FUNDAMENTALS OF SOOT FORMATION IN GAS TURBINE COMBUSTORS

Final Report
November 15, 1997 to November 14, 2000

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Principal Investigators:
Meredith B. Colket and Robert J. Hall

Co-Investigator:
David Liscinsky

United Technologies Research Center
Silver Lane, E. Hartford, CT 06108

Prepared with assistance from
M. D. Smooke
Yale University

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J. M. Tishkoff
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6. AUTHOR(S)
Meredith B. Colket, Robert J. Hall, David Liscinsky & Mitchell D. Smooke

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
United Technologies Research Center
411 Silver Lane
E. Hartford, CT 06108

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13. ABSTRACT (Maximum 200 words)

In this three year effort, particle extraction methods were evaluated for collecting soot particulates from sooting flames and significant enhancements to the models for physics of soot formation were developed. Through comparisons to the UTRC data as well as data obtained separately at Yale University, the models provided a reasonable simulation of physical phenomena related to soot production in flames. Four different techniques for characterizing soot were evaluated and compared including TPD, TEM, laser extinction, and electrical mobility. Evaluation of the last method led to an extension to quantitative measurements of soot emissions from military combustors. Advancements to the soot model include new PAH growth models, a revised particle inception model and more realistic treatment of soot particle physics. The detailed soot model aided development of a simplified code shown to be useful in modeling soot emissions in gas turbine combustors. This final report very briefly reviews the accomplishments of this program and includes some recent work performed in the last quarter on evaluating the effects of self-absorption on the temperature along the centerline of a coflow flame.

14. SUBJECT TERMS
Coflow laminar diffusion flames, premixed, sooting flames, soot formation, soot modeling, flame and soot diagnostics, particle agglomeration, soot inception, radiation

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I. Objectives

The initial objectives of this work were to obtain necessary fundamental data and to enhance and then validate modeling procedures in order to support modeling of soot production in practical gas turbine combustors. Several focused tasks of this effort include (1) extending measurements of surface growth rate constants to high temperatures, characteristic of rich zones in advanced combustors; (2) modeling of steady, laminar diffusion flames with different fuels to assist in validating the models; (3) advancing the modeling capabilities for describing known physical processes involved in soot production, including carbonization, ageing, and aggregate formation to enable more reliable extrapolation of existing models; (4) modeling of sooting, transient flames to offer some physical understanding of processes controlling soot formation and destruction in turbulent, diffusion flames; and (5) examining the use of a mobility particle sizer for measurement of particle size and quantity of soot.

II. Status of Effort

Significant accomplishments from this three-year effort include evaluation of experimental methods at UTRC for applications to measurements in sooting flames and advancements of modeling methods relative to predicting soot production in flames. In particular, extraction methods have been evaluated for collecting soot particulates from flames and significant enhancements to the models for physics of soot formation have been developed. Through comparisons to the UTRC data as well as data obtained separately at Yale University, the models have been shown to provide a reasonable simulation of physical phenomena related to soot production in flames. A main issue still unresolved is the accurate simulation of soot formation along the centerline of a coflow flame. Due to the extra effort focused in the hopes of resolving this issue and to our concern for applying the inexact model to transient processes, the modeling of transient processes in soot-forming flames has not been completed. This final report very briefly reviews the accomplishments of this program and includes some recent work performed in the last quarter on evaluating the effects of self-absorption on the temperature along the centerline of a coflow flame.

