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**INVITED SPEAKERS**

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**RESEARCH NEEDS FOR FIRE RESISTANCE DETERMINATION AND PERFORMANCE PREDICTION**

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Abstract

The scientific and engineering community have a responsibility to come to grips with the technical issues associated with the buildings that collapsed on Sept. 11, 2001. The Twin Towers withstood the physical impact of the aircraft, as designed, but succumbed to the thermal impact of the ensuing fire. Building 7, with unknown, but significantly less, structural damage collapsed hours later, apparently due to the fire that was allowed to burn unchecked, which would make it the first instance of a building of such a design to ever "burn to the ground." The relative amount of damage to the Pentagon due to the initial impact and due to the subsequent fire is unclear, but is important to discern if we are to learn the right lessons from the observed building performance, occupant behavior, and fire fighter response. Central to all these events is the fire resistance of the structure. No one did a calculation ahead of time to predict how resistant to heat these buildings were in the event of an extreme fire. Why? Reasons will be suggested in the paper. In response to these catastrophic building collapses, NIST has initiated a research program to improve structural fire protection. This presentation is a summary of the outcome of a workshop held to identify the fundamental research needed. The knowledge gained in this effort will lead, in general, to verified predictive tools and performance criteria to evaluate overall structural fire performance in real fires. The ultimate goal is to achieve cost-effective, assured structural integrity for high probability large fires, and predictability of time to structural failure in the case of extreme events or failures of suppression activities.

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## OPTICAL AND REACTIVE PROPERTIES OF SOOT IN FLAME ENVIRONMENTS

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### ABSTRACT

An understanding of soot optical and reactive properties critical for estimating the continuum radiation properties, the pollutant soot emission properties and the structure properties of most practical hydrocarbon-fueled nonpremixed flames. Motivated by these observations, recent progress concerning soot optical properties, soot formation properties and soot oxidation properties in flames are reviewed in this paper.

Soot in flame environments consists of nearly monodisperse (at a given flame condition) spherical primary soot particles that are collected into mass fractal aggregates having widely varying numbers of primary particles per aggregate. Experimental and computational studies have shown that these objects satisfy the Rayleigh-Debye-Gans scattering approximation, yielding a method of estimating soot optical properties called the Rayleigh-Debye-Gans/Polydisperse-Fractal-Aggregate (RDG/PFA) soot scattering theory. Given this theory, improved measurements of soot refractive indices have become available, finding that soot refractive index properties were relatively independent of the fuel used to create the soot, that dimensionless extinction coefficients were relatively independent of wavelength for wavelengths of 400-5000 nm and that the classical refractive index properties of Dalzell and Sarofim (1969), used by many workers in the field for reducing soot optical measurements, were surprisingly accurate.

Soot nucleation properties continue to be relatively poorly understood, but progress has been made toward a better understanding of soot surface growth rates. It has been found that these rates are similar in premixed and diffusion flames and that they are relatively independent of the fuel used to create the soot. In addition, soot surface growth rate properties are described reasonably well by the classical Hydrogen-Abstraction/Carbon-Addition (HACA) mechanism with steric factors on the order of unity as expected. More information about soot surface growth rates is needed, however, for high flame temperatures and for pressures other than atmospheric pressure. Finally, current controversy concerning the importance of Poly-Aromatic Hydrocarbons (PAH) in the mechanism of soot surface growth still must be resolved.

Early soot surface oxidation rates have recently been measured in diffusion flame environments, finding good agreement with the classical measurements of Neoh et al. (1980) in premixed flames. These results imply that soot oxidation in flame environments (when oxygen concentrations are smaller than 0.1 percent by volume) is dominated by reaction with OH with a collision efficiency on the order of 0.1. More information is needed, however, for soot oxidation at temperatures larger than 2000K, for oxygen concentrations larger than 0.1 percent by volume and for pressures other than atmospheric pressure. Finally, the properties of late soot oxidation, when primary soot particles become porous and internal particle oxidation becomes important, still must be resolved.

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**Lattice Boltzmann Simulation of Reactive Flow**

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## SI Engines

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A1.1

### Modeling Autoignition in Direct Injection Diesel Engines

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#### Abstract

Traditionally diesel ignition delay has been correlated using semi-empirical expressions which account for kinetic and thermodynamic aspects, but ignore the effects of mixing. Ignition delay results from experiments conducted using a 0.75 L single-cylinder direct injection (DI) diesel clearly show that changes in mixing caused by independently varying operating parameters such as injection pressure and engine speed affect the ignition process. A semi-empirical ignition model which includes the effects of mixing, as well as thermodynamic aspects, is derived and preliminary results provided. Future efforts will focus on continued development and validation of the model and incorporation of the model into a cycle simulation code for prediction of DI diesel performance and emissions.

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**Model Based Control of Cyclic Dispersion in Lean Spark Ignition Combustion**

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Abstract

We are investigating predictive symbol based and map based control algorithms using a simple spark ignition engine cyclic variability model. Data symbolization involves the conversion of a data series of many possible values into a symbol series of only a few distinct values. These values can be obtained from either a moving data window or a library of data at the specific operating condition. This technique is useful for characterizing predictability and identifying repeating temporal patterns in cycle-resolved combustion measurements (i.e., heat release). We are also investigating another predictive control technique that may be used in conjunction with or in lieu of the symbolic control technique. This technique utilizes low-order maps of the combustion instability to predict future combustion events. The low-order maps are developed by fitting data from either a moving window or library. We believe that these types of control algorithms can be useful in controlling steady state as well as transient cyclic dispersion under lean conditions.

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**A Multi-dimensional Combustion Model for Gasoline Direct-Injection Engine Design**

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## Abstract

A multi-dimensional combustion model suitable for direct injection gasoline engines is presented. As part of an engineering design tool, the model is constructed to enable early assessment of proposed combustion system designs and to facilitate in-depth understanding of engine behavior during prototype testing. The success of the model relies heavily on fuel spray models which have been discussed elsewhere [1]. A flame kernel submodel accounts for laminar chemical kinetic effects during kernel growth. Marker particles [2] are used to track the extent of the flame kernel allowing representation of small diameter flames on a relatively coarse unstructured mesh while avoiding numerical diffusion effects. Once the kernel is developed, combustion is governed by the combined time-scale turbulent combustion model [3], which balances the effects of turbulent mixing and chemical kinetics to identify the appropriate reaction rate across a range of in-cylinder conditions. The model is implemented in a KIVA-3V based code and applied to both homogeneous and stratified operating conditions. Single cylinder engine data is used to calibrate the model. The model is able to predict cylinder pressure, burn rates and NOx emissions under homogeneous operating conditions. The model is also applied to stratified charge conditions, using the same model calibration. Cylinder pressure predictions agree well with measured data, and predicted burn rates are similar to those deduced from measured pressure curves using heat-release analyses. Detailed examination of the in-cylinder combustion processes is possible with the model.

[1] Z. Han et al., SAE Paper 2001-01-3667, 2001.

[2] L. Fan, et al., SAE Paper 1999-01-0175, 1999.

