



## Project Summary

# Proceedings of the Fifth Fundamental Combustion Research Contractors Workshop

M. P. Heap

These proceedings are for The Fifth EPA Fundamental Combustion Research Contractors Workshop, held January 23, 24, and 25, 1980, in Newport Beach, CA. The purpose of the workshop was to exchange information between the various contractors engaged in fundamental combustion research for EPA and to coordinate their activities. In addition, the workshop provided for a review of EPA's Fundamental Combustion Research (FCR) Program by EPA's Science Advisory Board. The five conference sessions dealt with gas-phase chemistry and heterogeneous NO reduction, chemical and physical effects of thermal decomposition, bench-scale reactor studies, two-phase turbulent flames, and model development.

The main thrust of the FCR program is elucidating the mechanism of NO formation from fuel bound nitrogen. Several papers addressed the gas-phase conversion of fuel nitrogen species to NO, N<sub>2</sub>, HCN, or NH<sub>3</sub>. Advanced diagnostic techniques were used to investigate the physical changes taking place during the thermal decomposition of pulverized coal particles. Bench-scale reactor data were presented on the conversion of fuel bound nitrogen to NO in liquid- and solid-fuel flames. Studies on turbulent diffusion flames included detailed characterization of nonswirling coal flames and methods of measuring droplet size from fuel oil atomizers. Engineering analysis is a strong component of EPA's FCR program, and papers were presented on the analysis of turbulent diffusion flames.

*This Project Summary was developed by EPA's Industrial Environmental Research Laboratory, Research Triangle Park, NC, to announce presentations at the workshop that are fully documented in a separate report of the same title (see Project Report ordering information at back).*

### Introduction

This report summarizes the proceedings of the Fifth EPA Fundamental Combustion Research (FCR) Contractors Workshop, held January 23, 24, and 25, 1980, in Newport Beach, CA. The workshop brought together current EPA contractors engaged in combustion research activities, to ensure efficient technology transfer between the various groups working in related areas. Members of EPA's Science Advisory Board also attended the workshop to review the activities for EPA management.

The workshop was opened by W. S. Lanier of IERL-RTP, Project Officer for the FCR program. He welcomed the participants, expressing the hope that the workshop would be a forum for discussion and interchange which would benefit all of the projects. He informed the participants of EPA/IERL-RTP's Combustion Research Branch activities in the area of NO<sub>x</sub> control and how the research programs were planned to provide input for the technology development programs. It was stated that many of the research projects had relatively short-term goals because low-NO<sub>x</sub> systems were currently being developed and installed. However, in keeping with the fundamental nature of the program, several programs had been included which were expected to pay off in the long term.

The FCR program focuses on the control of NO<sub>x</sub> and primary related pollutants generated by large, confined, one-atmosphere, turbulent diffusion flames from pulverized coal, syngases, or residual oils which radiate to cold walls. The various projects funded by FCR were selected to provide a deeper insight into the spectrum of processes characterizing these flames.

W. S. Lanier, EPA/IERL-RTP, chaired Session I, Gas-Phase Chemistry and Heterogeneous NO Reduction, which included the following papers:

"Modeling of Fuel-Nitrogen Chemistry in Combustion: The Influence of Hydrocarbons," J. M. Levy, MIT Energy Laboratory.

"Development of a Kinetic Mechanism to Describe the Fate of Fuel Nitrogen in Gaseous Systems," T. L. Corley, Energy and Environmental Research Corporation.

"NO<sub>x</sub> Formation in Flat, Laminar, Opposed-Jet Methane Diffusion Flames," W. A. Hahn and J. O. L. Wendt, University of Arizona.

"The Formation and Destruction of Nitrogenous Species During Hydrocarbon/Air Combustion," D. W. Blair, Exxon Research and Engineering Company.

"Laboratory Scale Coal Studies," J. M. Beer, A. F. Sarofim, J. M. Levy, D. Altrichter, and L. Timothy, Massachusetts Institute of Technology.

