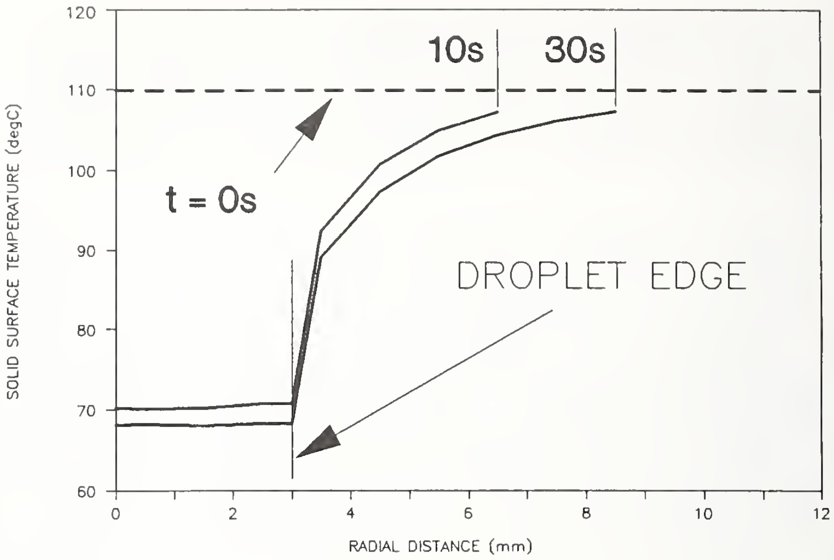


FIGURE TWO

Measured transient temperature distribution in Macor. Initial solid surface temperature 124 °C, initial droplet volume 30 μl.

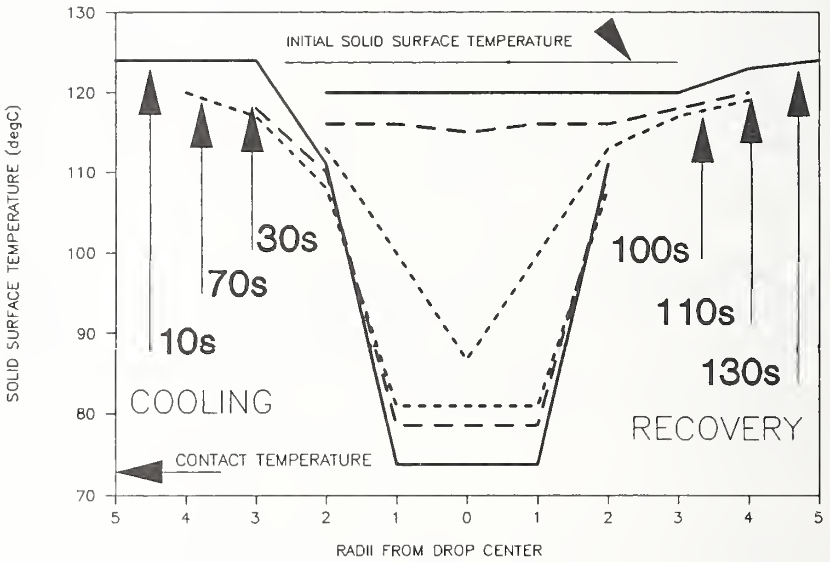
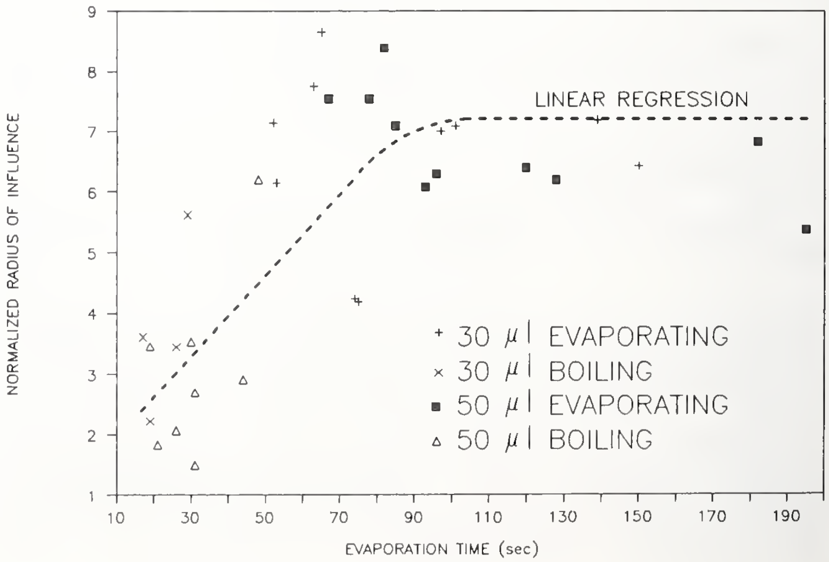


FIGURE THREE

Normalized radius of influence:

$$\frac{r_{\text{influence}}}{r_{\text{wetted-region}}}$$

versus evaporation time. Two linear regressions are computed for evaporation and boiling respectively.



CENTER FOR FIRE RESEARCH
NATIONAL BUREAU OF STANDARDS
FY 89

Institution: The University of California

Grant No: 60NANB6D0651

Grant Title: A Study of the Suppression and Extinction of Fires
by Water Sprays

Principal Investigators: Professors W. W. Yuen and W. Lick
Department of Mechanical Engineering
University of California at Santa Barbara
Santa Barbara, California, 93106

Other Professional Personnel: Neresh Kumar (M.S. Candidate)

NBS Scientific Officer: Dr. David Evans

1. TECHNICAL ABSTRACT

The objective of this study is to determine the fundamental mechanisms by which the spraying of water leads to fire suppression and extinction. During this reporting period, the research concentrated on two specific tasks: (1) the numerical simulation of the evaporation effect on water sprays in the thermal environment of a room fire; and (2) the effect of water spray on the thermal quenching of a flame at a vaporizing fuel surface. The first task contributes to the understanding of the "survivability" of the water sprays in a fire environment after injection. The second task contributes to the understanding of the interaction between the water droplets/vapor and the reacting species in a combustion/extinction process. Based on numerical results, the amount of water required for extinction will be correlated with fuel properties and external environmental parameters.

2. MODELING OF EVAPORATION EFFECT ON WATER SPRAY IN THE ENVIRONMENT OF A ROOM FIRE

A great deal of work has already been reported in the modeling of the interaction of water sprays in a general fire environment (Alpert, et. al. 1984, 1985, 1986). In most of these work, however, the computational domain covers a full-scale room and many important small scale phenomena are ignored. The emphasis of the present effort is to understand the penetration of the water spray through an adjacent smoke layer. Since the the smoke layer can have significant cross-stream momentum and high temperature (say, up to 270 C), the trajectory of the water sprays and its evaporation can be a dominant mechanism affecting the extinction effectiveness of the water spray.

The typical geometry considered by the current work is similar to that utilized by Chow (1989) and is presented in Figure 1. The computer fire code V (Mitler and Emmons, 1981) will be used to generate the temperature, flow field and thickness of the smoke layer. The effect of room geometry, sprinkler location and spray characteristics (i.e. initial droplet size distribution, velocity and trajectory, etc.) on droplet penetration will be predicted.

2. MODELING OF THE EFFECT OF WATER SPRAYS ON THERMAL QUENCHING

A stagnation flow "water mist" extinction model has been developed to illustrate the effect of water sprays on thermal quenching. As described in previous progress reports, the model considers the opposing stagnation flow geometry as shown in Figure 2. In the first year, the heat and mass transfer at the fuel surface are ignored and the model considers only two opposing gaseous fuel and oxidizer flow of equal free stream velocity. The effect of water evaporation on the extinction process was illustrated by the increase in the extinction Damkohler as shown in Figure 3.

To move toward our final objective which is to illustrate the effect of water spray on flames established on a solid/liquid fuel surface, the model is now expanded to include the effect of fuel surface heat/mass Transfer. Numerically, a two-step process is used. First, the analysis is expanded to allow for a vaporizing surface with constant wall temperature T_{wf} on the fuel side. This approach is similar to that utilized by other investigators (Krishnamurthy and Williams 1976) on conventional extinction analysis without water droplets.

The second step is to let the fuel surface temperature to be determined by the condition of heat and mass balance. Utilizing the concept of transfer coefficient originally introduced by Spalding (1963), this analysis will allow the extinction characteristics to be expressed entirely in terms of fuel properties and water concentration, a necessary condition for future experimental verification of the model.

3. REFERENCES

1. Alpert, R. L., "Calculated Interaction of Sprays with Large-Scale Buoyant Flows," *ASME Journal of Heat Transfer,* Vol. 106, May 1984, pp. 310-317.

2. Alpert, R. L., "Numerical Modeling of the Interaction Between Automatic Sprinkler Sprays and Fire Plumes," *Fire Safety Journal,* Vol. 9, 1985, pp. 157-163.

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4. Chow, W. K., "On the Evaporative Effect of a Sprinkler Water Spray," to be published at *Fire Technology.*

5. Krishnamurthy, L., Williams, F. A. and Seshadri, K. "Asymptotic Theory of Diffusion-Flame Extinction in the Stagnation-Point Boundary Layer," *Combustion and Flame,* Vol. 26, 1976, pp. 363-377.

6. Spalding, D. B., *Convective Mass Transfer,* McGraw Hill, New York, 1963.

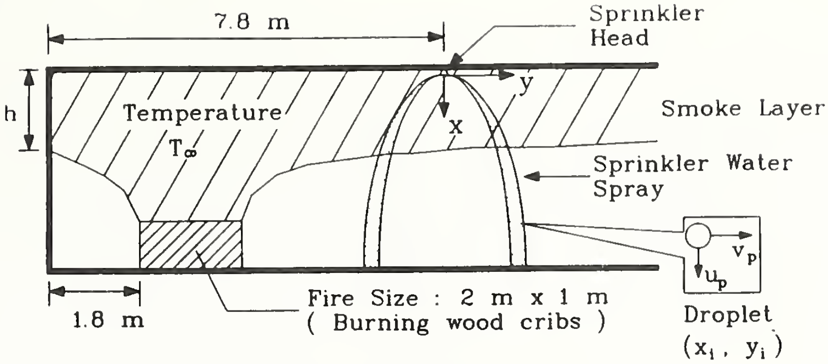


Figure 1. Geometrical configuration of the problem.