[3] J. Abraham, F.V. Bracco, and R. Reitz, Combustion and Flame, 60:309-322, 1985.

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## A1.4

### Local Fuel-Air Ratio Measurements in Internal Combustion Engines using Spark-Emission Spectroscopy

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#### ABSTRACT

Spectrally resolved visible and ultraviolet emissions are established as a basis for wide-range, individual-cycle measurement of the local fuel-air ratio in spark-ignition engines. The 388-nm CN emission intensity, normalized by the spark-discharge energy during the observation interval (typically 150  $\mu$ s at the start of the glow discharge), is demonstrated to provide a quantitative measure of fuel-air equivalence ratio over a range of at least 0 - 3 with random and systematic errors of 10% or less for engine operation on homogeneous fuel-air mixtures. Calibration data for both propane and isooctane fuels over a wide range of cylinder gas conditions at the time of ignition collapse to a single curve when the fuel concentration is expressed in terms of the number density of carbon atoms. Applied to an engine in which liquid fuel is injected directly into the cylinder, the technique reveals substantial cyclic fluctuations in the fuel-air ratio at the spark gap under conditions of both early fuel injection (intended to produce a homogeneous fuel-air mixture in the combustion chamber) and late fuel injection (which produces a highly stratified mixture). For stratified operation with a fixed fuel-injection timing, retarding the spark timing from optimum leads to incomplete combustion in many cycles due to fuel-air ratios that are too lean for good ignition and rapid flame development.

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**COMPARISON OF SIMULATIONS OF IMPINGEMENT FROM AN AIR-ASSISTED FUEL INJECTOR AND A SWIRL ATOMIZER**

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ABSTRACT

Reducing hydrocarbon emissions in Gasoline Direct Injection engines remains an important challenge. Fuel impingement has been identified as a major contributor to increased hydrocarbon emissions because a fuel film vaporizes more slowly than airborne droplets. Simulations of the impingement of an air-assisted fuel injector were made to determine whether fuel impingement from an air-assisted injector would be substantially less than that from a swirl atomizer, which is currently used in most production GDI engines. Normal and angled impingement were simulated under the assumption of an axisymmetric spray. Impinging droplet characteristics such as diameter, Weber number, normal velocity, position, and splashing were predicted for an air-assisted spray and a swirl atomizer spray. High-pressure cases were simulated to approximate a late-injection condition, and low-pressure cases were simulated to approximate an early-injection condition. In both sets of cases, the simulated air-assisted spray resulted in substantially less fuel impingement because of smaller droplets, faster vaporization, and slower penetration. Simulated results also predict that an air-assisted injector design change that increases the initial spray angle by 30% would reduce fuel impingement tremendously.

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**THE EFFECT OF WALL-WETTING ON HYDROCARBON EMISSIONS IN ENGINES**

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ABSTRACT

This study examines the relationship between wall-wetting and hydrocarbon emissions. To simulate emissions from practical fuels, a multi-dimensional code was used. It includes multi-component droplet and film vaporization models that account for both gas and liquid phase transport processes. To extend these models to simulate combustion, a multi-component fuel combustion model was developed. This combustion model combined the rate constants for each of the fuel components on the basis of mole fraction to form an effective fuel. The effective fuel was then used to calculate the reaction rates. These models were used to simulate hydrocarbon emissions resulting from wall-wetting in gasoline engines. Qualitative comparisons between the computed and measured results showed reasonable agreement. The computed results also provide insight to the causes of hydrocarbon emissions. It was revealed that the wall-wetting location has a significant effect on hydrocarbon emissions by allowing some of the unburned hydrocarbons an easy access to the exhaust, while making it difficult for others to escape into the exhaust. Injection timing affects the amount of film that survives past the combustion process. As film survived into the expansion and the exhaust stroke, the film's composition gradually shifted toward its heavier components. This new composition controls the vaporization characteristic of the film.

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**Effects of Engine Modifications on the Pollutant Emissions from Small Utility Engines**

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Abstract

Previously, it has been found that the hydrocarbon emissions from four-stroke, overhead-valve, small utility engines increase over the lifetime of the engines. It is believed that this increase is due to the formation of combustion chamber deposits (CCD) as the engines age. Based on the chemical composition of the CCD, the CCD appear to originate primarily from engine oil entering the cylinder. In an attempt to determine the primary source of this oil in the engine cylinder, various modifications are being made to the engines. There are three primary routes by which engine oil may enter the cylinder: (1) by passing from the crankcase into the intake system through the breather element, (2) through leakage from the valve stems, and (3) through the piston ring pack. In this ongoing study, the engines are being modified to isolate the effects of these three different routes on deposit formation and subsequently on hydrocarbon emissions. In this paper, the results of the effects of modification of the breather element arrangement on the hydrocarbon, NO<sub>x</sub>, and CO emissions will be presented. By comparing the hydrocarbon emissions from over the life cycle of the modified engines to those from unmodified engines, as well as by determining the nature of the CCD formed over the life cycle, it is possible to determine if the oil introduced to the engine combustion chamber through the breather element is significant enough to lead to large-scale CCD formation in these engines.

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## Multiphase Combustion

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### A2.1

#### **PREFERENTIAL VAPORIZATION MODEL FOR MULTICOMPONENT DROPLETS AND SPRAYS USING CONTINUOUS THERMODYNAMICS**

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#### ABSTRACT

A preferential vaporization model for droplets and sprays with large numbers of components is presented in this paper. Rather than using a set of discrete components to model the fuel, the composition of the fuel is described by a distribution function based on continuous thermodynamics and two parameters (i.e., mean and variance) are sufficient for tracking the composition of the mixture. This approach makes it possible to simulate commercial fuels with only a few distribution parameters rather than several hundred discrete components. Evaporation rates and heat flux to droplets are obtained with a quasi-steady assumption, and finite diffusion and preferential vaporization of the mixture are included in the liquid phase equations. A novel approach was used to reduce the equations to a set of zero-dimensional ordinary differential equations that are capable of accounting for the effects of the non-uniform temperature and concentration distributions inside a droplet. The resulting model is suitable for multi-dimensional spray simulations with a very small increase in computational costs compared to the widely used infinite-diffusion models, however, with a better accuracy. The model was used to study the vaporization process of diesel and gasoline fuel droplets. The results of the model were also compared against those obtained using the infinite-diffusion approximation and the discrete-component approach. The results show that this model is capable of modeling vaporization phenomena of complex mixtures of fuels, and that the finite diffusion and preferential vaporization effects on the temperature and composition of liquid droplets are successfully represented. Finally, the model was applied to study gasoline sprays under direct-injection engine conditions and the effects of multicomponent vaporization on the spray characteristics and vapor mixture are demonstrated.