III. Accomplishments/New Findings

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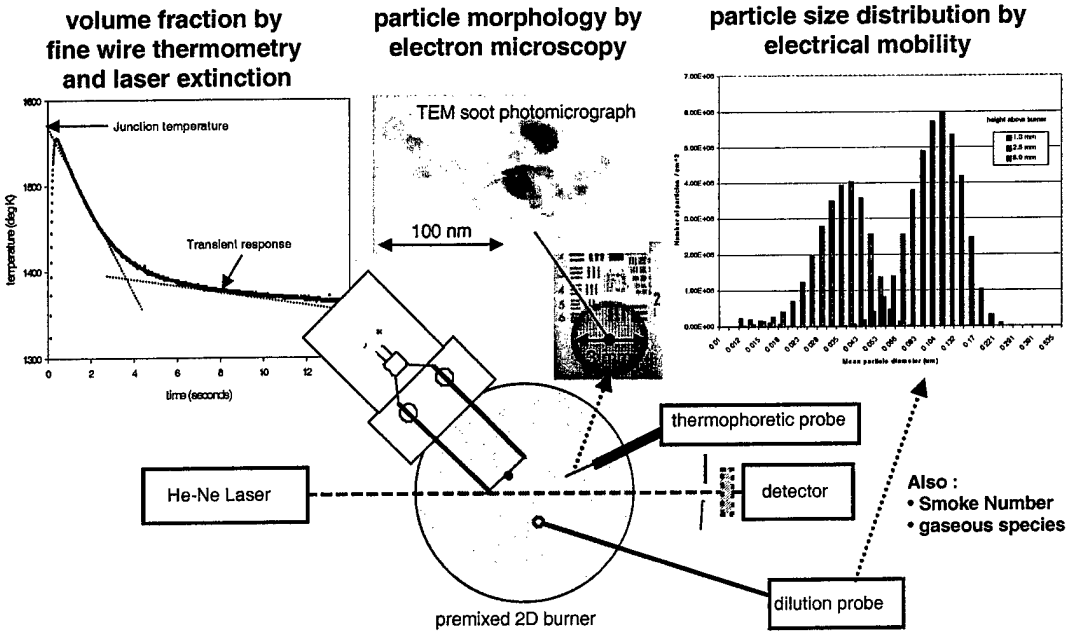
A. Particulate Measurements in Flames and Surface Growth Rates at High Temperatures

An important parameter for the prediction of soot production is the surface growth rate. Virtually all fundamental and reliable measurements of this parameter have been obtained over the temperature range of 1500-1950K. Yet for high performance gas turbine combusters the 'sooting' rich zone will be at temperatures well in excess of 2000K. In the current study, a series of fuel-rich, laminar premixed flames was examined. A variety of burner configurations was examined, including on a custom hastalloy burner containing 513 x 1.2mm diameter holes spaced 2.0mm (with 28% open area) surrounded by a co-flow. Also, several porous plug burners were examined; these burners provided more uniform flame structures, but the finest pore sizes suffered from leakage around the edges due to increased pressure drop. Four separate experimental techniques have been used for gathering information on soot particle growth. A schematic of the experimental set-up is provided in Figure 1.

Figure 1. Flame Laboratory with Diagnostics Set-up for Particle Characterization



Soot diagnostics include thermocouple particle densitometry (TPD); laser extinction (LE); transmission electron microscopy (TEM); and differential mobility. The first two of these methods provide soot volume fraction, TEM provides primary particle size and agglomerate structure, and the last provides information related to particle (agglomerate) size distribution and particle number density. This latter system utilized a Scanning Mobility Particle Sizer (SMPS) for classification of particles based on aerodynamm diameters (equivalent diameter of a charged spherical particle drifting through an E-field) and a Condensation Nuclei Counter (CNC) for particle counting, following extraction of particle-laden flame gases using a dilution probe. Using literature correlations for agglomerated particles [1,2] and definitions for the aerodynamic diameter [3], we have derived equations to convert data from the SMPS/CNC system into Feret's diameter for agglomerated particles and the soot volume fraction. Diameters of primary particles are needed and available from the TEM results. A SMPS/CNC system with sample analysis times of 90 s is attractive for use in combustor/rig environments in which sampling time is at a premium.

Volume fractions determined as a function of height in an ethylene/O2/Ar flame with C/O=0.80 from the three techniques (TPD, LE and SMPS/CNC) compare within a factor of two to each other and to other results [4] for the same flame. The SMPS/CNC data are slightly low, due to loss of particles in the sampling process. The TPD method is preferred; it is a point measurement and provides information on temperature as well. The largest uncertainty is in the deposit 'void' fraction, which we determined experimentally. The value of this parameter is high (~0.1) near the flame front location, but decreases rapidly to a constant value near 0.023 in the post-flame region. Details of this work are provided in [5,6].

Measurements have been obtained in several flames, although the goals of collecting data at and above 2000K have not been achieved due to poor flame structure. High flow rates are required to minimize loss of energy via conduction to the burner due to high adiabatic flame speeds. The existing data have been analyzed to examine the cause of the known rapid decay of surface growth rates from the 'young' soots to the 'aged' soots. Primary mechanisms examined are (1) decay of superequilibrium H-atoms, (2) surface aging, and (3) loss of PAH species (reservoir of surface growth species) produced near the flame front. Interpretations are incomplete, but we have been as yet unable to explain our data based on (1) or (2). A more accurate PAH production model should help resolve this problem.