"Mechanisms of Nitric Oxide Reduction on Solid Particles," G. G. de Soete, Institut Francais du Petrole.

Papers in Session II, Thermal Decomposition--Chemical and Physical Effects, chaired by A. F. Sarofim, MIT, were:

"Volatility of Fuel Nitrogen," R. Gay, A. E. Axworthy, V. H. Dayan, and H. L. Recht, Rockwell International.

"High Temperature Pyrolysis of Oil Droplet and Coal Particle Streams," J. M. Beer, A. F. Sarofim, S. P. Hanson, and A. K. Gupta, Massachusetts Institute of Technology.

"The Characterization of Coals During Thermal Decomposition," P. R. Solomon, United Technologies Research Center.

"The Physical and Chemical Effects Occurring During the Thermal Decomposition of Coal Particles and Oil Droplets," W. R. Seeker, G. S. Samuelsen, and M.

P. Heap, Energy and Environmental Research Corporation.

Session III, Bench-Scale Reactor Studies, was chaired by J. P. Longwell, MIT. The papers presented included:

"Pollutant Formation During the Combustion of Residual Fuel Oils in a Well-Stirred Reactor," M. Murphy, Battelle Columbus Laboratories.

"Pollutant Formation from Combusting Pulverized Coal Clouds," P. M. Goldberg, H. Tong, and R. Kendall, Acurex Corporation.

"Reactor Studies to Assess the Impact of Fuel Characteristics on Fuel NO<sub>x</sub> Formation," M. P. Heap, D. W. Pershing, G. C. England, S. L. Chen, R. Nihart, and D. P. Rees, Energy and Environmental Research Corporation.

"Pollutant Formation During Fixed-Bed and Suspension Coal Burning," D. W. Pershing, University of Utah.

The papers in Session IV, Two-Phase Turbulent Diffusion Flames, chaired by W. S. Lanier, were:

"An Experimental Approach to the Study of Heavy Oil Spray Combustion in Shear Layers," A. Vranos, United Technologies Research Center.

"Spray Characterization," W. R. Seeker, and G. S. Samuelsen, Energy and Environmental Research Corporation.

"The Application of Droplet Sizing Interferometry and Holography to the Measurement of Spray Droplet Size and Velocity," C. F. Hess and W. D. Bachalo, Spectron Development Laboratories.

"Characterization of Long Turbulent Pulverized Coal Diffusion Flames," R. Payne, The International Flame Research Foundation.

The chairman of Session V, Model Development, was T. J. Tyson, Energy and Environmental Research Corporation. He introduced the following papers:

"Development of a Coherent Flame Model for Turbulent Chemically Reacting Flows," F. E. Marble and J. E. Broadwell, California Institute of Technology.

"General Kinetic Analysis Codes," C. J. Kau and T. J. Tyson, Energy and Environmental Research Corporation.

## Abstracts of Papers

### **Introduction to the Fifth EPA Fundamental Combustion Research Contractors Workshop**

W. S. Lanier

Organizationally, the Fundamental Combustion Research (FCR) Program is funded through the Combustion Research Branch (CRB) of EPA's Industrial Environmental Research Laboratory at Research Triangle Park (IERL-RTP). The CRB charter calls for the development of emission control technology for pollutants generated by stationary combustion sources through modification of the basic combustion process. Consequently, the primary focus of the FCR program is the formation and destruction of NO<sub>x</sub> in flames. Boilers firing pulverized coal and high-nitrogen liquid fuels produce most of the NO<sub>x</sub> emitted by stationary sources. Thus, the projects funded as part of the FCR program concentrated on the mechanism of fuel nitrogen conversion in large two-phase turbulent diffusion flames.