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## A2.2

### **A Numerical Study of the Impacts of the Blending of Volatile Component on Spray Evaporation and Combustion**

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#### Abstract

Spray injections are widely used in the industries, such as, diesel engines, furnaces, fluid catalytic cracking reactor, and etc. The injected liquid droplets often contain multiple components of various thermal physical properties. The multiple components in the liquid have strong impacts on the evaporation and combustion characteristics of a spray. Computational fluid dynamics (CFD) codes have been used to simulate these processes. However, most simulations assume a single uniform thermal physical property for the liquid droplets. Argonne National Laboratory has developed an approach to account for the various boiling points of multiple components in the liquid droplets. The new approach was incorporated into a CFD code to simulate spray evaporation and combustion in a three-dimensional chamber. The CFD code uses an Eulerian approach to model the liquid droplet flow. The simulation includes turbulent mixing, interfacial drag and heat transfer, droplet evaporation, combustion reaction, radiation heat transfer, and pollutant kinetics.

The CFD code was used to simulate a spray of diesel fuel blended with a highly volatile component. A parametric study was conducted to investigate the impact of the blending on the spray evaporation and combustion characteristics. The final paper will describe the new modeling approach for a liquid spray with multiple components and present the results of the parametric study.

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**Combustion of Single Decane Droplets in Microgravity - Comparison of Experiments with a Simplified Numerical Model**

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Abstract

This paper presents both experiments and simplified modeling results of single decane droplets in microgravity. The experiments utilized fiber supported droplets with initial sizes ranging from 1.4 to 1.8 mm. The test ambient was an oxygen/nitrogen mixture with ambient oxygen mole fractions ranging from 0.15 to 0.19 at pressures ranging from 90 to 760 mm Hg. The data from the experiments were from two orthogonal views of the droplet burning, one backlit to image the droplet, the other showing the flame.

The experiments showed that the droplet burning history ( $D^2$ -vs. time) was non-linear, and nearly independent of pressure, initial droplet size, and ignition energy. The flame size (which showed dependence on pressure, initial droplet size, and ignition energy) typically increased with time, then reached a plateau and began to decrease at the end of the burn. The flame standoff ratio typically increased with time. At an ambient oxygen mole fraction of 0.15 and pressures below 190 mm Hg, the flame surrounding the droplet extinguished at a finite droplet size. The extinction droplet size increased with decreasing pressure, was a weak function of initial droplet size, and nearly independent of ignition energy (within the limited range tested).

The experiments are compared to a simplified numerical model of the droplet burning. The model is transient (from ignition to extinction), assumes constant Lewis number (although different species can have different Lewis numbers), single step chemistry, and gas-phase radiative loss. The model qualitatively predicts many of the trends observed experimentally.

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**MODIFIED FORM OF THE HELMHOLTZ VORTICITY EQUATION AND ITS SOLUTION FOR  
SPHERICAL FLOW WITHIN A DROPLET IN UNIFORM OR COUNTERFLOW STREAMS**

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ABSTRACT

Scale-invariant form of mass, energy, linear, and angular momentum conservation equations in reactive fields are described. The conservation of angular momentum is shown to result in a modified form of the Helmholtz vorticity equation. This equation is then solved to determine flow field within a droplet that is located either in a uniform stream or at the stagnation-point of axi-symmetric counterflow. For the former case, the classical solution of Hill spherical vortex is recovered. The latter case results in a spherical flow produced by two semi-spherical ring vortices.

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**Filtration Combustion of a Methane Wave in Air for Oxygen Enriched and Depleted Environment**

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Abstract

In this work, the fundamental properties, temperature and propagation rate, of a filtration combustion wave in an inert packed bed are studied experimentally for oxygen enrichment and depletion. This detailed experimental study was carried out for equivalence ratios from 0.1 to 1.0, for oxygen content of the oxidizer (OCO) of 10 to 30% and for equivalence ratio from 0.1 to 2.0 for OCO of 21% and 30%. Intrinsic properties of the filtration combustion waves are measured and comparatively analyzed for a single filtrating gas velocity in a packed bed of 3 mm alumina pellets. It was found that the peak flame temperature decreases with increasingly rich oxygen environment while the flame propagation rate increases. The opposite occurred with the depletion of oxygen in the oxidizer stream. To help understand this phenomenon, two important minor products, oxides of nitrogen (NO<sub>x</sub>) and carbon monoxide (CO) emissions were sampled from the product stream.

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**COMBUSTION OF LOW-EXOTHERMIC CONDENSED SYSTEMS FOR OXYGEN GENERATION**

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## Abstract

The combustion of low-exothermic compositions based on alkali metal chlorate and metal fuel similar to those used in emergency oxygen generators for aircraft is studied. The specific system investigated is a powder mixture of sodium chlorate ( $\text{NaClO}_3$ ), tin (Sn, 2-10 wt.%), and chlorate decomposition catalyst ( $\text{Co}_3\text{O}_4$ , 0-2.5 wt.%). The synchronized experimental data on temperature-time history of the process, combustion front velocity and product oxygen flow rate are obtained. The influence of reaction mixture composition on the process parameters is investigated. The combustion process is characterized by significant oscillations of the product oxygen flow rate. It is shown that the gas flow fluctuations are caused by unstable reaction front propagation. Increasing loading of catalyst or metal fuel accelerates combustion. In both cases, the relative amplitude of oscillations decreases with increasing the mean rate of process.

Structure of quenched combustion wave is studied by using X-ray diffraction analysis and scanning electron microscopy. It is shown that the metal oxidation zone is thinner by an order of magnitude as compared to the chlorate decomposition zone. The obtained results support the hypothesis that coupling of the two low-exothermic reactions (i.e. chlorate decomposition and metal oxidation) connected by production/consumption of oxygen is an important reason for oscillations in the investigated system.

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**ALO EMISSION TEMPERATURES FROM ALUMINUM BURNING IN CARBON DIOXIDE AT ELEVATED PRESSURES**

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## Abstract

Aluminum is often added to solid rocket motor (SRM) propellants to increase combustion temperatures and thus improve specific impulse. While the oxidation of Aluminum has been the subject of extensive study, a great deal of the previous work has been performed at atmospheric pressure in oxygen or air. Under SRM conditions, little oxygen is left for combustion of the Aluminum particles, and the Aluminum typically burns at pressures more than an order of magnitude above atmospheric pressure and in oxidizers such as CO<sub>2</sub> and H<sub>2</sub>O. Thus, there is a significant need for measurements of Aluminum particle combustion temperatures in environments similar to those seen in SRMs.

In the UIUC shock-tube facility, we conduct transient combustion experiments of fine Aluminum powders in highly controlled atmospheres and under similarly controlled temperatures and pressures. In this study, we report on the results of a study of Aluminum particle combustion in mixtures of CO<sub>2</sub> and Ar at pressures of 8.5 and 17 atmospheres. Spectra of the emission from the AlO intermediate are obtained at moderate dispersion (spectral resolution: 1-2 angstroms), allowing an emission temperature to be fit to the spectrum. Time-resolved spectra during the 1 ms combustion event are also obtained. Finally, particle ignition delay times and burn times are measured by photometry. These data are obtained for a range of CO<sub>2</sub> compositions in Ar (30-60%), and all combustion quantities show a significant variation over this range, with emission temperatures peaking at 40% CO<sub>2</sub>, while burn times continue to decrease with increasing CO<sub>2</sub> concentration. The relation of the emission temperature to the combustion temperature is discussed, and comparisons of emission temperatures with initial absorption measurements are made. The paper will conclude with discussions of the chemical rates for the reaction of Aluminum with CO<sub>2</sub>.