B. Models for Soot Inception

Detailed submodels for the inception, growth, oxidation, and dynamics of soot particulates, as well as effects of radiation, are included in the model. Inception rates used in the most of the papers published under this program were computed using steady-state expressions for the formation of naphthalenyl radical and phenanthrene; the expressions are based on presently understood reaction mechanisms and local concentrations of gas-phase species, (i.e., H, H_2, C_2H_2, phenyl, etc.). Several advancements to this inception model have been explored. In particular, the objective of this exploration was to resolve the issue of the underpredictions of soot along the centerline of coflow flames (see [7-9]).

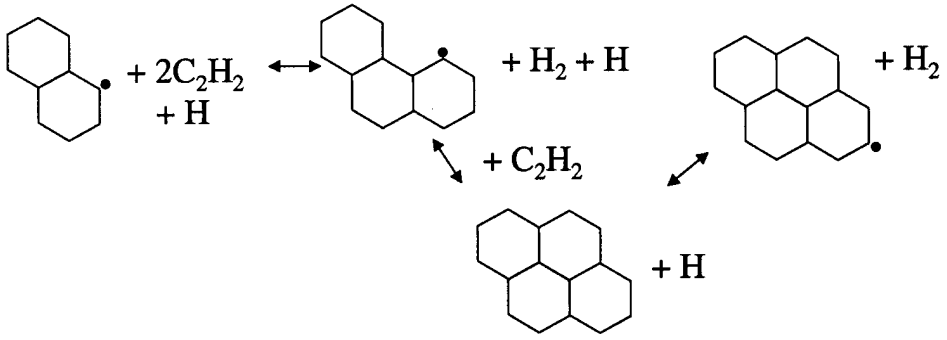
To test the possibility that another mechanism dominated polycyclic aromatic growth and soot inception along the centerline of the flame, four alternative PAH growth mechanisms recently promoted in the literature were considered. The reversible mechanisms include: (A) naphthalene formation via combination of benzyl and propargyl; (B) naphthalene formation via combination of cyclopentadienyl, (C) a reaction sequence involving vinylidene addition to the benzene ring; and (D) naphthalene formation via sequential addition of acetylene to phenyl but incorporating an H-atom shift in the intermediate adduct [10]. For each of these sequences, steady-state expressions were computed for the ethylene coflow flame [8] and net rates calculated at several different heights along the burner using the computed gas temperatures and local concentrations. Several other reaction sequences were investigated, including reactions initiated with phenyl-toluene combination. In general, these rates were very low at least for the ethylene system. The relative rates of this latter sequence and that of sequence (A) listed above increase substantially in the methane flame in which there is ready access to methyl radicals.

None of the reaction sequences approached the rate of production achieved by the original mechanism, except reaction sequence (D) is faster in the center of the flame, at heights below the main heat release and rapid soot production. Nevertheless, the absolute production rates at this location are very low so it is questionable whether sequence (D) can explain the underprediction of soot formation along the

centerline. However, the high relative inception rates along the centerline were consistent with the phenomena we were trying to reproduce. Hence, we added an inception rate term, following sequence (D), into the coflow code. The differences in the computed soot field were noticeable, but small.

An alternate approach was also investigated. In this sequence, instead of the presumption that naphthalene and phenanthrene lead directly to inception (a recognized weakness of the model), steady-state expressions have been derived for the formation of a high molecular weight condensed polycyclic aromatic hydrocarbon (PAH). Essentially, the model is based on subsequent growth analogous to the surface growth mechanisms:

Figure 2. Reaction Sequence for Growth from Naphthalene to Pyrene



Overall, the reaction can be written $C_{10}H_7 + 3C_2H_2 \Leftrightarrow C_{16}H_9 + 2H + H_2$. This sequence can be continued to form yet larger PAH structures with the overall balance of $C_{10}H_7 + 3nC_2H_2 \Leftrightarrow C_{10+2n}H_{7+2n} + 2nH + nH_2$. The assumption that all PAH intermediate species (including $C_{10}H_7$) rapidly attain steady-state concentrations leads to the conclusion that $\frac{d[C_{10+2n}H_{7+2n}]}{dt} \approx \frac{d[C_{10}H_7]}{dt}$. The latter is estimated using previously derived expressions [7]. Limitations to the use of this expression are related to (1) side reactions that may remove critical intermediate species from the reaction sequence and (2) the time it takes to achieve steady-state concentration levels. Utilization of this approximate reaction sequence for initiation has an effect similar to that of preventing coalescence for small particle sizes (<1nm). This approach has provided slightly better simulations of the experimental data and is preferred for use in future modeling, until a refined, validated PAH formation model has been developed.