As regards the mechanics of the FCR program, when a particular research topic is selected for investigation, a number of options are open. If the prime contractor Energy and Environmental Research (EE) Corporation, has an existing expertise, or no expertise is known to exist, there is the option to pursue the research topic at EE. This has been the dominant choice in numerical modeling activities. Other options open include sole-source, limited source, or full competitive procurement. In general, the sole-source or limited competitive route has been selected. Another option allows the CRB to fund the activity directly through either a contract or grant. Consequently, a variety of contracting options are available, and many have been used.

### **Modeling of Fuel Nitrogen Chemistry in Combustion: The Influence of Hydrocarbons**

J. M. Levy

Despite uncertainties in the currently available mechanistic and kinetic database, it is possible to model (albeit imperfectly) fuel nitrogen conversion in the presence of simple fuels. Unfortunately, there is a strong coupling between fuel nitrogen and hydrocarbon chemistry. In the heat release mechanism for real fuels, it is complex, it is necessary to develop methodology to treat the hydrocarbon

mechanism in some global manner which can be linked with the fuel nitrogen mechanism. Consequently, the conversion of fuel bound nitrogen in a hydrocarbon combustion environment requires a reaction mechanism which can be viewed as a synthesis of three subsets: fuel nitrogen, hydrocarbon oxidation, and hydrocarbon/nitrogen interactions. The outstanding phenomenological question raised in connection with the modeling of hydrocarbon chemistry pertains to the fate of the free-radical pool. Hydrocarbon fragments effectively catalyze radical recombinations, and free radical overshoots are much less in hydrocarbon systems than in hydrocarbon-free systems.

### ***Development of a Kinetic Mechanism to Describe the Fate of Fuel Nitrogen in Gaseous Systems***

T. C. Corley

This paper concerns the development of a kinetic mechanism which can predict adequately the conversion of fuel nitrogen compounds to NO in gaseous systems. A four-step approach was used to develop the mechanism: (1) assemble elements of the reaction model, (2) select data sets for analysis to resolve critical questions under well-defined reaction conditions, (3) identify and correct deficiencies by comparing with data generated in shock tubes and flames, and (4) use the completed sub-element of the reaction mechanism as a known element of more complex systems.

Application of the procedure to elements of the reaction model indicates:

- CH<sub>2</sub>O - CO - H<sub>2</sub> - O<sub>2</sub> system is complete.
  - HCO is important for chain-branching in rich, wet CO flames.
  - Decomposition and oxidation of CH<sub>2</sub>O is slower than previous predictions.
- NH<sub>3</sub>-O<sub>2</sub> mechanism requires additional analysis.
  - Chain-branching path required: NH<sub>2</sub> + NO = N<sub>2</sub> + H + OH.
  - Ignition delay controlled by: NH<sub>2</sub> + O<sub>2</sub> = HNO + OH.
  - N<sub>2</sub>H<sub>1</sub> species may be important for rich processing of NH<sub>3</sub>.
  - Overall oxidation of NH<sub>3</sub> too slow with present mechanism.
- HCN-O<sub>2</sub> reaction model must be compared with other data.
- Hydrocarbon mechanisms require further study.

— Ignition delays for CH<sub>4</sub>-O<sub>2</sub> predicted.

### ***NO<sub>x</sub> Formation in Flat, Laminar, Opposed-Jet Methane Diffusion Flames***

W. A. Hahn and J. O. L. Wendt

The detailed structure of a flat, laminar, opposed-jet diffusion flame can be modeled. By properly coupling the momentum and energy conservation equations and by using detailed finite rate combustion kinetics, it is possible to model the detailed structure of a flat, laminar, opposed-jet diffusion flame.