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## Rockets and SCRam Jets

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A3.1

### Magnetism, Equilibrium Combustion Compositions, and Theoretical Rocket Performance

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#### Abstract

The impact of magnetic fields on theoretical rocket performance for an infinite area combustor has been investigated. The limiting cases of frozen and equilibrium (shifting) rocket performance have been considered. A chemical equilibrium model based upon the minimization of Gibbs free energy was used to determine equilibrium combustion compositions. The expression for the Gibbs free energy was modified to account for the affect of a magnetic field on a mixture of paramagnetic and iamagnetic gases. The aforementioned chemical equilibrium model has previously been used to show that magnetic fields can significantly impact complex chemical equilibrium compositions. The model outlined in this paper was validated against existing equilibrium combustion models and previously published data on theoretical rocket performance (for the case of no applied magnetic field). A model reaction of RP-1 and oxygen was used to quantitatively examine the changes in rocket performance in the presence of a uniform magnetic field. The impact of magnetic fields on rocket performance in terms thrust, thrust coefficient, specific impulse, and characteristic exhaust velocity was considered. In addition, the impact of magnetic fields on the composition of the exhaust gases will be briefly discussed.

The results presented in this paper represent one of the first attempts to analyze the impact of magnetic fields on rocket performance in terms of the paramagnetic and diamagnetic nature of the constituent gases. Prior work, focusing upon the interaction between ionized gases and magnetic fields, has shown that externally applied magnetic fields can be used to control the burning rate in solid rocket motors. The work presented here has application to both solid rocket motors and rocket engines.

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**Solid Hydrogen Fueling of an Air Breathing Supersonic Combustor**

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Abstract

Wall injection of solid hydrogen into the supersonic airstream of a combustor has been investigated to provide ultrafast distributed fuel mixing for a practical large scramjet engine. A particle jet can penetrate the supersonic stream much better than a liquid jet can, and solid hydrogen has an extremely high dispersion/ablation rate. Modeling of a solid hydrogen particle ablating in a Mach 3 flow has been studied to understand the physics of the problem, to predict particle lifetime, and to define the dependence of particle lifetime on the parameters of the problem. Other research indicates that it is practical to pump and inject the solid as a 4 K Solid H<sub>2</sub>/liquid He with a very low helium fraction; the added helium will not decrease combustion efficiency. High speed single hydrogen pellet injection into an inert gas has been performed experimentally to examine actual ablation and verify modeling predictions. Solid hydrogen particle fueling has the potential to improve fuel distribution and mixing well beyond present concepts, eliminate injector drag, and take advantage of the more standard benefits of a higher fuel density.

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**A NUMERICAL STUDY OF VITIATION EFFECTS ON IGNITION IN TWO-DIMENSIONAL SUPERSONIC  
HYDROGEN/AIR MIXING LAYER**

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ABSTRACT

One associated complication for the use of vitiated air in laboratory studies of supersonic combustion to simulate the flight enthalpy is that the test media are contaminated by species, which are not of representative in the actual atmosphere. Particularly, since burning hydrogen in oxygen-enriched air is normally employed to produce vitiated air in the experimentation, the resulting high enthalpy airflow contains substantial amount of, for example, H<sub>2</sub>O, H, OH, O, and NO. Therefore, the primary objective of the present numerical study is to assess the effects of vitiated air on the ignition characteristics in the supersonic experiments.

Specifically, the ignition evolution in the supersonic hydrogen/air laminar mixing layer is computationally simulated using detailed chemistry and transport properties. Individual and combined influences of important contaminants on ignition are systematically examined over a range of pressure, air temperature, and free stream velocity variations. Vitiations of the active radicals, like H, O, and OH, are found to enhance ignition, as expected. Results also show that contaminations of H<sub>2</sub>O and NO can inhibit and promote supersonic ignition, respectively. The computed results on the net effect of simultaneous contaminations of H, O, OH, H<sub>2</sub>O, and NO on the ignition response further provide insight into the interpretation of the experimental data using the vitiated air facilities.

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## Diesel Engines

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A4.1

### An Investigation of Ignition and Heat Release Characteristics in Diesel Engines Using an Interactive Flamelet Model

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#### ABSTRACT

A multidimensional model is employed to model ignition and heat release rates in a Diesel engine. An interactive flamelet model is employed to model combustion. n-heptane is used as a representative fuel in the computations. Comparisons of computed and measured results are presented for a wide range of engine operating conditions: speed 1200-1500 rpm, start of injection 12.5 degrees before top dead center-9.5 degrees after top dead center and intake temperature 325-360 K. The primary objective of this work is to assess the ability of the model to reproduce ignition timings. The flamelet model uses detailed chemical kinetics and it is shown that it can reproduce the qualitative trends of changes in ignition delay and heat release rates with respect to changes in operating conditions of the engine. The capability to reproduce the measured changes in ignition delay is important because changes in injection timing lead to changes in ignition timing. Changes in ignition timing, coupled with changes in injection pressure and EGR, are employed to control NO and soot emissions in the engine. The interactive flamelet model is able to predict these changes.

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**Targeting the EPA HD-FTP 2007 Emission Standards Using a Modern Diesel Engine with EGR  
and a SCR/CRT Aftertreatment System**

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Ridge National Laboratory  
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Abstract

The EPA on-road emission standards for heavy-duty vehicles to be implemented in 2007-2010 loom as a huge technical challenge for compression ignition powertrain developers. A series of experiments based on the AVL-8 mode testing sequence were carried out on a low emissions diesel powertrain with included exhaust aftertreatment. The powertrain featured a 1999 Cummins ISB 5.9 L engine (6 cylinder, 24 valve) with an advanced cooled-EGR and low emissions fueling system. The aftertreatment system includes a continuously regenerating particulate trap in combination with a urea-based selective catalytic reduction system (for NOx removal). Ultra-low sulfur fuels were used in all testing.

Test results to date imply that the 2007+ emission standards for PM, CO and hydrocarbons could be met with such a powertrain but that NOx emissions would be quite problematic. The results strongly imply that controlling NOx to very low levels when the engine is operating at relatively low loads, including idle, is essential to meeting the 2007+ standard for NOx emissions. Even though low-load diesel engine operation produces modest amounts of NOx, the low temperature exhaust gas and SCR catalyst temperature greatly reduces the effectiveness of the aftertreatment system. This result likely applies to aftertreatment systems utilizing NOx adsorber systems, in addition to the SCR system explored in the current work. The results have strong implications for the near-term R&D needs for diesel engine combustion control.