C. Modeling the Growth and Oxidation of Soot Aggregates

The sectional soot formation model to describe the formation of soot aggregates has been extended considerably, and its application to premixed flames has been studied. The previous model dealt only with coalescing soot spheroids, and was not capable of describing the observed tendency of soot particles to form aggregates of small primary spheroids late in the soot growth process. The new computer model, which is based on an extension of the DISGLOM model [11-12], represents a significant increase in calculational sophistication. The aggregation process is important in soot formation because it affects the particle surface area available for growth, and it is now possible with these improvements in the algorithm to have a much more realistic description of the growth process. Three types of particles are now treated: incipient or nascent particles which are placed in one or more

discrete bins, liquid-like coalescing spheroids which are placed in sectional bins in a way similar to the previous model, and solid sections which consist of chain-like aggregations of small primary particles. The transition from liquid to solid particles occurs at a particle diameter that is an input item. The DISGLOM code did not have provision for surface growth and oxidation arising from gas phase species, and coefficients for these processes were added. Problems with the primary particle balance in the original program were also corrected. Within an aggregate section, particles of differing primary particle populations are allowed, but all primary particles within a bin are assumed to be the same size. These primary particles can grow by the conventional acetylene-driven surface growth processes, and also by coalescence with the smaller liquid particles. All collisional processes are now modeled as coalescence or coagulation processes with sticking probabilities that can be independently specified, and there is provision for continuum effects, so the program will be valid for high pressure soot growth as well. It is possible to specify a maximum primary spheroid size beyond which all growth processes affecting the primary spheroids are shut off. This feature represents a heuristic method for modeling surface ageing effects and the tendency of primary spheroids to reach maximum sizes largely independent of the type of flame and fuel.

The aggregate model features are illustrated with an application to the premixed ethylene flames of Harris and Weiner [13]. Profiles of temperature, velocity, and growth/oxidation species concentrations were generated using CHEMKIN. These profiles have been used to generate new soot growth predictions for these flames on a post-processing basis, assuming that soot growth scrubbing of gas phase species and temperature depression by radiative loss are small. Previous studies were based on the assumption that benzene formation determined the rate-limiting step in nucleation; these calculations are based on the nucleation/inception model in which a two-ring aromatic species of mass 127 amu. ($C_{10}H_7$) is the nucleation species (see Ref. 14). One discrete bin of this mass was included. Five liquid bins terminating at $D_0 = D_{max}$ (e.g., 20 nanometers diameter, where solidification was assumed to begin, were included, followed by seven aggregate bins terminating at a sphere-equivalent diameter of about 1000 nanometers. Two flames were modeled, with C/O ratios of 0.80, and 0.94. A surface growth rate was employed that is consistent with that reported in Ref. 13. The simulations were first carried out assuming no restriction on the size D_{max} of the primary spheroids. Significant divergence is observed between experiment and theory in the richer flame beginning at the point where aggregates start to occur, with the model significantly over predicting at the top of the flame. This arises because no surface area destruction occurs with solid aggregates as a result of coagulation, unlike the case for liquid-like particles. For the solid aggregates, surface area increases due to acetylenic surface growth, and the volume fraction grows more rapidly than is observed. The decay of surface growth rate with decreasing temperature at the top of the flame (31.8 kcal activation energy assumed) is insufficient to explain the fall-off in growth. The discontinuity in the growth curves arises from the unrealistic assumption that surface growth truncates sharply at D_{max} = 20 nanometers; in reality there would be a smoother variation with primary particle diameter. For the C/O=0.80 flame the effects are less pronounced because the particles remain predominately in the 'liquid' sections, with the aggregation effects less important. This procedure is felt to be reasonable in view of the uncertainties surrounding the spheroid size at which aggregation begins, and the way surface reactivity decays with particle age and provides a better agreement to the experimental data over a wide range of conditions.

Additional details of this portion of the effort are provided in [15].

C. Soot Predictions in CoFlow Flames

A noticeable discrepancy between our previous model predictions and the experimental data for both the coflow diluted, methane and ethylene flames [7,8] is the underprediction of soot mass along the centerline of the burner. Part of this underprediction is an incomplete PAH formation mechanism, as suggested previously. Possible explanations for the discrepancy have been analyzed in [16] and include the number of soot 'sections' utilized in our aerosol equations, particle ageing, and trade-offs between particle surface growth and inception rates. The applicability of our model to other flame parameters has also been investigated. In particular, predictions from our model [9] were compared to new data obtained under separate support for simulating the effects of variable fuel-dilution on the soot field and flame structure. The predictions utilize a modified version of the surface growth model utilized in [17]. The importance of a surface growth model that simulates the decay in growth rates with increasing flame temperatures (above 1900K) was demonstrated in the simulations presented in [18].