Such a flame is one-dimensional, if the proper velocity boundary conditions are used. Measurements with a laboratory CH<sub>4</sub>/N<sub>2</sub>/O<sub>2</sub> opposed-jet diffusion flame gave good agreement with predictions with respect to one-dimensionality, temperature, and species profiles within the reaction zone. However, the actual location of the reaction zone was displaced slightly. The theoretical/experimental tool developed was used to test kinetic mechanisms of NO formation from fuel nitrogen. In this case, anhydrous ammonia was introduced first with the fuel, and then with the oxidizer. The formation of NO was predicted reasonably well by using a detailed kinetic mechanism developed by others, when ammonia was introduced with the fuel; but agreement was poor when ammonia was injected in the air side. This indicates that there are some deficiencies in the ammonia pyrolysis kinetic mechanism when it is used in the absence of hydrocarbon fragments. The qualitative dependence of the NO profile on flame stretching was correctly predicted by the model.

### ***The Formation and Destruction of Nitrogenous Species During Hydrocarbon/Air Combustion***

D. W. Blair

An experimental investigation was carried out of the critical aspects of the formation and destruction of nitrogenous chemical species during hydrocarbon/air combustion. The primary purpose of the work was to provide reliable experimental information to aid in developing detailed kinetic models. The experiments were run in two significantly different laboratory combustors over a wide range of independent thermochemical variables (equivalence ratio, temperature, fuel species, fuel nitrogen species, and characteristic resi-

dence times). Two reactors, the jet-stirred combustor and the multiburner, both developed with EPA funds, were used. Conclusions drawn from this work include:

- With both equivalence ratio and flame temperature held constant, specific hydrocarbon chemistry influences both thermal nitrogen fixation and fuel nitrogen conversion.
- Fuel chemistry is more important in the multiburner than it is in the jet-stirred combustor. Contributions of combustion environment to this difference appear to exceed those of reaction time.
- While the conversion of fuel nitrogen depends on fuel nitrogen species, the dependency in the multiburner considerably exceeds that in the jet-stirred combustor. This argues that differences in combustion environment between the two combustors are important.
- Because production of fixed nitrogen products differs significantly between the multiburner and the jet-stirred combustor, choosing between these combustors, as models of given practical combustors, should be based on which one best approaches conditions that will exist in the given combustor.

### ***Laboratory Scale Coal Studies***

J. M. Beer, A. F. Sarofim, J. M. Levy, D. Altrichter, and L. Timothy

There is a possibility that, in pulverized coal flames, NO produced early in the combustion process is later reduced by char generated by the partial combustion of coal. Indirect evidence for the importance of NO reduction reactions in coal combustors is provided by the observation in pilot-scale combustors that the NO concentration passes through a maximum and undergoes substantial reduction in later stages of combustion, particularly under fuel-rich conditions. To assess the role of char in reducing NO, a three-part research program has been undertaken involving: (1) determining kinetics of the NO/char reaction under conditions of interest to pulverized coal combustion, (2) measuring temperature/time histories and burning times of coal particles to provide a basis for testing models for coal combustors, and (3) using the kinetic information to develop a model to predict (first) char loading and temperature profiles, and (then) the reduction of NO by char under different simulated coal combustion conditions. Preliminary data is presented on

NO/char reactions and on the burning temperatures and times of coal particles for conditions encompassing the range of interest in pulverized coal flames.

### **Mechanisms of Nitric Oxide Reduction on Solid Particles**

G. G. de Soete

In the last few years, attention has been focused on the role played by flame-born solid particles (e.g. soots, coal and char particles, fly ash) in the process of in situ (i.e., within the flame or in the hot combustion products) heterogeneous reduction of  $\text{NO}_x$ . Three main problems must be solved: (1) elucidating the kinetic mechanisms of heterogeneous NO reduction under typical flame and flue gas conditions, (2) determining the reaction rates which control the disappearance of NO, the formation of intermediate species, and the rate of their transformation of  $\text{N}_2$ , and (3) checking the relevance of heterogeneous reduction paths compared to homogeneous reduction mechanisms. This paper describes a study which will provide information on the first two problems using packed-bed reactors which will then lead into a general investigation of the heterogeneous NO reducing mechanisms. Data are presented which indicate that both  $\text{NH}_3$  and HCN can be formed during the reduction process, depending on the type of solid and the gas-phase composition.