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**A Comparison of Regulated and Unregulated Emissions from Light and Medium Duty Engines  
Operated on Diesel and Biodiesel Blends**

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ABSTRACT

Because of the great interest in many countries in biodiesel fuels, the International Energy Agency's Executive Committee on Advanced Motor Fuels sponsored Annex XIII, "Emission Performance of Selected Biodiesel Fuels." The objective was to produce emission and performance data on biodiesel and diesel-biodiesel-blends in different diesel engines with special attention to unregulated emissions. Fuels used were a baseline of ASTM 2D diesel fuel (351 ppm sulfur), the Swedish MK1 reformulated diesel fuel, rape methyl ester (both neat and 30% blended with the baseline fuel), soy methyl ester (both neat and 30% blended with the baseline fuel), UVOME30 - a 30% blend of used vegetable oil and the baseline fuel, and Oxydiesel - a 10% ethanol blend in a micro-emulsion with the baseline fuel. The test cycles were chosen to cover a range of engine operating conditions representing a large portion of the engines' operating range. An AVL 8-mode test was used to simulate the heavy duty transient test on the medium duty engine. Emissions results will be presented and will highlight the changes in emissions that occur between no. 2 diesel and the biodiesel blends. Differences in unregulated emissions will also be highlighted.

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**Resolving EGR Distribution and Mixing**

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Mike Ruth, Rob Smith and John Stang - Cummins, Inc.

Abstracts

Exhaust gas recirculation (EGR) is a strategy for reducing Nox emissions. Effective EGR implementation requires a well mixed and uniformly distributed EGR-air intake charge. A spatially resolved capillary inlet mass spectrometer (SpaciMS) has been used to map these EGR distributions based on local CO<sub>2</sub> concentration measurements. The SpaciMS physical probe is a 180-um diameter fused silica capillary which extracts ca. 10uL/min; this is sufficiently minimally invasive as to allow quantification of EGR distribution in actual engine systems.

We will describe the application of this instrument to the intake/EGR system of a Cummins V-8 medium-duty diesel engine. Two EGR hardware designs were evaluated in terms of EGR-air mixing at the intake manifold inlet and port-to-port EGR charge uniformity. Performance was assessed at four modalized-FTP engine conditions. The results indicated one design to be consistently better at three of the four engine conditions. We also characterized degraded performance for both designs at the highest mass air flows.

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**A MULTI-ZONED PHENOMENOLOGICAL MODEL OF NO FORMATION IN A DI DIESEL ENGINE**

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ABSTRACT

A cycle simulation developed by Bell for modeling coal fueled diesel engine performance is modified to predict combustion of conventional diesel fuel in a medium duty CIDI engine. The simulation code uses phenomenological models of the processes of fuel-air mixing, combustion and NO formation/destruction. The combustion rate is mixing controlled. The extended Zeldovich mechanism is applied to burning entrained fuel/air packets and the burned gas zone to calculate NO emissions. The computed data are compared with the experimental data collected in a single-cylinder test engine as a function of intake temperature and load. Good agreement is achieved for the engine performance. A methodology for adjusting an air entrainment constant model using a limited set of experimental data is described and was employed to achieve good NO emissions predictions. This model allows reasonably accurate, computationally rapid, predictions of NO emissions, and, considering its simplicity, allows a fairly detailed analysis of the principal sources of NO formation during the combustion process.

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**Boilers and Furnaces I**

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A5.1

**The Mercury Content of Ash Sampled from Various Locations in a 100MWth Wall-Fired Combustor**

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Abstract

Mercury emissions from coal combustion have become of recent environmental concern. Ash samples were collected from over 24 locations in a 100 MWth wall-fired combustor and measured for their mercury content. The highest mercury concentration was found in the ash collected from the bottom of the electrostatic precipitator. The lowest mercury concentrations were found in the ash collected from the burner area and economizer regions of the combustor. Additionally, mercury levels in the fly ash were compared to several factors including temperature and fly ash composition.

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**Investigation into Trace Elemental Composition in Ash on Mercury Emissions in a  
Utility PC Boiler**

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Abstract:

Trace elemental compositions, such as C, H, N, Hg, S, Ca, Cl, and ash content that existed in different locations of a utility PC boiler system, were collected and analyzed in order to investigate the formation of mercury and interactions among these elemental compositions as a result of coal fired combustion process. The relationship between mercury emissions and the temperature profiles in the boiler system was verified.

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**Field Testing of Reducing Mercury with High Chlorine Coals**

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Abstract:

Coal-fired utility boilers were identified as the largest source of mercury emissions in the United States. A study of mercury removal by firing with high chlorine coals in a pilot FBC system at the Western Kentucky University showed that the mercury releasing into the atmosphere had been lowered to only 5% of the total fuel mercury processed.

The field testing with high chlorine coals (Avg. Cl: 0.11%~0.45%) from Kentucky and Illinois has been conducted in a Power Station at Kentucky without further capital cost and additional equipment. The flue gases are trapped with the Ontario Hydro Method, consequently auto-sampled with Leeman Hydro Prep to analyze the elemental and oxidizing mercury with Leeman Hydro AA (simultaneously controlled by PS Analytical CEM for the measurement of the total mercury). The flue ashes are analyzed with LECO AMA-254.

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**Field Corrosion Testing with High Chlorine Coal in a Low NO<sub>x</sub> Burner Utility Boiler**

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Abstract:

Whether or not the chlorine in coal can corrode boiler components is not well understood, at least how and in which form it occurs during combustion. Some literature reports correlated corrosion of utility boilers with coal chlorine. However, some other studies recently indicated that there isn't apparent relationship between coal chlorine and corrosion in combustion process, such as corrosion testing conducted in a AFBC facility in the Western Kentucky University. In order to convince the utility industry, a new project of the short and long term field testing for corrosion are being conducted at a Power station. The objective of the project is to better understand the corrosion processes that take place in the test materials and the relationship between the metal's corrosion behavior and the corrosion conditions (including temperature, flue gases, and ash deposits).

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## Boilers and Furnaces II

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A6.1

### Integration of Coal Gasification and Reburning

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#### Abstract

Reburning (fuel staging) is a commercial technology to control NO<sub>x</sub> emissions from stationary combustion sources. Reburning involves injecting additional fuel above the existing burner zone followed by overfire injection for burnout and CO control. Although natural gas reburning is a proven technology for effective NO<sub>x</sub> reduction and reducing carbon losses, the cost of gas is significantly higher than the cost of the main fuel, coal. Coal reburning is more cost effective than natural gas reburning, but usually is less effective in NO<sub>x</sub> control. Coal reburning can also result in increased carbon-in-ash levels, precluding utilization of the ash by the cement industry.

To address these problems, GE EER is developing Fuel-Flexible Reburning (FFR) which will increase efficiency of NO<sub>x</sub> reduction in coal reburning and allow coal to be utilized under conditions that minimize carbon-in-ash. In FFR, coal is partially gasified before injection into reburning zone. The work includes a combination of analytical and experimental studies to identify optimum process configurations and develop a design methodology for full-scale applications. Tests were performed in a 1.0?10<sup>6</sup> Btu/hr Boiler Simulator Facility with two bituminous coals. The reburning fuel was partially gasified and injected into the furnace through an injector designed to provide rapid dispersion of the fuel into the flue gas. Tests showed that coal gasification improved reburning performance by 5-10% depending on coal nature, gasification temperature and residence time in the gasification reactor.