Modifications to the soot model have been tested. The most effective were (1) termination of surface growth at a predetermined diameter (e.g., about 30nm), (2) reducing the activation energy for surface growth to zero, and (3) cessation of coalescence at a predetermined size. Agreement with the experimental data set is much improved. The low activation energy for surface growth is unusual, although it has been reported for an acetylene diffusion flame [19]. In general, the agreement between the model and experiments is much improved.

Thermal Radiation Optical Thickness Corrections

It is commonly assumed that thermal radiation from small diffusion flames is emission-dominated, i.e., that the flames are in the optically thin limit. The calculation of the local radiative energy loss rate in this limit depends only on local temperature and species concentrations, and can be of such a magnitude as to significantly depress local gas temperatures [7,8,14]. Calculated temperatures lower than those measured, as have been observed in these investigations, might be caused by overestimation of this radiative loss. In principle, some reabsorption of thermal emissions can occur, particularly on or near the centerline, which receives emissions from all surrounding regions of the flame. This optical thickness effect acts to reduce the net rate of thermal radiation energy loss. To test whether this effect might be the cause of our centerline temperature underpredictions, calculations of the local rate of reabsorption were undertaken. This energy sink rate was then employed as a correction term in the flow energy equation.

The calculation used the "discrete transfer" method of Lockwood and Shah [20]. The algorithm fires rays into the interior of the flame from all calculation boundary surfaces. The path of each ray is registered, and then a line-of-sight, path-integrated calculation of radiative flux is performed using RADCAL, a narrow-band radiation model that includes both gas and soot emissions and allows for path inhomogeneities [21]. Subtracting the known optically thin emission rate from the flux divergence calculated in the program yields the local net rate of radiative reabsorption.

For the reference flame (with 32% ethylene/68% nitrogen flowing from the central tube), the optical thickness correction reduced net radiative emission along the centerline significantly, by about 33%. However, this reduction in energy loss rate translated into only about 15K increase in centerline temperature. We conclude that optical thickness effects, while more significant than initially expected, are not the cause of the approximately 100K discrepancy between experimental and theoretical temperatures along the centerline.

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IV. Personnel Supported

Key personnel contributing to this project are:
Dr. Meredith B. Colket, III of United Technologies Research Center

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Mr. Robert J. Hall of United Technologies Research Center
Mr. David S. Liscinsky of United Technologies Research Center
Dr. Anuj Bhargava of United Technologies Research Center
Professor Mitchell D. Smooke of Yale University

V. Publications

C. S. McEnally, A. M. Schaffer, M. B. Long, L. D. Pfefferle, M. D. Smooke, M. B. Colket, and R. J. Hall, "Computational and Experimental Study of Soot Formation in a Coflow, Laminar Ethylene Diffusion Flame," Twenty-Seventh Symposium (International) on Combustion, The Combustion Institute, pp.1497-1505, 1998.

M. D. Smooke, C. S. McEnally, L. D. Pfefferle, R. J. Hall, and M. B. Colket, "Computational and Experimental Study of Soot Formation in a Coflow, Laminar Diffusion Flame," Combustion and Flame, Vol. 117, pp.117-139, 1999.

C. S. McEnally, L. D. Pfefferle, R. K. Mohammed, M. D. Smooke, and M. B. Colket, "Mapping of Trace Hydrocarbon Concentrations in Two-Dimensional Flames Using Single-Photon Photoionization Mass Spectrometry", Analytical Chemistry, Vol. 71(2), pp. 364-372, 1999.

C. S. McEnally, L. D. Pfefferle, A. M. Schaffer, M. B. Long, M. D. Smooke, R. K. Mohammed, M. D. Smooke, and M. B. Colket, "Characterization of a Coflowing, Methane/Air Nonpremixed Flame with Computer Modeling, Rayleigh-Raman Imaging, and On-Line Mass-Spectrometry." To be published in the Twenty-Eighth Symposium (International) on Combustion, Vol. 28, 2001.

M. D. Smooke, R. A. Yetter, T. P. Parr, D. M. Hanson-Parr, M. A. Tanoff, M. B. Colket, and R. J. Hall, "Computational and Experimental Study of Ammonium Perchlorate/Ethylene CounterFlow Diffusion Flames." To be published in the Twenty-Eighth Symposium (International) on Combustion, Vol. 28, 2001.