### **Volatility of Fuel Nitrogen**

R. L. Gay, A. E. Axworthy, V. H. Dayan, and H. L. Hecht

An experimental program has been completed for the measurement of fuel nitrogen volatility using a quartz two-stage pyrolysis reactor. Solid and liquid fossil fuels were heated in helium in the first stage of the reactor at temperatures up to  $1100^\circ\text{C}$ . The volatile nitrogen compounds released were measured by converting them to HCN in the second stage of the reactor at  $1100^\circ\text{C}$ . The HCN was collected in dilute sodium carbonate solution and measured colorimetrically.

Twenty fossil fuel samples were studied, consisting of petroleum-based fuel oils, synthetic oils from coal and shale, and coals. All of the samples tested produced the greatest yield of volatile nitrogen compounds at a first-stage temperature of  $1100^\circ\text{C}$ . The maximum yields of volatile nitrogen from petroleum fuel oils were 35-

48 percent of the nitrogen in the sample. The yield curves increased continuously from  $300^\circ\text{C}$  with a slight dip at  $600-750^\circ\text{C}$ . The maximum volatile nitrogen yields from shale oils were 70-79 percent, while the coal liquids yielded 50 percent. The nitrogen species in shale oils were very volatile at low temperatures, giving HCN yields of about 65 percent at a pyrolysis temperature of only  $200^\circ\text{C}$ .

A variety of bituminous and lignite coals were tested. In general, the coals exhibited much lower fuel nitrogen evolution than did the fuel oils. Maximum coal volatile nitrogen yields obtained at a pyrolysis temperature of  $1100^\circ\text{C}$  were about 15-25 percent. A plot of the percentage of fuel nitrogen converted to NO during combustion (measured elsewhere) vs the percentage of fuel nitrogen volatilized at  $1100^\circ\text{C}$  was found to give a strong linear correlation with a variety of coals. This correlation may provide an excellent means of predicting NO formation for any given coal, simply by measuring its nitrogen volatility at  $1100^\circ\text{C}$ .

### **High-Temperature Pyrolysis of Oil Droplet and Coal Particle Streams**

J. M. Beer, A. F. Sarofim, S. P. Hanson, and A. K. Gupta

A series of high-temperature flow reactor experiments were carried out with coal particles under pyrolysis and combustion conditions. Techniques are described to study the pyrolysis of heavy liquid fuel droplets. The purpose of these investigations was to provide kinetic data on fuel nitrogen evolution and general volatile release. In addition, experimental evidence was sought to determine if the ignition of volatiles in the vicinity of coal particles influences the further evolution of nitrogenous compounds from the pyrolyzing particle. Preliminary results indicate during droplet pyrolysis the evolution rates of fuel-nitrogen compounds are affected strongly by rapid heating to high-temperature conditions similar to those encountered in practical flames. The development and application of a technique to obtain time-resolved particle temperatures are reported. The nature of the data acquisition, storage, and analysis permits statistical studies to be made of coal particle time/temperature histories. Information of this type would perhaps explain the observations which indicate different yields of  $\text{NO}_x$  from fuel of seemingly similar fuel characteristics.

### **The Characterization of Coals During Thermal Decomposition**

P. R. Solomon

A relation between coal organic structure and the products of thermal decomposition has been developed by measuring the modeling vacuum devolatilization of 12 bituminous coals and a lignite. The relation allows the prediction of the time and temperature dependent evolution of the major products of pyrolysis from knowledge of the coal's functional group distribution using a general kinetic model with rate constants independent of co-rank. The model assumes that large molecular fragments (monomers) are released from the coal "polymer" with only minor alteration to form tar, while simultaneous cracking of the chemical structure forms the light molecules of the gas. As a chemical component of the coal can, therefore, evolve as part of the tar or as independent species. The model may be used to predict the amount of volatile fuel nitrogen evolved in pyrolysis, which is essential in estimating the conversion of fuel nitrogen to  $\text{NO}_x$ .