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**A Numerical Investigation of Combustion Patterns in Various Furnaces**

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Abstract

Furnaces are widely used to provide energy in industries. A computational fluid dynamics (CFD) code has been developed at Argonne National Laboratory to simulate turbulent mixing, combustion reaction, radiation heat transfer, and pollutant kinetics of the combustion flow. The code employs an integral approach to incorporate a lumped combustion reaction model in the flow calculation and a separate hybrid technique to perform pollutant kinetics calculations for  $\text{NO}_x$  and soot. The lumped combustion reaction model considers five major species, i.e., natural gas, oxygen, nitrogen, and two lumped products. A five-step kinetic mechanism was modified and used to calculate methane burning and NO formation. Since soot particles are small, they are treated as a gaseous subspecies. A soot model was developed based on kinetic models to calculate soot concentration for the radiation heat transfer calculation. Both soot formation and oxidation are considered. The CFD code has been validated with experimental data collected from industrial furnaces.

The validated code was used for a parametric study of various furnace geometries. The parameters studied were the air to fuel ratio, air inlet temperature and velocity, and fuel inlet velocity. These parameters were investigated to determine their effect on species concentration and mixing as well as the temperature and velocity distribution of the combustion products. Preliminary results show that the air to fuel ratio has an important effect on the temperature of the combustion products and improved species mixing near the nozzle with increased velocity. The study also demonstrates that CFD can be a useful tool for analyzing the flow field of the combustion space in industrial furnaces. The details of the combustion model and results will be discussed in the paper.

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**Numerical Simulation of Industrial Nozzle-mix Burners Per Strain**

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## Abstract

In industrial combustion systems, the heat generator consists of one or more burners where a fuel is burned with an oxidizer, ranging from air to pure oxygen. Different types of burners are in use, depending on the specific requirements. However, the high heat load required for such burners necessarily implies that the burners have to operate in the turbulent regime. For an industrial burner, the most important characteristic feature is the flame height. Flame height plays an important role in NO<sub>x</sub> emission and is controlled by several factors like fuel stoichiometry, fuel jet momentum, presence of coflow air and presence of confinements. Consequently, flame heights of turbulent flames have been studied for several decades. However, most of the available studies discuss turbulent combustion in unconfined burners only. The objective of the present work is to simulate a nozzle-mix non-premixed burner for aluminum remelt furnace. The burner is modeled as an axisymmetric vertical arrangement of fuel duct at the center, surrounded by a coaxial annular duct of air. The ducts discharge into a confined environment, formed by a chimney, placed coaxially with the ducts. The available results cannot be directly applied to the present case as, based on the requirements of the application, (1) the coflow air velocity is nearly of the same order as the fuel velocity and (2) the confinement is much closer to the jets than in the studies available in literature. The flow field, temperature and species distributions and the flame profile were obtained from solution of the equations for conservation of mass, momentum, energy and the species. The flow was considered turbulent and modeled using RANS-based approaches. The equations were solved using commercial CFD software, FLUENT Version 5.4. The different turbulence, combustion and radiation models, available in the software, were employed in the modeling to assess the sensitivity of the results to the choice of model. Based on comparison with experimental data on turbulent burners available in literature, we finally adopted the standard k-epsilon model for turbulence and eddy dissipation model for combustion. Different definitions of flame lengths used in the literature were employed to assess the sensitivity of the flame lengths obtained from simulations to the definition adopted. This kind of sensitivity analyses are not readily available in open literature. The effects of fuel velocity and air coflow on flame lengths were studied for both buoyancy-dominated and initial momentum-dominated regimes of combustion. It was observed that the flame length was relatively insensitive to fuel velocity in the momentum dominated regime but showed strong dependence in the buoyancy-dominated regime. However, flame length decreased with increase in coflow velocity for both the cases.

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**Combustion Characteristics of a Natural Gas Burner Using Inert Porous Media**

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ABSTRACT

Recent interest in combustion of hydrocarbon fuels within porous inert media has arisen due to the desire to create efficient burners to meet increasingly stringent emissions requirements. Combustion within porous inert media is designed to recirculate product enthalpy to precombustion zone reactants. Increasing the enthalpy of reactants promotes more complete combustion, which decreases unburned hydrocarbon and carbon monoxide emissions. The increase in radiant heat output is a result of radiative heat transfer from the porous material, as opposed to the weak gas radiation in conventional combustors. An experimental investigation of premixed methane-air combustion is described in this paper. The burner section consisted of four interchangeable open-cell silicon carbide foam materials with pore sizes ranging from 10 to 80 ppi. The premixer section also utilized the open cell silicon carbide foam materials. Experiments were performed to determine the configuration of pore sizes that would yield stable combustion over the widest range of flowrates and equivalence ratios. Measurements included determination of the lean flammability limit at various flowrates, emissions of NO<sub>x</sub> and CO, and temperature of the product gas. The results of this experimental study can be used in further development of porous medium combustion for gas turbines and other applications.

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**Lattice Boltzmann Simulation of Laminar Jet Diffusion Flame**

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Abstract

This paper reports simulation of laminar jet diffusion flames based on a two-distribution lattice Boltzmann algorithm. One distribution function represents the transport of the Schvab-Zeldovich coupling function, the mixture fraction that combines the energy and species equations. The other distribution function models the compressible Navier-Stokes equations. The modified equilibrium distribution functions recover the macroscopic governing equations up to second order accuracy. The characteristic-based Galerkin finite element method is used to discretize the set of lattice Boltzmann equations on unstructured mesh, and to capture large gradients near the jet nozzle exit. A 2-D slot-jet burner is tested. The results are in agreement with Roper's theoretical prediction of a steady Burke-Schumann diffusion flame. The lattice Boltzmann algorithm is also used in the time-dependent simulation of a laminar jet diffusion flame. The simulation predicts the flame flicker phenomena in normal gravity, with a realistic flicker frequency in the range of 10 to 15 Hz.

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## Diffusion Flames

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B1.2

### Dynamics of Radiative Edge Diffusion Flames

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#### ABSTRACT

Dynamics of nitrogen-diluted hydrogen edge flames burning in air were computationally studied using a constant density, one-step reaction model in a plane counter flow configuration. Both adiabatic and radiative edge diffusion flames were investigated and compared. A simple grey gas model with an optically thin assumption was used to investigate the effects of gas phase radiation on flame dynamics and structure, with emphasis on the flames near the low stretch radiatively induced extinction limit. Due to the effects of sub-Lewis number, these kinds of flames were observed to give rise to strong cellular instabilities, like advancing flame edges, stationary and moving warps of flame strings, close to the extinction Damkholler numbers in the high stretch region. Some sub-limit structures were also observed for Damkholler numbers below the 1D blowoff extinction limit, indicating the ability of the cellular structures to resist 1D high-stretch quenching. Furthermore, the ability of the flame to resist quenching by radiative heat loss was tested by checking for two-dimensional flame structures for Damkholler numbers above the 1D radiative extinction limit.