Meeting Proceedings:
D. Liscinsky, M. Colket, B. True, R. Hall, A. Bhargava, "Growth of Soot Particulates in Laminar, Premixed flames", Combustion and Physical Processes of Combustion, pp. 340-343, NCSU, 1999.

M. D. Smooke, M. B. Colket, and R. J. Hall, "Toward Quantitative Modeling of Soot Formation in CoFlow Diffusion Flames, " Combustion and Physical Processes of Combustion, pp. 344-347, NCSU, 1999.

R. J. Hall and M. B. Colket, "Calculations of Soot Aggregate Growth and Oxidation Using a Sectional Size Representation" Combustion and Physical Processes of Combustion, pp. 348-351, NCSU, 1999.

D. S. Liscinsky, M. B. Colket, R. J. Hall, A. Bhargava, B. True, and S. Morford, "Comparison of Particulate Sizing Techniques in Sooting Premixed Flames," AIAA 2000-0954, 38th Aerospace Sciences Meeting, Reno, NV, 2000.

Copies of each of the above documents have been provided as appendixes in the annual reports and are also available in the literature and hence are not duplicated here.

VI. Interactions/Transitions

VI. A. Meetings

Personnel supported by this contract attended:

1. 19th Annual Combustion Conference for the Office of Basic Energy Sciences, Dallas, TX, March 29-April 1, 1998.
2. 27th International Symposium on Combustion in Boulder, August 2-7, 1998.
3. 37th Aerospace Sciences Meeting in Reno, NV on January 11-14, 1999.
4. First Joint Meeting of the United States Sections of the Combustion Institute at the George Washington Institute in Washington, D. C., March 14-17, 1999.
5. Advanced Gas Turbine Systems Research, Combustion Workshop IV at the Virginia Polytechnic Institute in Blacksburg, VA, on April 19-21, 1999.
6. Atmospheric Effects of Aviation Meeting at Virginia Beach, VA, April 21-22, 1999.
7. Fall Technical Meeting of the Eastern States Section of the Combustion Institute, at Rayleigh, NC, on October 10-13, 1999.
8. 38th Aerospace Sciences Meeting in Reno, NV on January 10-13, 2000
9. 21st Annual Combustion Conference for the Office of Basic Energy Sciences of the Department of Energy, Chantilly, VA, May 30-June 2, 2000
10. 28th International Symposium on Combustion, held in Edinburgh, Scotland. July 30th – August 4th
11. Advanced Gas Turbine Systems Research, Combustion Workshop V in Berkeley, CA, September 2000.

Special seminars were given by the Program Manager, including:
"Particulate Emissions from AeroEngines: Measurements, Modeling and Future Concerns" on September 22nd, 1998 at Cornell University.

"Mechanisms and Models of Soot Formation" at University of Connecticut on September, 26th, 2000, at Cabot Corporation on Dec. 1st, 2000 and Worcester Polytechnic Institute, on January 25th, 2001.

VI. B. Advisory Functions

Mitch Smooke and Med Colket are members of the NASA Discipline Working Group in Combustion.

Mitch Smooke is Editor in Chief for Combustion Theory and Modeling.

In December, 1998, Med Colket participated in the final review of the "Assessment of the Effects of High-Speed Aircraft in the Stratosphere - 1998," NASA/TP-1999-209237.

Med Colket contributed to the Workshop on Research Needs for Air Quality Compliance on June 2-3, 1999 sponsored by the American Academy of Environmental Engineers and the Strategic Environmental Research and Development Program (SERDP) in support of program planning for SERDP.

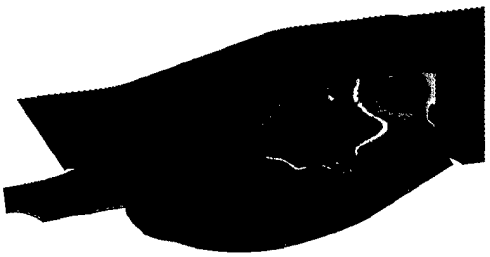
Med Colket was a member of the Committee of Visitors, for the Chemical and Transport Systems Division of NSF, 2000.

VI. C. Transitions

Med Colket developed a simplified, computationally fast (Phase I) algorithm for soot/smoke formation in a gas turbine engine and transferred it to Pratt and Whitney (Dr. Saadat Syed) for installation into a CFD design code. In addition, he has refined a previously developed model for predicting equilibrium temperatures during combustion in vitiated air streams. Also, he participates on design/development teams at Pratt and Whitney for validation of a CFD code for combustor and augmentor applications.