### **The Physical and Chemical Effects Occurring During the Thermal Decomposition of Coal Particles and Oil Droplets**

W. R. Seeker, G. S. Samuelsen, I. P. Heap, J. O. Trolezer, and C. F. Hess

Events occurring during the thermal decomposition of liquid droplets and coal particles in the initial stages of heat release in turbulent diffusion flames are of considerable significance to the designers of low pollutant emission combustors. In pulverized coal flames the partition of fuel nitrogen between the volatile and char fractions, for example, will impact the production of fuel NO. Earlier studies have demonstrated that holography could be used to observe the behavior of coal particles during combustion. The approach taken in the present study was to observe particles/droplets under well-controlled conditions which simulated those encountered in real systems. This was accomplished by the construction of a reactor which allowed the particle/droplets to be injected into high temperature gas whose temperature and composition could be varied. Diagnostics were designed to allow visualization of the particles/droplets during combustion, both by hologra-

and high-speed photography. Two-color particle pyrometry was used to measure particle temperatures, and solid and gaseous samples were extracted to investigate the variation of composition with time. Initial evaluations of the results obtained to date, on the physical phenomena which occur during the thermal decomposition of pulverized coal particles, indicate that:

- Volatile coal fractions are ejected from coal particles in jets; for large bituminous coal particles, these jets produce a trail of small particles.
- Coal composition and volatile evolution rate influence particle temperature.
- Large soot structures can be formed from the bulk gases produced when bituminous coal particles decompose.

### ***Pollutant Formation From Combusting Pulverized Coal Clouds***

P. M. Goldberg, H. Tong, and R. Kendall

The objective of this experimental study was to provide information on the mechanisms of coal combustion and subsequent NO<sub>x</sub> formation under conditions similar to those found in the near-burner region of a high-intensity pulverized coal flame. A jet-stirred reactor system is used in this study to simulate this type of combustion environment. The stirred combustor can roughly simulate a flame region where a high degree of recirculation is present. The first goal of the program was to design a well-mixed coal reactor capable of operating at residence times of 20-200 ms. After completing the design and fabrication, noncombusting mixing studies were conducted to verify that a high level of gas-phase mixing exists in the reactor. Once gas-phase mixing performance was verified, subsequent experiments were directed at quantifying particle mixing behavior. Combustion experiments began after completion of this task.

Combustion results show that devolatilization may be essentially completed in the 50-100 ms time range. The exhaust concentrations and temperature dependence on equivalence ratio are similar to those expected in larger time scale systems. This might lead to the conclusion that enhanced volatile yields play a major role in combustion. It has been observed that fuel nitrogen conversion is correlat-

able with equivalence ratio, reaction efficiency, and temperature. It was also found that the nitrogen depletion of the char corresponds roughly to the weight loss exhibited by the char, although a limited range of weight loss (75-95 percent) was examined.

### ***Reactor Studies to Assess the Impact of Fuel Characteristics on Fuel NO<sub>x</sub> Formation***

M. P. Heap, D. W. Pershing, and G. C. England

This paper describes results obtained to date in two ongoing investigations to assess the impact of fuel properties on pollutant formation. The approach taken in both investigations was experimental, wherein both solid and liquid fuels were burned in the absence of molecular nitrogen. The oxidant consisted of a mixture of O<sub>2</sub>, Ar, and CO<sub>2</sub> (21 percent by volume O<sub>2</sub>). The CO<sub>2</sub> was added to maintain the same adiabatic flame temperature for both the artificial oxidant and air. NO formed during combustion with this artificial N<sub>2</sub>-free oxidant is called fuel NO.