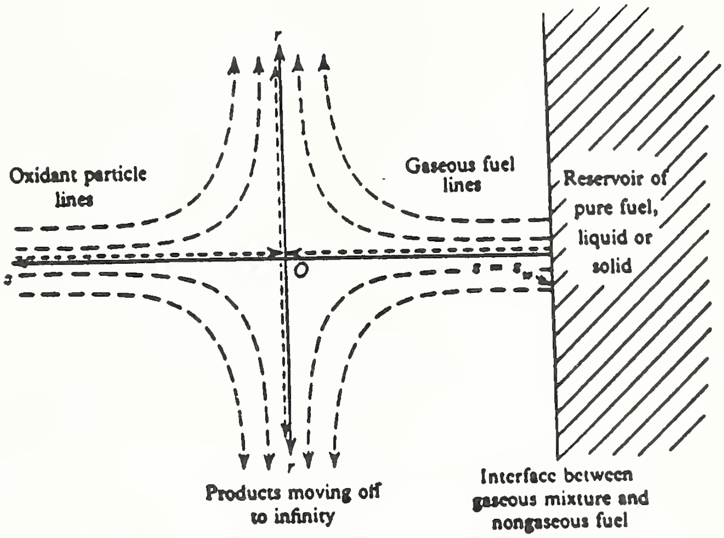


Figure 2. Oxidant, fuel, and product particle lines in an axially symmetric stagnation-region flow.

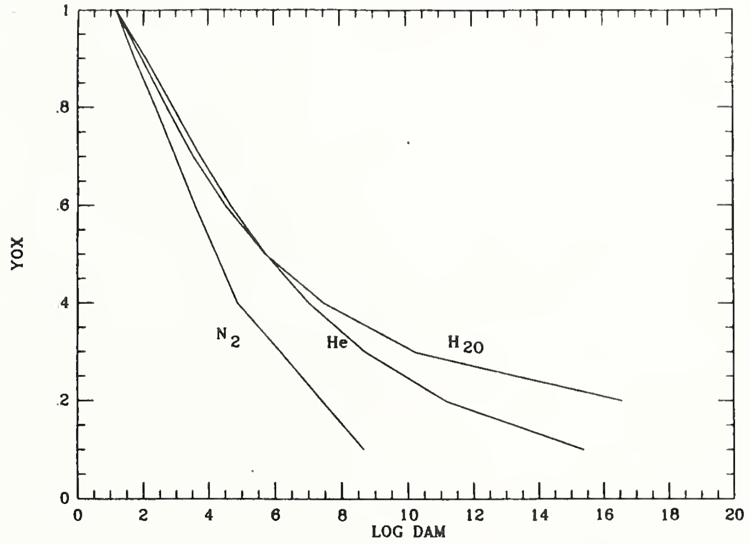


Figure 3. Critical Damkohler number required for extinction for oxidizer streams with different oxygen mass fraction and inert gases.

L. Cone Calorimeter

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

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 FY89 included: (a) Cone Calorimeter round robins for both ASTM and ISO; (b) assistance to users; (c) completion of Bldg. 205 controlled-atmospheres Cone Calorimeter.

Technical Accomplishments

The main focus of this year's work has been the round robins being sponsored by ASTM and by ISO. Both of these required identifying a number of hardware and software problems that participating laboratories were having, and then correcting them. The data analysis is nearly finished for both round robins. The results were generally good, with two exceptions: (1) For materials tested at heating fluxes only slightly higher than their minimum ignition flux, repeatable results can never be obtained; it was not intended to create such conditions for the round robin tests, but some were found to occur and had to be excluded *a posteriori*. (2) Charring materials showed wide scatter on the total-heat-released variable. This is because the test termination time was not adequately pegged down in the draft standards. Both of those issues were resolved in updating the standard documents — a caveat was inserted into the appendix to point out that rate of heat release testing (on any instrument, not just the Cone Calorimeter) cannot give repeatable results if the irradiance used is too close to the specimen's minimum ignition flux. Also, a detailed rule was developed for when the test operator should declare the end of test time to be. Both the ASTM task group and the ISO working groups met several times during the course of this year and made numerous other modifications to the draft standards. These modifications were based on the experience now accumulated by the laboratories and serves to pin down, quite a bit more closely, various operational details of the Cone Calorimeter. One other change of significance is that the wire grid specification, which was rigidly set forth in the original draft, was changed to permit wide latitude for the testing lab. It was recognized that samples can show various ways of mechanically misbehaving, and a single restraint method will not be optimum for all. The standard now will specify that if an alternative grid or restraint method is used, that the method used must simply be specified in the test report.

Within ASTM, the Task Group agreed to supplement the ASTM round robin with a 'proficiency round.' Some of the laboratories which had conducted the original round robin were brand new users of the Cone Calorimeter. By now, these labs have had a significant amount of experience; thus, it was felt that this proficiency round would indicate the difference between the performance of an experienced lab, as compared to an inexperienced one.

Also during this year, the controlled-atmosphere Cone Calorimeter in Bldg. 205 was finally placed into operation. A number of features on this unit are quite different from the standard, open-air unit; data gathering is now underway.

A number of changes were also made to the User's Guide. This document will be re-issued in approximately one year, when enough revisions are accumulated.

Also, during this year, data formats were established for how Cone Calorimeter data can be handled within the proposed Fire Data Management System (FDMS). A significant number of other laboratories, on a worldwide basis, will be participating in the new standard for fire test data exchange which is contained in FDMS. The data formats have been worked out with the cooperation of a number of European fire laboratories. Thus, it was ensured that the formats would have general acceptability within the community. (Similar data formats have also been worked out for a number of additional other fire tests, once the Cone Calorimeter definitions were completed.) Actual programming work, however, was not started.

Reports and Publications

Braun, E., Shields, J.R., and Harris, R.H., Flammability Characteristics of Electrical Cables Using the Cone Calorimeter (NISTIR 88-4003). [U.S.] Natl. Inst. Standards and Technology, Gaithersburg, MD (1989).

Babrauskas, V., Smoke and Gas Evolution Rate Measurements on Fire-retarded Plastics with the Cone Calorimeter, **Fire Safety J. 14**, 135-142 (1989).

Brown, J.E., Cone Calorimeter Method for Determining the Flammability of Composite Materials, pp. 141-150 in **How to Apply Advanced Composites Technology (Proc. of the Fourth Annual Conf. on Advanced Composites)**. ASM International, Dearborn, MI (1988).

Babrauskas, V., Effective Measurement Techniques for Heat, Smoke, and Toxic Gases, pp. 4.1 to 4.10 in **Fire: Control the Heat...Reduce the Hazard**, QMC Fire & Materials Centre, London (1988).

Babrauskas, V., and Wickström, U.G., The Rational Development of Bench-Scale Fire Tests for Full-Scale Fire Prediction, pp. 813-822 in **Fire Safety Science – Proc. of the Second International Symposium** (1988). Hemisphere Publishing, New York (1989).

Mulholland, G.M., Henzel, V., and Babrauskas, V., The Effect of Scale on Smoke Emission, pp. 347-357 in **Fire Safety Science – Proc. of the Second International Symposium** (1988). Hemisphere Publishing, New York (1989).

M. Technology Transfer

CENTER FOR FIRE RESEARCH
PRIORITY PROJECT - 1989

TECHNOLOGY TRANSFER

Professional Personnel

R. Bukowski, Manager
N. Jason, Information Specialist

Project Objective

To facilitate the assimilation and use of new science and technology by all aspects of the fire community.

Scope

CFR should be responsive to the technological needs of the fire community. This involves (1) identification of their needs, (2) finding solutions to these problems, (3) tailoring the results in a manner in which they can be utilized by the recipient and (4) providing access to those results. The Technology Transfer Office facilitates the flow of information between CFR and the fire community.

Technical Accomplishments

I. HAZARD I

CFR has released a method for quantifying the hazards to occupants of buildings from fires, and the relative contribution of specific products (e.g., furniture, wire insulation) to those hazards. The culmination of six years of development, HAZARD I represents the most comprehensive application of fire modeling in the world (see HAZARD I Priority Project). The role of HAZARD I in the Technology Transfer project is as a vehicle by which technology developed by the Center can be utilized in the solution of problems. By building a technology into the framework of HAZARD I, it can be applied without the need to deal directly with the mathematics or theories.

II. Application of HAZARD I

The newly-released fire hazard assessment software HAZARD I was successfully employed by CFR in a litigation against the United States. The suit asked $26M for the deaths of a mother and two of her children in a fire in base housing at Ft Hood, TX in 1982. The claim was based on the fact that the base fire department was delayed in responding to the fire by troop movements, and that an earlier arrival would have allowed one or more of the victims to have been rescued. At the request of the Justice Department, the HAZARD I software was used to recreate the fire and evaluate the impact of the fire department delay on the outcome. The analysis reproduced many details of the fire including damage patterns to the building, the successful escape of three older children, and the three fatalities including the locations of the bodies and the autopsy results. The analysis also showed that the fatalities occurred as the fire department was being first notified, and that their delayed arrival played no significant role. Faced with this detailed analysis, the plaintiff agreed to settle for less than $200k. The US Attorney stated that this outcome was almost exclusively based on the HAZARD I analysis. This application will serve as an example of the power of HAZARD I in the fire reconstruction area.

III. Training on HAZARD I

The Center for Firesafety Studies at Worcester Polytechnic Institute has developed a 5 day, intensive course on HAZARD I aimed at fire safety professionals with significant experience in the fire field. The course combines formal lecture on the underlying science, assumptions and limitations of the models and procedures with "hands on" training on the mechanics of using the HAZARD I software. The students then apply the software to a class project of their choice. The course will be offered by WPI beginning in January.

IV. Acceptance by Code Authorities

In most regulated applications, the success or failure of HAZARD I will depend on whether the responsible authority is comfortable with the analysis performed with it. To this end, efforts have been undertaken to work with code authorities (the model code organizations and the Fire Marshals) in training their staffs in the use of HAZARD I. As they then begin to use HAZARD I to evaluate code change proposals, they might identify areas in which they feel that the system works properly, and can offer suggestions on changes which will improve its usefulness in their applications. Additionally, the State Fire Marshals section of the International Association of Fire Chiefs is sponsoring a person (a Deputy State Fire Marshall in California) to spend a year at CFR working with us on HAZARD I.

V. FRIS

The Fire Research Information Service (FRIS) is being more closely integrated into the Technology Transfer Office. This means that we are looking for more ways in which FRIS can serve our customers through better access to information. Such things as broadening the scope of the databases currently on line are being explored. The document entry into FIREDOC is proceeding at a good pace with about 2/3 of the entire collection now available to users of the system. In the past year, a new security system with user passwords has been implemented which should eliminate some "hacker" problems encountered and give us better statistics on user interest.