Based on AFOSR-sponsored research, Med Colket updated a simplified, computationally fast (Phase IIA) algorithm for semi-quantitative predictions of smoke formation in a gas turbine engine and transferred it to Pratt and Whitney (Dr. Saadat Syed) for installation into a CFD design code. Also, Med Colket modified and delivered a detailed chemical kinetics mechanism for treating fuel-rich chemistry and preprocessing routines for use in a combustor design code for treatment of kinetically-limited processes. An example of predicted soot production in the new PW6000 combustor is shown in the following figure.

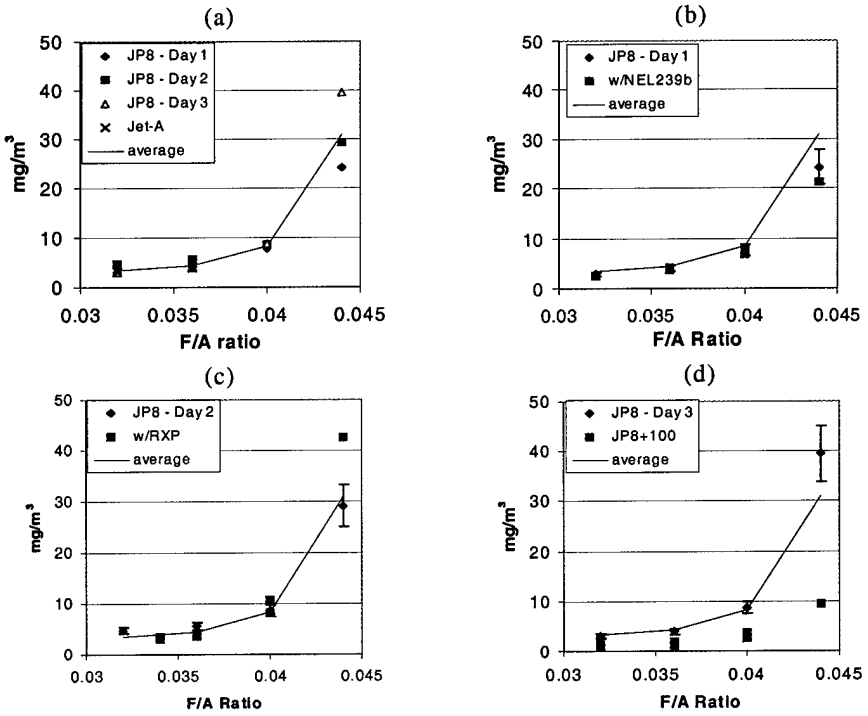
Figure 3. Predictions of Soot Evolution in a PW6000 Combustor



CFD Model of Soot Contours

Dave Liscinsky and Med Colket have applied the soot/particle diagnostic methods refined under this AFOSR program to a AF/UTC DUST program to make quantitative measurements of soot particles emitting from a F119 simulated burner and to identify fuel additives that reduce soot emissions by 60%. This information has been transmitted to Don Phelps and Mel Roquemore of the Air Force Research Laboratories. For inlet conditions of 200psia and 500F, estimated soot mass from a series of JP-8 runs (along with Jet-A) are shown in Figure 4a and compared to comparable results using a series of fuel additives in Figs 4b-d. The results strongly suggest a significant reduction in soot mass when burning JP8+100.

Figure 4a-d. Additive Effects on Emissions of Soot Mass from Simulated F119 Burner.



VII. Record of Inventions

There were no inventions during this reporting period. (DD Form 882, Interim Patent Report to be submitted under separate cover)

VIII. Honors/Awards

M. Colket, as a member of a CFD development team, has been nominated and was a finalist for the 1998 Pratt and Whitney Leadership Award.

Mitch Smooke was elected a Fellow in the Institute of Physics in 1999.

Med Colket received a 2000 AIAA Best Paper Award by the AIAA Terrestrial Energy Systems Technical Committee for a paper entitled *Comparison of Measurements and Predictions of Flow in a Gas Turbine Engine Fuel Nozzle*, presented the at 38th Aerospace Sciences Meeting, AIAA 2000-0331, Reno, NV, Jan. 2000.

Principal Investigator Annual Data Collection (PIADC) Survey Form

NOTE: If there is insufficient space on this survey to meet your data submissions, please submit additional data in the same format as identified below.