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**Soot and NO Formation in Counter-flow Diffusion Flames under Oxygen-enriched Conditions**

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Abstract

Soot and NO formation are studied as a function of the amounts of methane in the fuel stream and of oxygen in the oxidizer stream at a global strainrate of 20 1/s. As the percent methane in the fuel stream increases, less percent oxygen in the oxidizer stream is required for soot inception. A detailed soot model suggests that incipient soot formation is consistent with a peak flame temperature near 2550 K. Oxy-fuel flames are more sooting as they contain less than 10% N<sub>2</sub> in both the fuel and oxidizer streams. Peak soot volume fractions in these flames correspond to a temperature near 1500 K. Laser-saturated fluorescence measurements of nitric oxide concentration ([NO]) in six different oxy-fuel flames are compared with predictions from an opposed-flow diffusion flame code by using an optically thin radiation model for major gaseous species along with the GRI kinetic mechanism (version 3.0) for NO formation. The results indicate that peak [NO] is over predicted, especially at higher temperatures associated with lower N<sub>2</sub> dilution levels. Better agreement between measurements and computations occurs when enhanced radiative heat loss from soot is included in the kinetic model.

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**Diffusion Flame Stabilization and Reaction Kernel Structure in Microgravity**

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Abstract

The structure of laminar methane jet diffusion flames in normal earth gravity (1g) and zero gravity (0g) has been simulated numerically. Computations of the time-dependent full Navier-Stokes equations with buoyancy were performed using an implicit, third-order accurate numerical scheme and a detailed C2-chemistry model. An optically thin-media radiation model for heat losses from CO<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>, and CO is included. Observations of the flames were also made at the NASA Glenn 2.2-Second Drop Tower. The parametric computational results are as follows: (1) In a quasi-quiescent oxidizing environment in 1g, buoyancy induced the entrainment of the surrounding oxidant into the flame base and formed a peak reactivity spot, i.e., reaction kernel, responsible for flame stabilization. (2) In a quasi-quiescent, 0g environment, diffusion-dominated transport processes reduced the peak reactivity an order of magnitude smaller. (3) In a coflowing oxidant stream in 0g, the flame structure became similar to that in the 1g environment as a result of a 'blowing' effect. (4) The 2D flames were generally larger than the axisymmetric flames because of geometrically limited transport processes in 2D directions. (5) The flames in an oxygen-enriched environment were generally smaller than those in air as a result of higher reaction rates and stoichiometry. This paper extends the previously proposed correlations between the reaction kernel reactivity and velocity and the reaction-kernel hypothesis for diffusion flame stabilization to the near-zero velocity conditions in microgravity.

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**Influence of Gravitational Level on Laminar Diffusion Slot Flame Behavior**

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Abstract

This paper provides the results of an investigation into the premise that, in the buoyancy-controlled regime, the flame height of a laminar diffusion flame produced using a slot burner is inversely proportional to the buoyant acceleration raised to the one-third power. The validity of this premise is examined by examining the behavior of a laminar diffusion flame under different gravitational levels. Variation in the gravitational level was produced by conducting a series of experiments aboard the KC-135a at the NASA Johnson Space Center. Luminous flame heights and shapes for laminar diffusion slot flames burning propane (99.999% purity) in quiescent air at gravitational levels in the range of 0.1g to 1.7g were measured. Test conditions involved burner widths of 0.245mm and 0.508mm and burner length of 3.81mm. Images of flame behavior were recorded using a color CCD camera and a Hi8 video recorder. Stoichiometric flame height was determined for the non-sooting flames by examining the peak blue luminosity of the video images of the flames. The data is compared to several different flame models and conclusions are drawn as to the validity of these models for laminar diffusion slot flames.

The results presented in this paper represent one of the first attempts to analyze the fundamental behavior of laminar diffusion flames using slot burner ports. To date, reduced gravity combustion research has focused almost exclusively on flames produced using circular burner ports. As a result of the seminar work of Roper, it is now recognized that the behavior of laminar diffusion flames produced using different burner port geometries are fundamentally different.

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**Laminar Slot Diffusion Flames in Non-Uniform Magnetic Fields: Experimental Flame Height Correlations**

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Abstract

The impact of non-uniform magnetic fields on laminar diffusion flame behavior is quantified through the use of experimentally determined correlations. Luminous flame heights and shapes for laminar diffusion slot flames burning propane (99.5% purity) in quiescent air at were measured both with and without an applied magnetic field. Non-uniform magnetic fields were established using two Neodymium-Iron-Boron (NdFeB) magnets and two gray steel prisms. Test conditions involve a maximum magnetic field strength of 1.000, 0.750, 0.500, and 0.000 Tesla. Images of flame behavior were recorded using a single reflex camera with a 1-5X macro lens. Flame behavior was recorded for flow rates from the "near extinction" point to the visible soot inception point. Luminous flame height and shape were determined using digitized images of the flames and image analysis software. The flame height data was nondimensionalized and experimental correlations were developed. These correlations are compared to existing correlations for flames with no applied magnetic field and conclusions are drawn with respect to the impact of magnetic fields on flame height. The results indicate that an applied magnetic field with a decreasing magnetic field gradient decreases the height of a diffusion flame. The impact of non-uniform magnetic fields on flame shape is also discussed relative to flame behavior with no applied magnetic field.

It is well known that non-uniform magnetic fields can significantly affect diffusion flame behavior as a result of the diamagnetic and paramagnetic gases in the flame region. The results presented in this paper represent the first attempt to develop experimental correlations of flame height behavior in a non-uniform magnetic field. Such correlations can be used to predict flame behavior and to validate future mathematical model of laminar diffusion flames in non-uniform magnetic fields.

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## Partially-Premixed Flames

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B2.1

### Transition of Propagating Triple Flames to Burner Attached Flames in an Axisymmetric Jet

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#### Abstract

The characteristics of propagating triple flames in axisymmetric partially premixed jets are both experimentally and numerically investigated at relatively low velocities. Rich mixtures of methane and air from an inner tube and air from a concentric outer tube are ignited downstream with a pulsed Nd:YAG laser. Flame propagation images are recorded by a high-speed video camera and the flame propagation speed is determined. A time-dependent, implicit numerical model that employs a detailed description of the chemistry and includes buoyancy effects is used to simulate the flame structures. The numerical results are validated through comparisons with experimental measurements. Both experimental and numerical results show that the edge of the propagating flame exhibits a triple flame structure and the flame propagation speed has a good correlation with flame curvature and flame stretch rate. However, with the flame approaching the burner wall, the triple flame degrades into an edge flame structure, which its lean premixed wings lost under the influence of various parameters in the system, such as Lewis number, flame stretch, heat loss rate etc.