VI. CFRBBS

The CFR electronic bulletin board continues to be very popular, logging over 5000 calls in its 2½ years of operation. The system operator (Doug Walton) has included much information of interest to the fire service, and their response is great. At several of their annual gatherings a large fraction of those who stop by the CFR booth have been on the CFRBBS.

PART II. Timely Response to Current Fire Problems (mostly projects funded by other agencies and private sector organizations)

A. Fire/Materials Interactions

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

RADIATIVE IGNITION AND SUBSEQUENT FLAME SPREADING IN MICROGRAVITY ENVIRONMENT

Funding Agency:	NASA Microgravity Science Program
Professional Staff:	Takashi Kashiwagi, Project Leader Howard Baum, NIST Fellow Colomba Di Blasi, Guest Researcher Hidesaburo Nambu, Guest Researcher

Project Objective:

Develop a theoretical model to be able to predict ignition and subsequent flame spreading over a cellulosic material in a microgravity environment using the material characteristics determined in one G environment.

Technical Accomplishments:

Ignition characteristics, ignition delay time vs. external radiant flux and surface temperatures of a black paper vs. external radiant flux, were measured in one G under the bottom surface ignition configuration with upward external radiation from a tungsten lamp. Surface reflectance of the black pepper was measured from 0.3 to 2.5 μm. Thermal and thermal oxidative degradation characteristics of the black paper are being determined by Thermal Gravimetric Analysis with multiple heating rates and by continuous evolved gas analysis of CO, CO_2, H_2O and O_2. A two-dimensional axisymmetric time-dependent ignition model is being developed. Its gas phase model is based on irrotational flow mainly controlled by gas expansion with energy and species equations. Its condensed phase model is based on the thermally thin black paper with two step global degradation mechanisms. At present, the gas phase chemical reaction has not been included in the model.

Reports and Publications

"Radiative Ignition in a Microgravity Environment - The Preheating Problem", Baum, H.R., Kashiwagi, T., and Di Blasi, C., 1988 Fall Technical Meeting, Eastern Section of the Combustion Institute, Dec. 5-7, 1988.

"Radiative Pyrolysis of Thin Fuels in a Microgravity Environment", Baum, H.R., Kashiwagi, T., and Di Blasi, C., to be presented at 1989 Fall Technical Meeting, Eastern Section of the Combustion Institute, Nov. 1989.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

HEAT RELEASE FROM AIRCRAFT COMPOSITES

Funding Agency FAA

Professional Staff: Bill Parker, Project Leader
Angel Perez, Computer Scientist

Project Objective

Develop a theoretical and/or empirical or estimating methodology for predicting an aircraft panel's 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 to calculate the temperature, mass loss rate and heat release rate of aircraft cabin panels based on the measured thermophysical and thermochemical properties of the panel materials. It takes the thermal radiation exchange in the honeycomb cavities into account along with the heat conduction through the solid material and the air. Single first order reactions are assumed in calculating the mass loss rates. The calculations are being compared with measurements in a burning rate apparatus and in the Cone and OSU Calorimeters.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

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. Combustion Sensitivity Index Methodology

The dependence of rate of heat release (RHR) on external flux was determined using the NIST Cone Calorimeter for various composite materials under constant fluxes indicative of small and large (flash over) fires. Figure 1 shows a plot of an average RHR versus external flux for a vinylester resin/glass fiber composite. The slope of the curve, called the thermal sensitivity index, indicates the effect of external flux on the average burning rate for various periods of the flaming combustion; while the intercept indicates the external flux requirement for sustained flaming combustion.

2. Ignitability

Ignition delay time as a function of external radiant heating was measured also in the Cone Calorimeter over a broad range of fluxes. Figure 2 demonstrates the flux dependence of the ignition delay time. Minimum external fluxes required for ignition in reasonably finite periods can be predicted.

3. Testing of Materials

Fire testing of Navy candidate composite materials for surface ships was initiated. The results from these tests are being used to propose requirements for submarine applications.

4. Flammability Assessment of Composite Deckhouse Materials

Ignitability and lateral flame spread characterization was accomplished for two composite materials utilized in the construction of full-scale deckhouse compartments. These results were utilized to help guide the full scale testing of those compartments; they are being prepared for publication.

Reports and Publications:

"Cone Calorimeter Method for Determining the Flammability of Composite Materials" J.E. Brown, Proceedings of the fourth Annual Conference on Advanced

Composites: "How to Apply Advanced Composites Technology" Dearborn, MI 13-15 Sept. 1988, pp. 141 - 150.

"Assessing the Flammability of Composite Materials", T. Ohlemiller, National Institute of Standards and Technology NISTIR 89-4032, January, 1989

"Ignition and Lateral Flame Spread Characteristics of Certain Composite Materials", T. Ohlemiller and S. Dolan, National Institute of Standards and Technology NISTIR 89-4030, January, 1989

FIGURE 1. Orientation Effect on the Average (180 s) RHR of a 4.5 mm Thick Vinylester Resin composite with Respect to External Flux

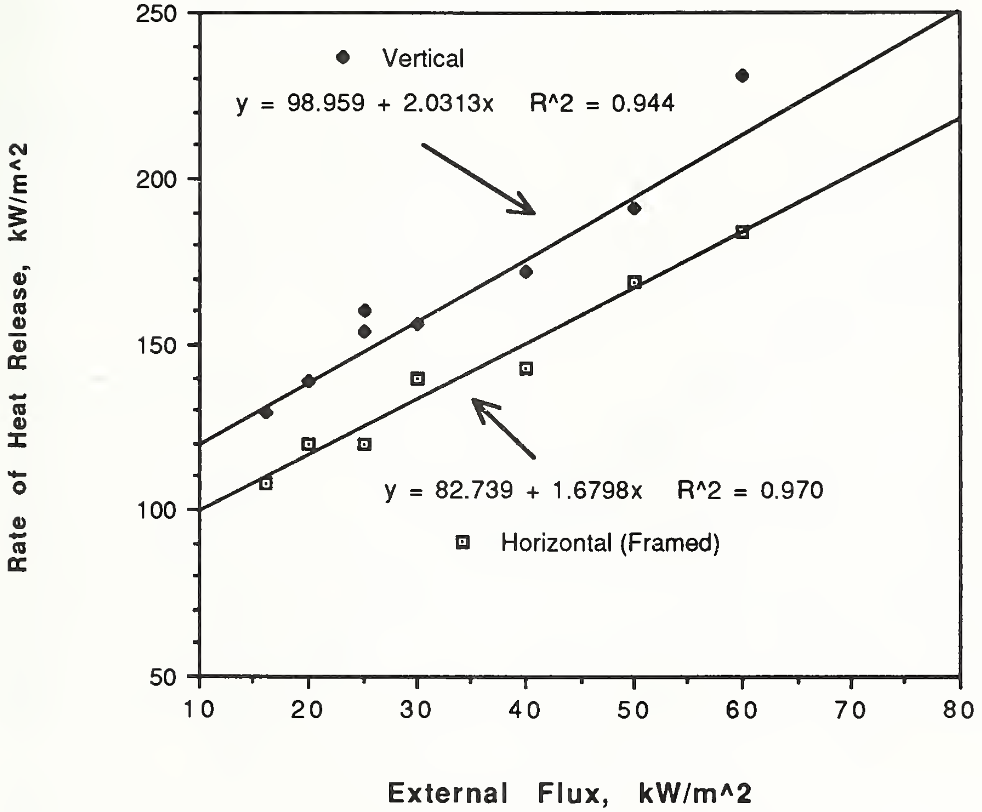
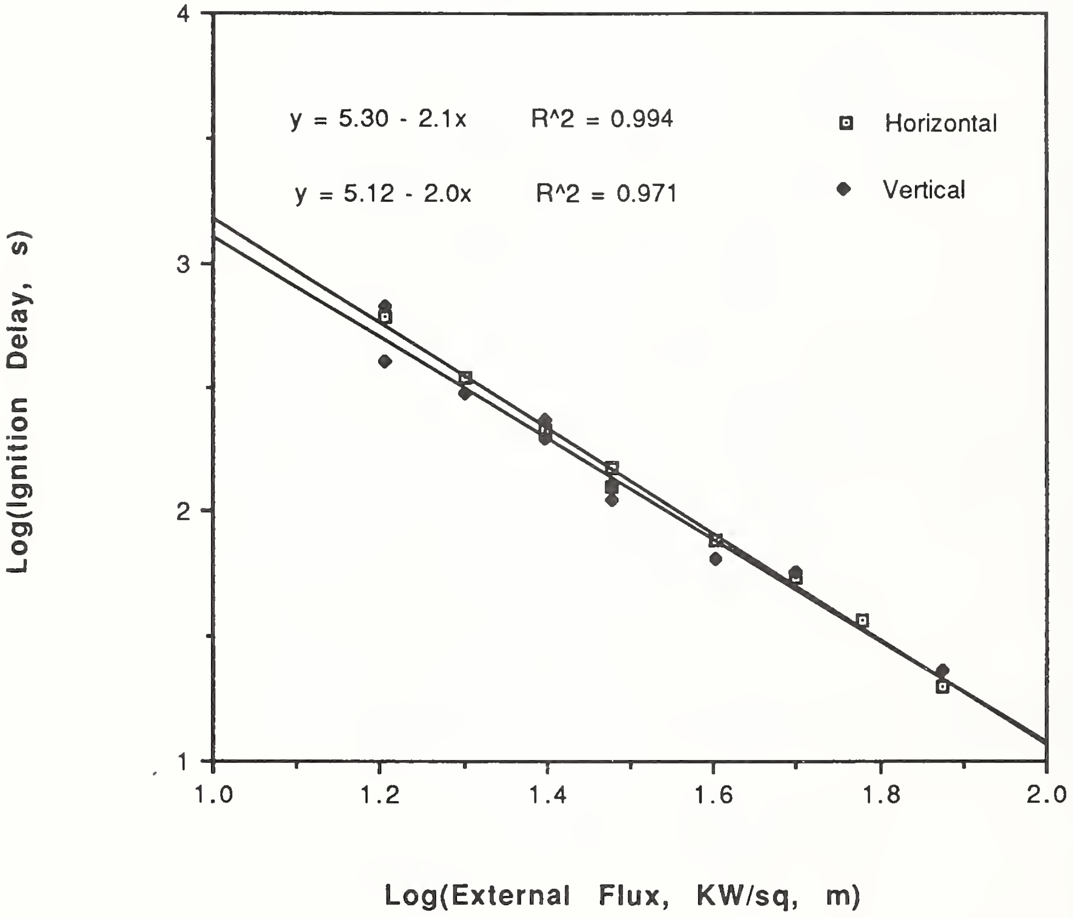


FIGURE 2. Flux Dependence of the Ignition Delay Time of a 4.5 mm Thick Vinylester Resin Composite in Two Orientations



CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

FIRE PERFORMANCE OF SCHOOL BUS INTERIORS

Funding Agency: The National Highway Traffic Safety Administration

Professional Staff: Sanford Davis, Project Leader
Emil Braun, Physicist
Barbara Levin, Toxicologist
Maya Paabo, Chemist
Richard Harris, Chemist

Project Objective

Assess the fire performance of school bus seat assemblies when exposed to internal and external fuel sources 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 experiments.