PI DATA

Name (Last, First, MI): Colket, Meredith B. III

Institution: United Technologies Research Center

Contract/Grant No: F49620-98-C-0008

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Project/Subarea
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NX _____

FY _____

NUMBER OF CONTRACT/GRANT CO-INVESTIGATORS

Faculty _____ Post Doctorates_____ Graduate Students_____ Other_____

PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

NOTE: List names in the following format: Last Name, First Name, MI

Include: Articles in peer reviewed publications, journals, book chapters, and editorships of books.

Do Not Include: Unreviewed proceedings and reports, abstracts, "Scientific American" type articles, or articles that are not primary reports of new data and articles submitted or accepted for publication, but with a publication date outside the stated time frame

Name of Journal, Book, etc: Twenty-Seventh Symposium (International.) on Combustion

Title of Article: Computational and Experimental Study of Soot Formation in a Coflow, Laminar Ethylene Diffusion Flame

Author(s): McEnally, C. S., Schaffer, A. M., Long, M. B., Pfefferle, L. D., Smooke, M. D., Colket, M. D., and Hall, R. J.

Publisher (if applicable) _____

Volume: _____ Page(s): 1497-1505 Month Published: _____ Year Published: 1998

Name of Journal, Book, etc: Combustion and Flame

Title of Article: Computational and Experimental Study of Soot Formation in a Coflow, Laminar Diffusion Flame

Author(s): Smooke, M. D., McEnally, C. S., Pfefferle, L. D., Hall, R. J. and Colket, M. D.

Publisher (if applicable) _____

Volume: 117 Page(s): 117-139 Month Published: _____ Year Published: 1999

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Do Not Include: Unreviewed proceedings and reports, abstracts, "Scientific American" type articles, or articles that are not primary reports of new data and articles submitted or accepted for publication, but with a publication date outside the stated time frame

Name of Journal, Book, etc: Analytical Chemistry

Title of Article: Mapping of Trace Hydrocarbon Concentrations in Two-Dimensional Flames Using Single-Photon Photoionization Mass Spectrometry

Author(s): McEnally, C. S., Pfefferle, L. D.,. Mohammed, R. K, Smooke, M. D., & Colket, M. B.

Publisher (if applicable) _____

Volume: 71(2) Page(s): 364-372 Month Published: _____ Year Published: 1999

Name of Journal, Book, etc: Twenty-Eighth Symposium (Inter.) on Combustion

Title of Article: Characterization of a Coflowing, Methane/Air Nonpremixed Flame with Computer Modeling, Rayleigh-Raman Imaging, and On-Line Mass-Spectrometry

Author(s): McEnally, C. S., Pfefferle, L. D., Schaffer A. M., Long, M. B., Smooke, M. D., Mohammed, R. K., & Colket ,M. B.

Publisher (if applicable) _____

Volume: 28 Page(s) _____ Month Published: _____ Year Published: 2001

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NOTE: If there is insufficient space on this survey to meet your data submissions, please submit additional data in the same format as identified below.

PI DATA

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Institution: United Technologies Research Center

Contract/Grant No: F49620-98-C-0008

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PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

NOTE: List names in the following format: Last Name, First Name, MI

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Name of Journal, Book, etc: Twenty-Eighth Symposium (Intern.) on Combustion

Title of Article: Computational and Experimental Study of Ammonium Perchlorate/Ethylene Counter Flow Diffusion Flames

Author(s): Smooke, M. D., Yetter, R. A., Parr, T. P., Hanson-Parr, D. M., Tanoff, M. A., Colket, M. B., & Hall, R. J.

Publisher (if applicable) _____

Volume: 28 Page(s): _____ Month Published: _____ Year Published: 2001

Name of Journal, Book, etc _____

Title of Article _____

Author(s) _____

Publisher (if applicable) _____

Volume _____ Page(s) _____ Month Published _____ Year Published _____

UTRC01-5.100.0016-1

HONORS/AWARDS RECEIVED DURING CONTRACT/GRANT LIFETIME

Include: All honors and awards received during the lifetime of the contract or grant, and any life achievement honors
such as (Nobel Prize, honorary doctorates, and society fellowships) prior to this contract or grant.

Do Not Include: Honors and awards unrelated to the scientific field covered by the contract/grant.

Honor/Award Pratt & Whitney Leadership Award (finalist) Year Received: 1998

Honor/Award Recipient(s) Dr. Meredith B. Colket (with CFD development team)

Award Organization Pratt & Whitney

Honor/Award Fellow Year Received: 1999

Honor/Award Recipient(s) Professor M. D. Smooke

Award Organization Institute of Physics

Honor/Award 2000 AIAA Best Paper Year Received: 2000

Honor/Award Recipient(s) Dr. Meredith B. Colket

Award Organization AIAA