Data are presented showing the impact of fuel properties on NO<sub>x</sub> formation from liquid fuels under both excess air and staged conditions. These data indicate that:

- The formation of fuel NO from petroleum and alternative liquid fuels mainly depends on their total fuel nitrogen content.
- NO<sub>x</sub> control techniques for high nitrogen fuels, which rely on the generation of a high-temperature primary fuel-rich zone, appear to give the maximum opportunity for NO<sub>x</sub> reduction.

Twenty-six coals have been tested under fuel-lean conditions: it appears that, although fuel nitrogen content is important, it is not the only fuel characteristic dictating fuel NO formation. It appears that the volatility of the fuel nitrogen has an important impact on fuel NO formation, particularly under well-mixed conditions. Under fuel-rich conditions, the coal composition impacts the gas-phase nitrogen species distribution. With bituminous coals, ammonia represents a substantially smaller fraction of the total fixed nitrogen than with subbituminous or lignite coals. Of the nine coals tested in detail, only one—a Utah bituminous—formed substantial amounts of HCN under well-mixed conditions. Contrary to liquid fuel, increasing the temperature of a fuel-rich primary zone

does not appear to reduce stack emissions from a coal-fired staged combustor.

### ***Pollutant Formation During Fixed-Bed and Suspension Coal Combustion***

G. P. Starley, S. L. Manis, S. P. Pearcell, D. M. Slaughter, and D. W. Pershing

Recent large-scale pilot and field tests have (at least partially) demonstrated the potential of combustion modifications for NO<sub>x</sub> control in stoker-fired boilers. The overall objective of this program is to study the formation of NO<sub>x</sub> and SO<sub>x</sub> under carefully controlled experimental conditions typical of stoker-fired boilers. In particular, the following major research areas are being considered: (1) the evolution and oxidation of fuel nitrogen and sulfur, (2) the retention of SO<sub>x</sub> by ash and/or solid-chemical sorbents in both suspension- and fixed-bed burning, and (3) the effectiveness of distributed air addition for NO<sub>x</sub> control in stoker-fired coal systems.

Results with the suspension furnace do not support the hypothesis that a large fraction of the NO<sub>x</sub> is formed in the over-throw phase; however, many additional heating rates must be studied before any firm conclusions can be reached. The following tentative conclusions have been reached regarding the formation of NO<sub>x</sub> in a fixed-bed combustion system:

1. NO formation is not uniform throughout the burning time of the bed. The formation maximizes early in the process, prior to the peak combustion rate, and then gradually decreases.
2. Staged air addition is a potentially effective means of NO control. Exhaust concentrations decrease approximately linearly with decreasing bed stoichiometry.

### ***An Experimental Approach to the Study of Heavy Oil Spray Combustion in Shear Layers***

A. Vranos and B. A. Knight

This paper describes a two-phase program: (1) design and fabrication of an apparatus, and (2) preliminary combustion experiments. A unique shear layer mixing and combustion apparatus was developed which simulates high-shear diffusive combustion with heavy oil drop-

let injection as found in the near-field combustion zone of boilers and furnaces. The apparatus provides: (1) two-dimensional mixing and combustion of uniform streams of air and rich combustion products fed from opposite sides of a splitter plate, (2) uniform injection of a mono-disperse heavy oil spray into the shear layer by a linear array of fuel injectors beneath the combustor wall, (3) control of droplet path, residence time, and extent of vaporization, (4) control of hot and cold stream inlet properties, and (5) three-dimensional probing of the flow field.

The design phase of the program consisted of two tasks: aerodynamic and thermodynamic design and mechanical design. A wind tunnel, hot gas generator, combustion chamber, droplet injection system, and phase-sensitive sampling probe were designed in the first task. The design of the apparatus was influenced most strongly by the diverse requirements of the fuel injection system. The injector was designed so that the angle of droplet penetration into the shear layer could be varied over a wide range. Droplet trajectories were computed for vaporizing No. 6 oil droplets injected from the floor of the combustor into a hot rich environment provided by a hot gas generator. Hot gas generator dimensions and injector locations were selected to accommodate the required droplet trajectories, provide complete vaporization if desired, and provide sufficient hot soak time for substantial conversion of fuel nitrogen compounds to molecular nitrogen.