Technical Accomplishments

Guidelines for the development of material acceptance criteria intended to limit the fire growth in school buses are being investigated. This study is directed towards defining material selection parameters that affect the rate of development of hazardous conditions in a school bus geometry. The largest source of combustible material in a school bus interior is the seat assemblies. Padding required in other interior area typically employ the same materials as the seats; however, this study is limited to currently used and state-of-the-art materials assemblies for school bus seats. Six different seat assemblies having a range of expected fire performance were purchased from a major manufacturer of school buses.

Small- and large-scale tests were performed to characterize material fire performance in easily measured parameters, such as ignitability, flame spread, rate of heat release, smoke development, and toxicity. Preliminary experiments were carried out in the furniture calorimeter using single seat assemblies to determine the level of fuel exposure necessary to carry out full-scale experiments in a school bus geometry. With three rows of seats, one of which was exposed to a 100 kW natural gas fire, only the assembly composed of an untreated polyurethane foam covered with an untreated vinyl cover succeeded in flashing over the compartment; the other five constructions did not cause fire spread beyond the seat of fire origin, although there was damage to the adjacent seat. Small-scale tests of composite materials are still in progress and will be evaluated for their predictive capabilities.

The acute inhalation toxicity of the combustion products of the five foams and three cover materials was assessed by the N-Gas Model using the NBS Toxicity Test Method apparatus under flaming conditions. LC_{50} values ranging from 10 to 85 mg/ℓ were estimated based on the model; the toxicity does not necessarily track with the burning propensity.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

SMOKE EMISSION AT LABORATORY SCALE

Funding Agency: Defense Nuclear Agency

Professional Staff: George W. Mulholland, Project Leader
Nelson P. Bryner, Chemical Engineer

Project Objective

To measure the emission, optical properties, and cloud scavenging tendency of smoke produced by urban fuels.

Technical Accomplishments

Cribs were constructed with a wide range in stick spacing to simulate the range in packing densities expected for free standing structures versus blast damaged structures. The smoke emission and burning rate were measured during tests performed on small (10 cm stick length) and intermediate scale (50 cm stick length)cribs. The cribs were made of wood, wood and gypsum, and wood, gypsum, and plastic. For the more densely packed cribs, less flaming combustion occurred and large amounts of pyrolysis products were evident as white smoke.

The performance of the Transmission Cell - Reciprocal Nephelometer (TCRN), which is used for measuring the extinction, scattering, and absorption coefficients of smoke, has been improved about 10 fold in regard to stability (drift reduced to about one part in 10,000 over 10 minutes) and in regard to the time for data analysis. The improved TCRN was used in joint study with Desert Research Institute on the effect of humidity on the optical properties of acetylene smoke. Preliminary results with haze chambers indicate no significant humidity effect on the optical properties of smoke at humidities less than 100%. The single scattering albedo increased by about 50% at high moisture supersaturation produced by an expansion chamber and appeared to increase by a few percent at a supersaturation of about 1.5%, which is similar to the supersaturation observed in clouds.

Reports and Publications

G. W. Mulholland, V. Henzel, and V. Babrauskas, Fire Safety Science - Proceedings of the Second International Symposium, 347 (1988). The Effect of Scale on Smoke Emission.

G. W. Mulholland and Nelson P. Bryner, Proceeding of Global Climatic Effects of Aerosols to be published in Atmospheric Environment. Smoke Emission and Burning Rates for Urban Fires.

Related Grants

"A Study of the Scavenging and In-Cloud Processing of Combustion Aerosols", D. Hagen, University of Missouri-Rolla.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: University of Missouri - Rolla

Grant No.: 60NANB9D0953

Grant Title: A study of the scavenging and in-cloud processing of combustion aerosols.

Principal Investigator: Donald E. Hagen
Physics Dept. and Graduate Center for Cloud Physics Research
University of Missouri - Rolla
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e-mail: C3102@UMRVMB.UMR.EDU

Other Professional Personnel:
Dr. John C. Carstens
Dr. Josef Podzimek
Dr. John L. Schmitt
Dr. Daniel R. White
Mr. Max B. Trueblood
Mr. Alfred R. Hopkins

NBS Scientific Officer: Dr. George W. Mulholland

Technical Abstract: 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. In this effort we are pursuing 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 our laboratory 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, crude oil in particular. An existing combustion aerosol generation system is being modified to handle crude oil combustion on a laboratory scale. These studies will cover a wide range in temperature encompassing both warm (liquid cloud drops) and cold (ice) conditions, and will cover both static and time-dependent thermodynamic conditions. The experimental results will be translated into a form suitable for use as inputs into the numberical models used to describe the overalll evolution of combustion aerosols in the atmosphere.

Reports and papers: There are none. The project has just started.

CENTER FOR FIRE RESEARCH
STANDARDS REFERENCE MATERIAL PROJECT - 1989

PARTICLE CONTAMINATION STANDARD AND 0.1 μm PARTICLE SIZE STANDARD

Staff

George W. Mulholland, Project leader
Nelson P. Bryner, Chemical Engineer

Project Objective

Develop a prototype particle contamination standard for the semiconductor industry involving the deposition of a known number of 1 μm silicon particles on a silicon wafer. Prepare about 300 samples of an 0.1 μm particle size standard and measure the particle size to an accuracy of about 2%.

Technical Accomplishments

An aerosol generation system was developed with staff at the Particle Technology Laboratory at the University of Minnesota for producing monodisperse 0.9 μm silicon particles. First a polydisperse aerosol was generated by nebulizing a suspension of silicon particles in water, and then a monodisperse fraction of the aerosol was isolated by using a bipolar charger and an electrical mobility analyzer. A laminar flow chamber was used to uniformly deposit the monodisperse aerosol on 10 cm diameter silicon wafers. A commercially available wafer scanner was used to determine the number of particles deposited on the wafer. Fifteen wafers were prepared in this manner and will be distributed to selected facilities for evaluation of the utility of the prototype standard.

A detailed analysis of the feasibility of using the electrical mobility analyzer for accurately measuring the diameter of 0.1 μm polystyrene spheres was carried out. A conservative estimate of the uncertainty in the particle size measurement is 3.8 %. Preliminary measurements indicate that this uncertainty can be reduced by a factor of two by using the existing 1.0 μm SRM particle size standard to "calibrate" the electrical mobility classifier.

Publications

Patrick D. Kinney, David Y.H. Pui, and George W. Mulholland, to be published as NBSIR. Use of the Electrostatic Classification Method to Size 0.1 μm SRM Particles - A Feasibility Study.

B. Fire Protection Technology

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

SAFETY IN OFFSHORE DRILLING

Funding Agency: Minerals Management Service, U.S. Department of Interior

Professional Staff:
David Evans, Project Leader
Doug Walton, Fire Protection Engineer
Howard Baum, NIST Fellow
George Mulholland, Chemist
Dan Madrzykowski, Mechanical Engineer

Project Objective:

Examine technologies that can mitigate the effects of fire and oil spills from offshore platform accidents.

Technical Accomplishments:

Measurements of the effects of water spray on methane jet flames that simulate gas well blowout fires were continued and expanded to include methane with heptane and methane with crude oil. Temperature and radiation measurements were taken on fires with heat release rates up to 15 MW. The effect of water spray on these fires was also examined. A detailed analysis of the data has been performed under a grant by Dr. Gore of the University of Maryland.

The Center for Fire Research has conducted research focused on examining the phenomena associated with crude oil combustion and the impact of using burning as a spill response method. The process of burning crude oil on water as a means to mitigate oil spills has been investigated with a research effort combining both small scale experiments and calculations. As a result of these studies, there has been increased understanding of the burning process including burning rate, fire radiation, smoke emission, smoke composition and smoke dispersion in the atmosphere.

A key to gaining acceptance of burning as a spill response technique is the demonstration that the favorable results obtained at laboratory scale can be shown to continue to operational conditions at field scale. Field scale burn tests are being planned and coordinated by MMS to document the use of burning technology under conditions simulating actual oil spill clean-up operations. The Center is undertaking a new project to develop measurement techniques suitable for field use, verify these techniques and make measurements under field scale burning conditions. These measurements will provide the information that can be used by local officials and oil spill response professionals as part of the decision making process in the event of an oil spill.

Reports and Publications:

Burning, Smoke Production, and Smoke Dispersion from Oil Spill Combustion, D. Evans, G. Mulholland, D. Gross, H. Baum, K. Saito, National Institute of Standards and Technology Interagency Report, NISTIR 89-4091, June 1989.

In-Situ Burning of Oil Spills, D. Evans, Alaska Arctic Offshore Spill Response Technology, Workshop Proceedings, NIST SP 762, April 1989.

Alaska Arctic Offshore Spill Response Technology, Workshop Proceedings, N. Jason Editor, NIST SP 762, April 1989.

Smoke Plumes for Crude Oil Burns, D. Evans, H. Baum, G. Mulholland, N. Bryner, G. Forney, Proceedings of the Twelfth Arctic and Marine Oil Spill Program Technical Seminar, Calgary Alberta, Canada, June 7-9, 1989.

Generation and Dispersion of Smoke from Oil Spill Combustion, D. Evans, G. Mulholland, D. Gross, H. Baum, K. Saito, Proceedings, 1989 Oil Spill Conference (Prevention, Behavior, Control, Cleanup), February 13-16, 1989, San Antonio, TX.

Related Grants:

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 STANDARDS AND TECHNOLOGY
FY89

Institution: University of Kentucky

Grant No.: 60NANB7D0739
Grant Title: A Study of Pool Combustion of Crude Oil Supported on Water
Principal Investigator: K. Saito
Associate Professor
Dept. of Mechanical Engineering
University of Kentucky
Lexington, KY 40506-0046
Tel.: (606)257-1685

Other Professional Personnel: Takao Inamura (Visiting Scientist)
Shyam Venkatesh (Ph.D Candidate)

NIST Scientific Officer: Dr. Dave Evans

Technical Abstract:

Under certain circumstances, the water on which a burning pool of liquid fuel is supported may begin to boil. The water vapor that is released and escapes through the fuel surface tends to atomize the oil, which results in an emulsive-droplet flame above the fuel surface. This phenomenon, called boilover, has been observed for large scale pool fires, but the mechanism causing it to occur has not been fully investigated yet. We studied fundamental aspects of the effect of a boiling water sublayer on the behavior of pool fires.

A burner system in which the burning surface of the fuel can be fed into the flame so that the fuel/water interface with respect to the edge of the container remains fixed was used. Ten different single-component and six different multicomponent fuels were tested. Conventional flow visualization techniques were applied to study the liquid motion, and results for an ethylbenzene pool in a 4.8 cm diameter pan are presented. Data obtained include temperatures and mass loss history of the liquid fuel and water, flame height, and irradiance from the flame. Results show that when the water sublayer starts to boil, the temperature gradient across the fuel layer vanishes, the temperature level of the fuel decreases, and the burning rate of the fuel decreases. Contrary, the large pool fires show an opposite result that when the boilover occurs, the burning rate of the fuel increseases. Thus it was suggested that for the small pool fires, additional external radiant heat is required to simulate quantitatively the boilover phenomenon for the large pool fires.

Background:

Studies on the combustion of liquid fuel have covered a wide range of problems, e.g., from the combustion of a small droplet to a large oil tank fire (Williams, 1985), and some of these have been left as unresolved problems that merit further investigation (Glassman and Dryer, 1980). Here we report the results of an experimental effort aimed at improving our understanding of the effects of a boiling water sublayer in an open tank combustion system that is similar to the burning of an oil slick supported on a water sublayer. Oil-slick fires may occur as unwanted fires following an oilspill, or they may be initiated as a control measure. In either case, when the heat transfer from the fire plume back through the oil slick is sufficient to boil the water an intense spattering of water and oil droplets (boilover) may occur that poses a hazard to containment efforts.

The so-called boilover phenomenon has usually been observed when a relatively large fuel surface area (say larger than 0.5 m in diameter) was burning (Hall, 1925; Blinov and Khudyakov, 1961; Seeger, 1974; Brzustowski and Twardus, 1982; Evans et al., 1986 and 1987). To elucidate the physics of this occurrence, it is important to study local temperature histories of the water sublayer and the fuel during the progress of combustion. These measurements can be performed with accuracy in a small scale pool combustion system because the flame is stable, fuel surface waves due to gravity are negligible, and the boiling of the water sublayer begins nearly uniformly over the entire fuel/water interface. Larger scale pool combustion systems are easily disturbed by these factors (Evans et al., 1988). The characteristics of the small scale system make a one-dimensional simulation model simple to develop and useful in interpreting the physics of the boilover process.

The combustion behavior of different crude oils under different conditions has been studied in several laboratories, and large variations were observed for different crude oils. Direct comparison of test results is difficult, and it is, therefore, difficult to draw any general conclusions. The studies by Evans et al. (1986, 1987 and 1988), Brzustowski and Twardus (1982) and Twardus and Brzustowski (1981) are of particular interest to us because their studies are rather recent and were performed using a system similar to the one used here.

In the NBS studies (Evans et al., 1986, 1987 and 1988) burning rate, flame height, radiant heat loss to the surroundings, and the formation of toxic products and soot were studied. Boilover was found to occur near the end of the combustion process, and a considerable amount of oil spilled over the rim of the test tank. Using their qualitative observations as a guide, we performed a series of small scale pool fire tests aimed at developing an understanding of the effects of the boiling water sublayer on boilover.

SUMMARY AND CONCLUSIONS:

The burning characteristics of pools of liquid fuel floating on a water sublayer that are reported here lead to the following observations:

1. Boilover occurs for fuels whose boiling point temperature is higher than that of water, regardless of whether the fuel is pure or a multicomponent fuel.
2. The intensity of boiling of the water sublayer largely depends on the boiling point temperature of the fuel; the higher the boiling point of the fuel, the more intense is the boiling.
3. When boiling of the water sublayer occurs in the small pool fire system, the average flame height and irradiance from the flame decrease slightly, the fuel layer temperature becomes uniform and then decreases, and the fuel mass burning rate decreases with progress of combustion.
4. The large pool fires show an opposite result from the small pool fires that when the boilover occurs, the burning rate of the fuel increases. Thus for the small pool fires, additional external radiant heat is

required to simulate quantitatively the boilover phenomenon for large pool fires.

5. Occasionally following the onset of an intense boiling accompanied with active frothing a fire-ball-like flame appears, which radiates intensely (see Fig. 1).
6. The fuel temperature near the fuel/water interface is somewhat limited by the presence of the boiling water and cannot reach the boiling point of the fuel, thus flame is extinguished and unburnt fuel is left. For fuels whose boiling point is less than that of water, the fuel temperature near the fuel/water interface eventually reaches nearly the boiling point temperature of fuel.
7. To predict temperature profiles in liquid, the following equation was solved using finite difference method.

$$\rho c(\partial T/\partial t) = \partial(\lambda \partial T/\partial y)/\partial y + q\mu\ e^{-\mu y}$$

The calculation results are favorably compared to experimental ones (see Fig. 2).

<u>Papers:</u>

1. Evans, D., Mulholland, G., Gross, D., Baum, H., and Saito, K. (1987). Environmental Effects of Oil Spill Combustion. Proceedings of the Tenth Arctic Marine Oil Spill Program Technical Seminar, June 9-12, Edmonton, Alberta, Canada.

2. Evans, D., Mulholland, G., Gross, D., Baum, H., and Saito, K. (1988). Burning, Smoke Production and Smoke Dispersion from Oil Spill Combustion. Proceedings of the Eleventh Arctic Marine Oil Spill Program Technical Seminar, June 7-9, Vancouver, British Columbia, Canada.

3. Inamura, T., Taghavi, K., and Saito, K. (1989). A Simplified Model to Predict Boilover Phenomenon. Proceedings of the Central States Section/The Combustion Institute, Dearborn, MI, April 30-May 3.

4. Elam, S.K., Tokura, I., Saito, K., and R.A. Altenkirch (1989). Thermal Conductivity of Crude Oils, Experimental Thermal and Fluid Science, 2,1.

5. Arai, M., Saito, K. and Altenkirch, R.A. (1989). A Study of Boilover in Liquid Pool Fires Supported on Water: Part I --- Effects of a Water Sublayer on Pool Fires, Combustion Science and Technology (submitted).

6. Inamura, T., Taghavi, K. and Saito, K. (1989). A Study of Boilover in Liquid Pool Fires Supported on Water: Part II --- A One Dimensional Analysis of Onset of Boilover Phenomenon, Combustion Science and Technology (submitted).

7. Ito, A., Masuda, D. and Saito, K. (1989). Holographic Interferometry Temperature Measurement of Liquid Phase under Spreading Flame Condition, the 26th ASME/AIChE National Heat Transfer Conferance, Philadelphia, PA, August.

8. Ito, A., Masuda, D. and Saito, K. (1989). A Study of Flame Spread Over Alcohols Using Holographic Interferometry, Combustion and Flame (submitted).

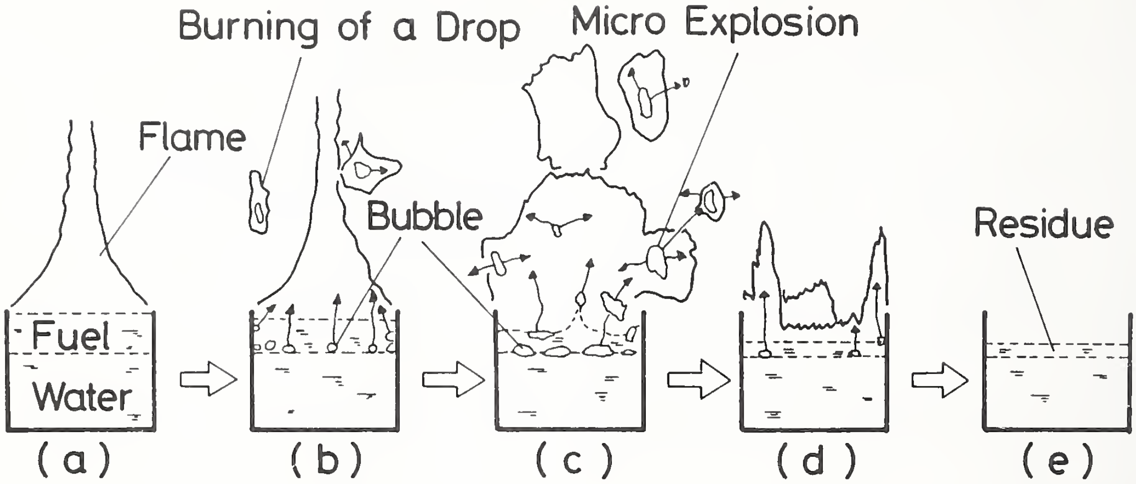

Fig. 1 Schematic illustration of boilover process.

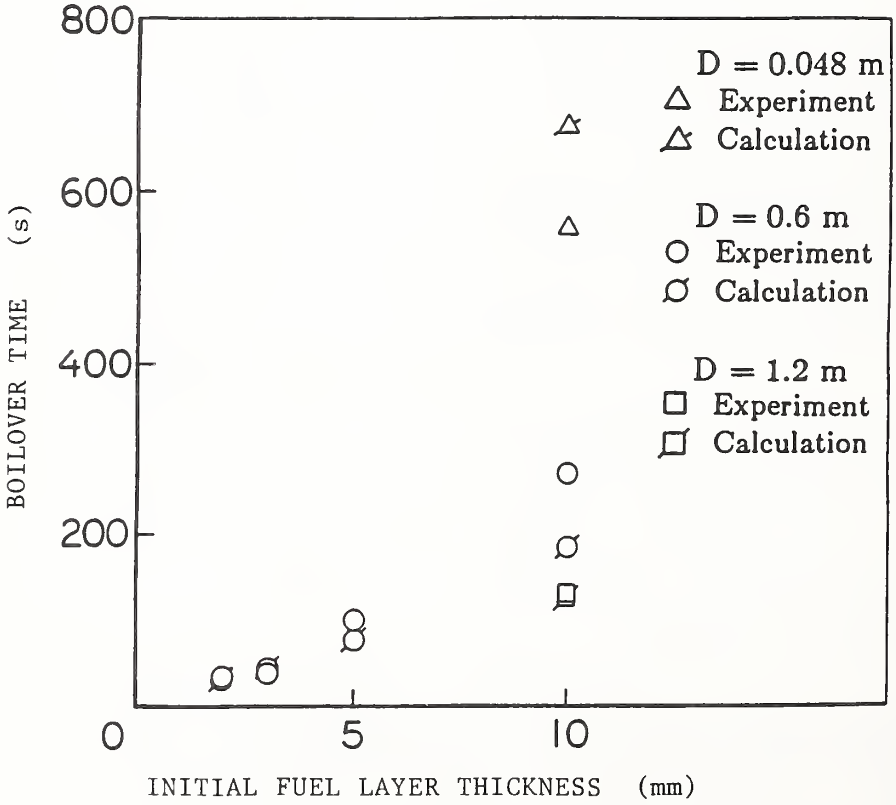

Fig. 2 Boilover time as a function of initial fuel layer thickness.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 89

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) 454-8869

Other Professional Personnel: S. M. Skinner (M. S. Candidate)
C. Q. Jian (Ph. D. Candidate)
D. W. Stroup (N. I. S. T.)
D. Madrzykowski (N. I. S. T.)