### ***Spray Characterization***

W. R. Seeker and G. S. Samuelsen

A program has been established to explain the dependence of  $\text{NO}_x$  emissions from fuel-oil fired combustors on atomizing nozzle type, and nozzle operating conditions. Toward this end, a cold chamber spray rig, patterned after the firetube simulator at EER, was built to characterize nozzle spray behavior. As the initial step in the program, nonintrusive optical techniques are being applied and evaluated for (1) consistency of data, and (2) applicability to the study of spray behavior which impacts  $\text{NO}_x$  emission. The optical techniques include diffraction, visibility, and holography. At this juncture in the program, visibility measurements are concluded. Significant differences exist between these data and data acquired in an independent program conducted at the IFRF. The resolution of these differences is not in progress.

### ***The Application of Droplet Sizing and Interferometry and Holography to the Measurement of Spray Droplet Size and Velocity***

C. F. Hess and W. P. Bachalo

Droplet sizing interferometry (DSI) and laser holography are used in a fuel spray study. The size and velocity distributions of the fuel droplets produced by a Sonicore nozzle in a cylindrical rig are obtained. The two techniques are evaluated and compared. The power and flexibility of the interferometer in the study of the fuel droplet size and velocity are demonstrated. The data obtained by the two techniques are compared and are shown to agree very well. Although holography is adequate for sizing droplets, the analysis of the holograms is time-consuming. The DSI measures size and velocity of the individual droplets, provides an immediate data display, and is therefore a very powerful diagnostic tool for liquid sprays.

### ***Development of a Coherent Flame Model for Turbulent Chemically Reacting Flows***

F. E. Marble and J. E. Broadwell

The coherent flame model is applied to the methane/air turbulent diffusion flame with the objective of describing the production of NO. The example of a circular jet of methane discharging into a stationary air atmosphere is used to illustrate application of the model. In the model, the chemical reactions take place in laminar flame elements which are lengthened by the turbulent fluid motion and shortened when adjacent flame segments consume intervening reactant. The rates with which methane and air are consumed and NO generated in the strained laminar flame are computed numerically in an independent calculation. The model predicts NO levels of about 80 ppm at the end of the flame generated by a 30.5 cm (1 ft) diameter jet of methane issuing at  $3.05 \times 10^3$  cm/sec (100 ft/sec). The model also predicts that this level varies directly with the fuel jet diameter and inversely with the jet velocity.

### ***General Kinetic Analysis Codes***

C. J. Kau and T. J. Tyson

A computer code, capable of predicting or analyzing premixed or diffusion flames, is reported. The generality of the code allows the computation of various configurations; e.g. one-dimensional time-

dependent planar/spherical, steady two-dimensional planar, and steady axisymmetric nonrecirculating reacting flow systems. Physical phenomena such as laminar unequal species diffusivities, radiation, flame holder recombination effect, and heat loss are treated. Several phenomenological turbulent eddy viscosity models, based on mixing length theory, are also incorporated into the code. Kinetically the code can treat up to 200 two- or three-body basic reactions and up to 52 species.

A linearized implicit finite difference network is used. Thus, all the dependent variables, except cross-stream velocity, of all the grid points at the same coordinate line (or at the same integration step) are solved simultaneously in coupled fashion. The inversion of a block tridiagonal matrix is required at each integration step.

For illustrative purposes, detailed calculation of four types of laminar flames are presented: a flat flame, an opposed-jet diffusion flame, a coflowing diffusion flame, and a nonrecirculating confined flame.

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*W. Steven Lanier is the EPA Project Officer (see below).*

*The complete report, entitled "Proceedings of the Fifth Fundamental Combustion Research Contractors Workshop," (Order No. PB 83-164 483; Cost: \$44.50, subject to change) will be available only from:*

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