N. I. S. T. Scientific Officers: Dr. D. D. Evans
Mr. W. D. Walton

Technical Abstract:

The overall objective of this project is to develop predictive capabilities for scaleup of suppression techniques for oil and gas-well blowout fires. The suppression techniques under study involve application of water spray and are aimed at reducing flame radiation to allow containment and capping of the blowout fires. Our research thus far has emphasized: (1) structure and radiation properties of single and two phase mixtures of fuels with and without water suppression and (2) coupled radiation and structure properties of turbulent diffusion flames. The results from the study of radiation under the effect of water suppressant were discussed in the last meeting. In the following results from studies involving mixtures of fuels are described. Both turbulent and laminar flames burning fuel mixtures are considered.

Large Scale Turbulent Fires:

Tests involving measurements of temperature and radiative heat loss fractions for methane+heptane and methane+Alberta sweet crude oil were conducted at N. I. S. T. by D. W. Stroup and D. Madrzykowski. Water was applied during portions of the tests to study suppression. Five fully instrumented tests with approximately 15 MW heat release rates were conducted. The heat release rates from the two fuels were approximately equal. Methane flames with approximately 8 MW heat release rates were studied as a baseline.

Figure 1 shows the measurements and predictions of temperatures along the axis of the CH_4/air flames. The predictions show good agreement with the data. Figure 2 shows the measurements and predictions of radiative heat flux parallel to the axis of the CH_4/air flames. Again, the data and predictions agree reasonably well. Together with earlier results, this shows that the capabilities of the analysis for CH_4/air flames is established.

Approximate state relationships for flames burning heptane/methane mixtures with air were constructed by using those of the individual fuels based on a mixing rule. The mixing rule is based on the observation that the measurements of major gaseous species for three different paraffins could be correlated in terms of a generalized state relationship for a paraffin C_nH_{2n+2}. The radiative heat loss fraction for the mixture flames is estimated based on a linear interpolation of those of the individual fuels. The radiative loss fraction for heptane was obtained from auxiliary tests involving small pool flames.

Measurements and predictions of axial temperature profile and radiative heat fluxes parallel to the axis of the mixture flames are shown in Figures 3 and 4. The temperatures are underpredicted by 10 % and the radiative heat fluxes are underpredicted by 30 %. We are carrying out measurements of state relationships for laminar flames burning fuel mixtures to check the reason for these discrepancies. Measurements of temperature profiles and radiative heat fluxes for flames burning Alberta sweet crude oil+methane mixtures(not shown here) show remarkable similarities to those of heptane+methane. In view of the higher soot concentrations for the crude oil flames, this result is somewhat unexpected. The reasons are probably associated with the optical depths of the flames. In particular self absorption in methane+crude oil flames may be higher than that in methane+heptane flames.

Laminar Flames Burning Fuel Mixtures:

As a first step mixtures of two gaseous fuels are considered to test the mixing rule for state relationships without the complications of phase change. Acetylene (due to its high propensity for soot) is selected to be mixed with methane in different proportions. The burner configuration is a laminar jet diffusion flame in a coflow of air similar to past studies. Measurements of soot volume fractions and total radiative heat loss fractions for eight flames have been completed.

Figure 5 shows the maximum soot volume fractions in ppm plotted as a function of mass fraction of methane in the fuel stream. The maximum soot volume fractions decrease from approximately 40 ppm for pure acetylene/air flames to negligible (transmittance of greater than 99.5%) for the pure methane flames. For the mass fractions of methane at which measurements were obtained, the peak soot volume fractions seem to decrease linearly with methane mass fraction. As a result the minimum transmittance in the flame goes from 10% to 70% when the methane mass fraction increases from 0 to 0.5.

Figure 6 shows the measurements of total radiative heat loss fractions for the flames burning fuel mixtures. The radiative heat loss fraction decreases from about 0.45 for pure acetylene flames to 0.2 for pure methane flames. The change in radiative loss fractions is smaller for high acetylene concentrations. A small change in radiative heat loss fractions for a large change in soot volume fractions confirms the effects of optical depth suspected from the turbulent flame results. Work in progress will verify the mixing rule for state relationships, address the problem of two phase mixtures and separated flow effects in multiphase fires with and without suppression.

Reports and Papers:

1. J. P. Gore, 1988, "Coupled Structure and Radiation Analysis of Turbulent Diffusion Flames," Collected Papers in Heat Transfer 1988, Vol. 2, (K. T. Yang, ed.), ASME, New York, pp. 77-86.

2. J. P. Gore, D. D. Evans and B. J. McCaffrey, 1988, "Temperature and Radiation of Large Methane/Air Jet Flames with Water Suppression," Proceedings of the Twenty-First Fall Technical Meeting of the Eastern States Section of the Combustion Institute, Pittsburgh, PA., pp. 60.1-60.4.

3. J. P. Gore and U.-S. Ip, 1989, "Coupled Radiation Structure Analysis of Acetylene/Air Flames," J. Heat Transfer, submitted.

4. J. P. Gore, S. M. Skinner, D. W. Stroup, D. Madrzykowski, and D. D. Evans, 1989, "Structure and Radiation Properties of Large Two Phase Flames," ASME 1989 Winter Annual Meeting, Session on Combustion of Solids and Liquids, San Francisco, CA, December, 1989.

5. J. P. Gore and U.-S. Ip, 1989, "Temperature Fluctuations in Strongly Radiating Turbulent Flames," Twenty-Second Fall Technical Meeting of the Eastern States Section of the Combustion Institute, submitted.

6. J. P. Gore, S. M. Skinner and U. S. Ip, 1989, "A Study of Simulated Oil Well Blowout Fires," Annual Report for Grant No. 60NANB8D0834, University of Maryland, College Park, sponsored by N. I. S. T., Center for Fire Research, in progress.

7. U. S. Ip, 1989, " A Study of Strongly Radiating Diffusion Flames," M. S. Thesis, University of Maryland, College Park, in preparation.

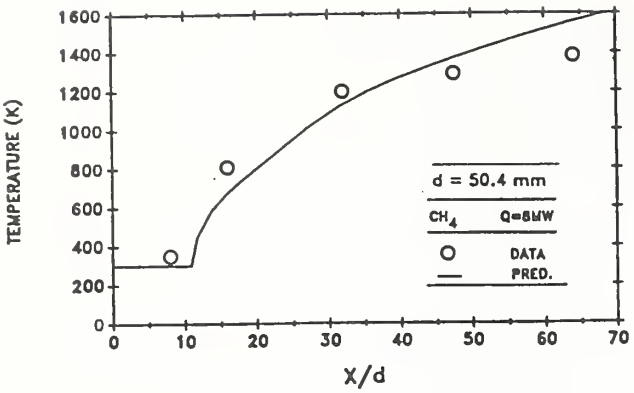

Figure 1: Temperature Profile along the axis of CH_4/Air Flames

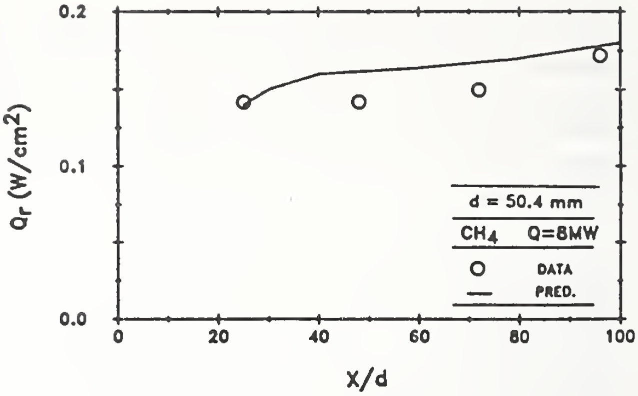

Figure 2: Radiative Heat Fluxes Parallel to the Axis of CH_4/Air Flames

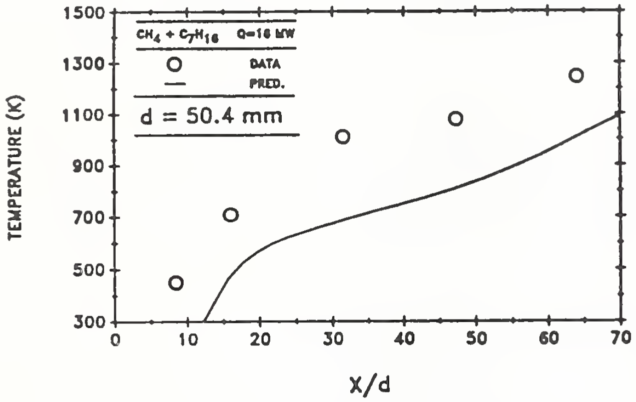

Figure 3: Temperature Profile along the Axis of $CH_4+C_7H_{16}$/Air Flames.

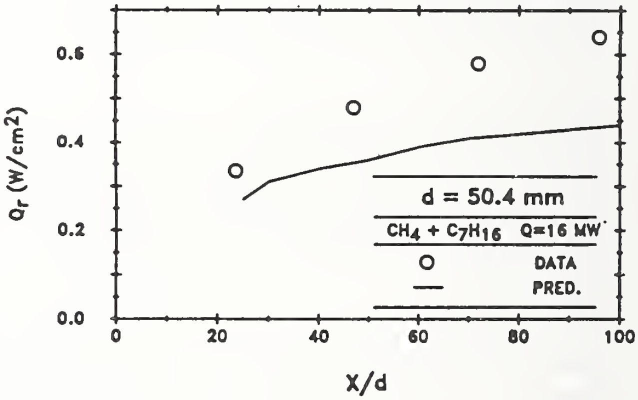

Figure 4: Radiative Heat Fluxes Parallel to the Axis of $CH_4+C_7H_{16}$/Air Flames.

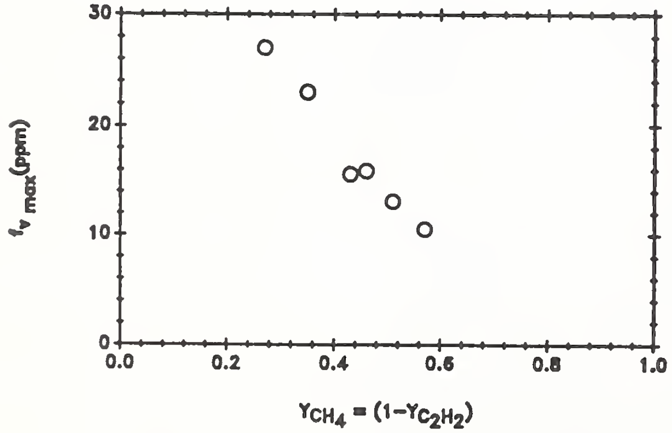

Figure 5: Peak Soot Volume Fractions for $C_2H_2+CH_4$/Air Flames.

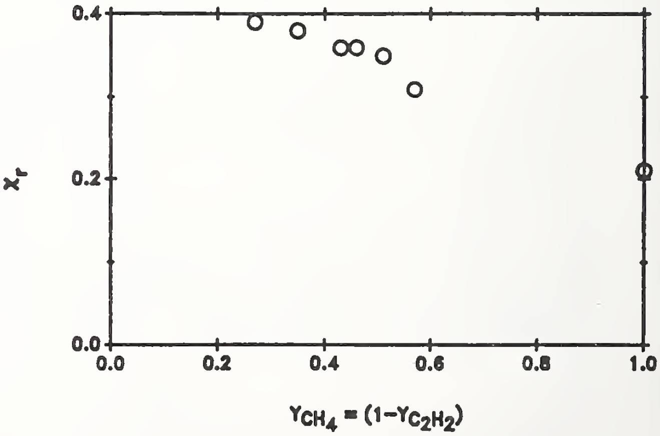

Figure 6: Radiative Loss Fractions for $C_2H_2+CH_4$/Air Flames.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

SPRINKLER RESPONSE

Funding Agency: U.S. General Services Administration
U.S. Fire Administration

Professional Staff: Doug Walton, Project leader
Randy Lawson, Physical Scientist
Kathy Notarianni, Fire Protection Engineer

Project Objective:

To develop an understanding of the response of sprinklers in various mounting configurations and the response of secondary sprinklers in the presence of operating sprinklers.

Technical Accomplishments:

The first phase of this project focuses on the understanding of the response of sprinklers mounted in various configurations. These include varying distances below a smooth ceiling, recessed into a smooth ceiling, and in the sidewall position. All of the sprinkler activation models in use, with the exception of the newly developed LAVENT, assume the sprinkler is mounted at an optimum distance below a smooth ceiling in a large unconfined space. LAVENT can predict the operation of sprinklers mounted at variable distances below a smooth ceiling in spaces confined by draft curtains.

Experiments in this study were conducted in a room approximately 9 by 18 m (30 by 60 ft) with a smooth ceiling height of 2.4 m (8 ft). Ventilation was provided at the ends of the room to simulate a large unconfined space. The fires for the experiments were generated with a propane diffusion burner with steady state heat release rates from 56 to 504 kW. Measurements include gas temperatures as measured with bare bead thermocouples located at various distances below the ceiling and at various radial distances from the fire. Metal disks with known response time indices were used to provide temperatures of simulated sprinkler heat responsive elements. Gas velocities were also measured at selected locations. The response of actual sprinklers were used in selected cases.

The analysis of the test results has not been completed. The preliminary results show that sprinklers located from 25 to 152 mm (1 to 6 inches) below the ceiling are subject to nearly identical heating from the fire. These results are being compared to those predicted with the DETACT and LAVENT models to determine the suitability of those models and to provide corrections for recessed and sidewall sprinklers.

The second phase of this project focuses on the response of secondary sprinklers in the presence of operating sprinklers. With the advent of quick response sprinklers a concern has been raised that the use of these sprinklers could result in the operation of large numbers of sprinklers. If a large number of sprinklers were activated, the water supply to the building could be over taxed resulting in reduced sprinkler performance and the potential for extensive loss. The operation of large numbers of sprinklers has been observed in industrial occupancies with the potential for high heat release rates. This project examines the potential for the operation of large numbers of sprinklers in light hazard occupancies such as office buildings.

Experiments were similar to those in the first phase except that a manually operated sprinkler was used and temperatures were measured on the up and down stream side of this sprinkler with respect to the fire. Although the analysis of the results has not been completed, temperatures on the down stream side of the sprinkler are considerably lower than temperatures measured without the intervening sprinkler operating. Correlations for these temperatures are being developed.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

DYNAMICS AND SPREAD OF LARGE CONFLAGRATIONS

Funding Agency: Defense Nuclear Agency

Professional Staff:
J. Quintiere, Project Leader
T. Ohlemiller, Research Engineer
H. Baum, NIST Fellow
H. Mitler, Physicist

Project Objective:
1) Critically assess the state of knowledge of the dynamics of mass fires
2) Conduct supplemental measurements during a Canadian prescribed burn of logging slash to estimate the heat release rate pattern
3) Develop an integrated report on the Canadian prescribed burn with emphasis on fire dynamics

Technical Accomplishments

Twelve sets of thermocouples were placed within the central region of a Canadian prescribed burn that encompassed some 400 hectares of logging slash. These supplemented similar sets placed by Forestry Canada. In both cases the goals were to obtain measures of the duration of flaming and smoldering phases of combustion as the fire passed through the logging slash. These data are being combined with measurements of the flaming/smoldering areas obtained from aerial infrared cameras to obtain an estimate of the time-dependent overall rate of heat release from this very large fire. This estimate will be utilized in a plume model to test its ability to predict the measured ground-level fire-induced winds. These data and those from several other experimental groups will be integrated to assess the adequacy of our current understanding of the behavior of very large fires.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

FIRE AND THERMAL CHARACTERISTICS OF NAVY FIRE FIGHTING TRAINERS

Funding Agency: Navy Training Systems Center, Orlando, Florida

Project leader: R. S. Levine

Project Objective:

To support the development and implementation of prototype fire fighter trainers at Mayport Naval Station, Jacksonville, Florida, and the Submarine Base at Groton, Connecticut.

Technical Accomplishments:

Using fire compartment models, wall and gas temperatures, radiant fluxes, oxygen concentrations, and ceiling layer heights were predicted for the trainer compartments with large fires in them. Measurements were made during Navy acceptance tests of the prototype trainers, and the results used to validate FIRST9X as a design tool for the sponsor and for related CFR use. A model under development, FPETOOL, will be evaluated.

The upper layer temperatures calculated by the model were similar to those measured near the upper part of the room, but were significantly higher than those measured at trainee head height. In most cases the temperature gradient from floor to near the ceiling was nearly linear. The models assume an abrupt discontinuity.

The project leader participated in a design review meeting to decide changes to the prototype 19F3 trainer for the 25 production trainers.

Measurements will be made on the 21C12 prototype submarine trainer in October 1989 at Groton, CT, and measurements on the 19F1A advanced surface ship trainer will be performed in November 1989.

Reports and Publications:

Most results to date are incorporated in project letters to the Naval Training Systems Center.

NBSIR 88-3755, Stroup, D.W., Naval Fire Fighting Trainers-Thermal Radiation Effects Associated with the 19F4 FFT.

NIST Report of Test FR3979, Levine, R. S., and Rinkinen, W., Fire Tests of the Prototype 19F3 Navy Firefighter Trainers.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

COMPARTMENT FIRE MODEL TO SIMULATE THE EFFECTS 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.

Scope

The scope of the effort is defined by the generic fire scenario depicted in Figure 1. The analysis and the corresponding computer code to be developed will be 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 code will also account for first sprinkler actuation by a fused link and the effect of subsequent sprinkler-spray cooling of the accumulating ceiling-level smoke layer on subsequent

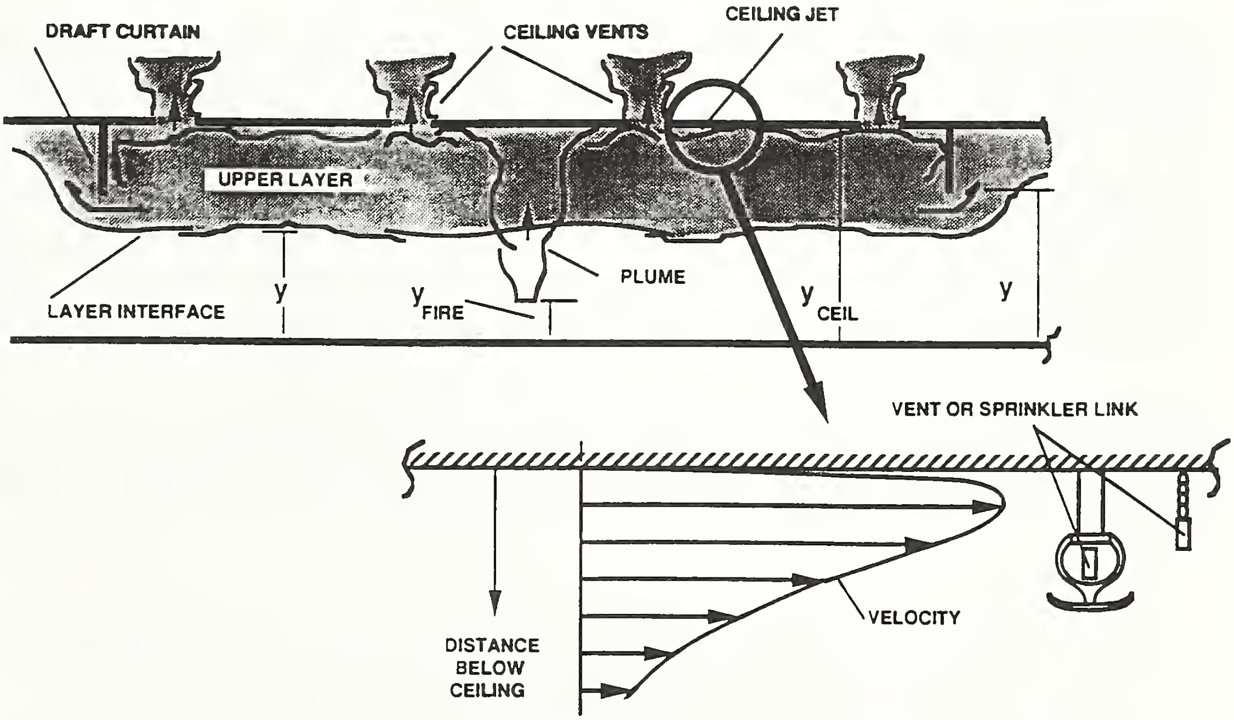

Figure 1. Fire in a building with draft curtains and fusible-link-actuated ceiling vents and sprinklers.

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.

Technical Accomplishments

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 this year. This resulted in the user-friendly computer code LAVENT (Link Actuated Vents) and its comprehensive User Guide [3]. This code implements the model equations developed and presented in [1] and discussed in the overview of [2]. 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.

LAVENT is written in FORTRAN 77. The executable code operates on IBM PC-compatible computers and requires a minimum of 300 kilobytes of memory. The software is available on the CFR computer bulletin board.

Reports and Publications

"Estimating the Environment and the Response of Sprinkler Links in Compartment Fires with Draft Curtains and Fusible Link-Actuated Ceiling Vents - Part I: Theory," Cooper, L.Y., NBSIR 88-3734, National Institute of Standards and Technology (formerly National Bureau of Standards), Gaithersburg, MD, 1988.

"Estimating the Environment and the Response of Sprinkler Links in Compartment Fires with Draft Curtains and Fusible Link-Actuated Ceiling Vents - An Overview," Cooper, L.Y., Proceedings of the 10th Joint Meeting of the UJNR Panel on Fire Research and Safety, pp. 87-91, Tsukuba, Japan, June 9-10, 1988; also Proceedings of the 1988 Annual Technical Meeting of the Eastern Section of the Combustion Institute, Clearwater FL, Dec. 5-7, 1988.

"Estimating the Environment and the Response of Sprinkler Links in Compartment Fires with Draft Curtains and Fusible Link-Actuated Ceiling Vents - Part II: User Guide for the Computer Code LAVENT," Davis, W.D. and Cooper, L.Y., NISTIR 89-4122, National Institute of Standards and Technology, Gaithersburg, MD, 1989.

Related Grants

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 - 1989

FIRE RISK ASSESSMENT

Funding Agency: National Fire Protection Research Foundation

Professional Staff: S. Wayne Stiefel
Richard W. Bukowski

Project Objective

To develop a generally applicable methodology for the proper evaluation of the expected life-safety risk associated with the fire performance of new and existing products.

Technical Accomplishments

The first phase of the project involved the development of a general purpose methodology for quantitative prediction of the fire risk associated with a product. This general method was then tested against a diverse set of three products and occupancies (these were upholstered furniture in residences, carpet in offices, and wire insulation in hotels). The experience gained was used to identify refinements in the method for resolution in phase 2.

The second phase of the project was completed this year. A fourth case study was completed (interior finish in restaurants) to examine the defined method and to test the model cap;abilities on another physical situation of significant interest (flame spread on walls). Also, a large number of sensitivity analyses were performed to examine key data and assumptions. Some simplifications identified in this process which allow a more efficient operation without sacrificing detail or accuracy were incorporated into the method. Finally, the resulting methodology and the four case studies addressed with it were documented in reports. These reports have been submitted to the sponsor for eventual release as NFPRF documents.

The third and final phase of the project is yet to be undertaken. In this work, a Users' Guide to the software developed to implement the methodology should be prepared as a companion document to the software itself. This should be made available on tape for specific mainframe computers.

Related Grant

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

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY89

Institution: University of California, Los Angeles

Grant No.: 60NANB6D0647

Grant Title: Fire Risk Analysis Methodology

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Technical Abstract:

The objective of this work is to develop probabilistic models to characterize phenomena which occur during a building fire scenario (primary ignition, detection, suppression, secondary ignition) and to integrate them with the current state of the art in building fire risk analysis. We recently completed the development of a methodology for the assessment of the frequency of ignition of a consumer product. Deterministic thermal models of the heat transport processes are coupled with parameter uncertainty analysis of the models and with a probabilistic analysis of the events involved in a typical scenario. This leads to a distribution for the frequency of ignition for the product. Work is currently in progress on the development of probabilistic models for secondary ignition.

Methodology:

The frequency with which a fire begins is an important input to the analysis of a fire scenario. For many building/room/material combinations, fire occurrence data give us various statistics to work with, including the frequency of primary fire ignition involving the material. However, when a new product is introduced and analysis is being performed on a scenario involving it, the applicability of statistics which describe other materials is subject to doubt. This is because physical/chemical/thermal changes in the material may cause it to become either easier or more difficult to ignite. The pertinent question then is how would these numbers change if a product's "ignitability" were to change. If we define ignitability as the probability of ignition of the item given exposure to the ignition source (fr(ig/exp)), and define fr(exp) as the frequency with which the product is `exposed' to the source, we have the frequency of ignition of the product given as:

$$fr(ignition) = fr(exp)\ fr(ig/exp)$$

The value of fr(ig/exp) will be the result of physical modeling and experimental evidence for both old and new products. For the status quo, we have data on fr(ignition), but not on fr(exp). For a new product, we have neither fr(ignition) nor fr(exp) and in reality, it is fr(ignition) for the new product case which we wish to assess (to compare with the status quo value).

The value of fr(exp) can be interpreted in one of two ways. These interpretations involve the exposure intensity and duration. The intensity is important since for most materials, there is some minimum intensity of exposure below which the material will not ignite (e.g., a 100W light bulb may ignite a piece of tissue dropped on it, but not a piece of wood in contact with it). Duration is important for all scenarios since even a very intense source may not cause ignition, if it is only briefly exposed to the product (e.g., someone places a cardboard pizza box on an electric burner, quickly realizes his mistake and removes it). Thus, the two possible interpretations of fr(exp) are as follows:

1. The frequency with which the product is exposed to the ignition source for any length of time or intensity of exposure.

2. The frequency with which the product is exposed to an ignition source of adequate intensity and duration to cause ignition (product dependent).

In 1), the ignition source intensity and duration information will have to be combined with Pr(ig/exp) in a meaningful way. In 2), an analysis would have to be performed to screen out any non-significant events.

A significant portion of fires in the U.S. are caused by fixed or portable area heaters igniting combustible items. As an example of analyzing a primary initiating event, this is the type of ignition source we have considered. "Fixed or portable area heaters" consist of several different forms and fuel types. Fuels can be gas, liquid, solid or electric. Solid fuels are almost exclusively wood, liquid fuels are dominated by kerosene, and gas is usually propane or natural gas. Fixed heaters range from small electric wall or baseboard units to medium/large wall gas units, to (normally wood-fueled) wood-stoves and fireplaces. Portable heaters are usually small (hence portable) and either electric or liquid fueled.

Inherent in a fire scenario is the knowledge that somehow an ignition source (our heater) transferred enough heat to some item to cause that item to begin burning (to ignite). Given a particular target item and ignitor (as well as building type, room, etc.), statistics exist (NFIRS, NFPA) on the frequency with which an ignitor caused a fire by igniting that item. Obviously, at a higher level, the number of fires caused by the ignitor igniting any item is also available. In many instances there is also information on how the ignitor came to ignite the item. Thus, we know, for the status quo products and ignition sources, a variety of statistics on the `average' time rate of occurrence of fires involving them.

The methodology for the estimation of the distribution of f(ig/exp) proceeds as follows:

1. Select a piece of furniture from the set of furniture by sampling from the relevant distributions describing the thermophysical properties of the furniture covering and padding (surface emissivity, ignition temperature, thermal conductivity, specific heat, and density).

2. Select a heater type and the physical characteristics of that heater from the relevant distributions for the different types of heaters.

3. Select the physical placement of the piece of furniture with respect to the heater within the critical area using the uniform or triangular distribution assumption discussed above.

4. Using the computer code that has been developed under this grant, calculate the thermal response of the furniture cushion and see if and when the ignition temperature is exceeded. If it is exceeded, then this scenario contributes an ignition to the f(ig/exp) calculation for this piece of furniture.

5. Using the same description of the piece of furniture, repeat steps two through four to generate another ignition/non-ignition trial.

6. After a suitable number of trials, the number of ignitions observed divided by the number of trials is an estimate of the f(ig/exp) for this piece of furniture.

7. Repeat steps one through six to generate another estimate of f(ig/exp) for another piece of furniture from the set of furniture. Repeat this for a suitable number of pieces of furniture and thus generate a set of estimates for f(ig/exp) for the set of furniture throughout the U.S. with the cover fabric that we are analyzing. This set of values is a sample from the state-of-knowledge uncertainty distribution of f(ig/exp) for the set of furniture. Thus, from this sample, we form the distribution of f(ig/exp).

Details of the methodology are described in the report entitled "Fire Risk Analysis Methodology: Initiating Events" by Brandyberry and Apostolakis (NIST-GCR-89-562), published in March, 1989. Current efforts are directed toward the development of models for secondary ignition.

CENTER FOR FIRE RESEARCH
OTHER AGENCY PROJECT - 1989

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 knowledge based system (or expert system) EXPOSURE was nearly completed. EXPOSURE offers 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 buildings 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 shows the single line floor plans and the wall elevation view.

Reports and Publications

"Expert Systems Applied to Spacecraft Fire Safety" by Richard L. Smith and Taskashi Kashiwagi, NASA Contractor Report 182266, June 1989

"Maximum Radiation at Various Regions of a Vertical Wall Due to N-Openings in a Wall of a Burning Building" by Richard L. Smith NISTIR in process.

APPENDIX

ALPHABETICAL LISTING OF CENTER FOR FIRE RESEARCH GRANTS

NBS-114A (REV. 2-80)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** *(See instructions)*	1. PUBLICATION OR REPORT NO. NISTIR 89-4188	2. Performing Organ. Report No.	3. Publication Date October 1989

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"Summaries of Center for Fire Research In-House Projects and Grants - 1989"

5. AUTHOR(S)

Sonya M. Cherry (Editor)

6. PERFORMING ORGANIZATION *(If joint or other than NBS, see instructions)*

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE
GAITHERSBURG, MD 20899

7. Contract/Grant No.

8. Type of Report & Period Covered

Final Report

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS *(Street, City, State, ZIP)*

10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

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 FY1989.

12. KEY WORDS *(Six to twelve 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

13. AVAILABILITY

☒ Unlimited
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