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**A Study of Effects of Radiation Including Absorption on a Methane/Air  
Partially-Premixed Flame**

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Abstract

Experimentally verified significant effects of a very small amount of radiation heat loss in a partially premixed flame (1 - 2 % of local heat release for the rich premixed flame and 6 to 11% of the local heat release for the diffusion flame) are reported and discussed. The objective is to improve our understanding of the interactions between radiation including the effects of emission and absorption and detailed chemistry. An opposed flow partially premixed flame burning methane and air with a rich side equivalence ratio of 1.8 is considered using a one dimensional code including the treatment of radiation emission and absorption suitable for plane parallel layers represented by this configuration. The spectral properties of CO<sub>2</sub>, H<sub>2</sub>O, CO and CH<sub>4</sub> are considered using a weighted sum of gray gases model derived from a previously validated narrow band model. The effects of the small radiation heat loss (1 to 2% of heat release) on the rich premixed flame were more pronounced than those of the relatively larger heat loss (6 - 11% of heat release rate) on the diffusion flame. This somewhat surprising finding is explained using the basic differences in the structure of the two types of flames. The results show that the effects of radiation heat loss on the major species concentrations and temperature can be accounted for by defining an appropriate reaction progress variable and a radiation-adjusted flame speed. However, such simple adjustments are not adequate for capturing the effects of radiation on the volumetric heat release rate in the premixed flame and

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**Effect of Unequal Fuel and Oxidizer Lewis Numbers on Flame Dynamics**

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Abstract

The presence of a large disparity of diffusion rates of various species and unequal rates of heat and mass transfer cause the Lewis number to vary significantly in a flame. The interaction of non-unity Lewis number with the coupled effect of radiation, chemistry and unsteadiness alters several characteristics of a flame including its structure and stability. The consideration of this interaction is important for obtaining the improved quantitative predictive understanding of turbulent flames. The present study numerically investigates this interaction with a particular emphasis on the effect of unequal and non-unity fuel and oxidizer Lewis numbers. The effect of fuel (oxidizer) Lewis number is investigated by varying the fuel (oxidizer) Lewis number from 0.5 to 2 while keeping the oxidizer (fuel) Lewis number equal to unity. The unsteadiness is simulated by considering the flame subjected to modulations in reactant concentration and by the degree of partial premixing. Flames with different strain rates and subjected to different modulating frequencies are considered. The results show various similarities and differences of the fuel and oxidizer Lewis numbers effects on flame dynamics.

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**Extended Flame Stability for Partially Premixed Acetylene-Air Flames by Acoustic Control**

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Abstract

An axisymmetric, co-flow acetylene-air diffusion flame was driven by an acoustic source at frequencies ranging from 230 to 3100 Hz and powers of 0 to 10 W. Soot formation and total production from the flame was determined by laser extinction measurements and also by soot sampling. The 940 Hz driving most strongly modified the concentration of soot released from the flame. For large acoustic forcing (power), the soot concentration was reduced by almost three orders of magnitude, essentially suppressing soot release from the flame. In the same burner, partially premixed flames were characterized over a range of equivalence ratio. While initial addition of air into the fuel stream slightly raised the soot released, further addition of air would suppress soot production. The mechanisms responsible for modification of the soot properties under acoustic forcing were consistent with a partial premixing process. The same levels of soot suppression could not be achieved by partial premixing as by acoustic forcing because stability considerations limited the amount of air that could be directly premixed with the fuel. This suggests that acoustic mixing is more stable at the same overall level of premixing than conventional mixing. This study aids in clarifying the enhanced soot production in some acoustically pulsed systems described in the literature and also describes the stabilizing effect of the acoustic field.

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**Laser-induced Fluorescence Measurements and Modeling of Nitric Oxide in  
High-Pressure Partially Premixed Flames**

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**Abstract:**

Quantitative laser-induced fluorescence (LIF) measurements of nitric oxide concentration ([NO]) have been obtained along the centerline of methane-air counter-flow partially premixed flames between one and five atmospheres. Fuel-side equivalence ratios of 1.45, 1.6, 1.8 and 2.0 and global strain rates of 20, 30 and 40 s<sup>-1</sup> are investigated at each pressure. Linear LIF measurements of [NO] are corrected for variations in the electronic quenching rate coefficient by using major species concentrations obtained from an opposed-diffusion flame code and quenching cross-sections for NO available from the literature. Corrected linear LIF measurements of [NO] are compared with numerical predictions from an opposed-flow flame code by utilizing the GRI chemical kinetic mechanism (version 2.11 as well as 3.0). The effect of radiative heat loss is accounted for by using an optically thin radiation model. A sensitivity analysis is used to identify key reactions having an influence on NO chemistry in these high-pressure partially premixed flames. A pathway analysis is also performed to study relative contributions of different NO formation pathways for the flames under investigation.

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## Turbulent Flames

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B3.1

### Flow Structure in Lean Premixed Swirling Combustion

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Swirling flows have been widely used in industrial burners, furnaces, and gas turbine combustors to improve blowoff characteristics, ignition stability, mixing enhancement, flame stabilization, and pollutant reduction. Mean flow structure of the swirling flows with and without combustion has been extensively studied over the last forty years. Some important phenomena in swirling combustion, such as combustion instabilities, depend on the multipoint instantaneous flow structure. However, the multipoint instantaneous flow structure in swirling flows has not been revealed in the past work because of measurement difficulties in the complex flow environment. Motivated by this, a cross-correlation particle image velocimetry (PIV) system was used to measure the multipoint instantaneous velocity fields in strongly swirling flows with a theoretical swirl number of 2.4 and a Reynolds number of 72,000. The mean flow structure based on the present measurements is consistent with the literature. However, the multipoint instantaneous flow structures show significantly different characteristics compared to the mean flow structure. Many smaller scale vortices with both directions of vorticity appear in the instantaneous flow in contrast to a single large vortex observed in the mean flow. Heat release seems to help a breakdown of the multiple vortices to produce a more homogeneous field. The turbulence intensity has a spatial distribution similar to that of the mean velocity. The heat release significantly increases the magnitude of the mean and the instantaneous vorticity. The differences in the flow structure and length scales of the vortices between the mean and the instantaneous fields suggest that the latter should be used in evaluations of transient phenomena and simulations.

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**Hydroxyl Time-series Measurements in Turbulent Non-premixed Swirling Flames**

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Abstract

Time-series measurements of OH are reported for turbulent, swirling, non-premixed, methane-air flames. The [OH] data are consistent with a mean reaction zone surrounding a central recirculation zone, with residual OH in the recirculation zone approaching chemical equilibrium. Modeling of the OH electronic quenching environment, when compared to fluorescence lifetime measurements, suggests that the reaction zone burns as a partially-premixed flame. The time series and probability density functions indicate the presence of thin flamelet-like regions based on the relationship between swirl-induced turbulence and fluctuations of [OH] in the reaction and recirculation zones. The OH integral time scales are found to qualitatively correspond to mean velocity measurements in similar methane-air swirling flames. In particular, quantitative dependences can be established on axial position, Reynolds number, and global equivalence ratio. Based on these relationships, the OH time scales, and thus the reaction zone, appear to be dominated by convection-driven fluctuations. These results for OH time-scales in non-premixed swirling flames are the first obtained in a recirculating flow and are similar to previous OH results in non-premixed jet flames.

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**Measurements of OH Time Series in Turbulent Non-Premixed Jet Flames**

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Abstract

Quantitative hydroxyl time-series measurements have been obtained using picosecond time-resolved laser induced fluorescence (PITLIF) in a series of turbulent H<sub>2</sub>/N<sub>2</sub> jet diffusion flames. Radial profiles and temporal results are reported, including probability density functions, autocorrelation functions and integral time scales, for a range of Reynolds numbers (6200-13,000) and axial locations ( $x/D = 5-50$ ). The autocorrelation functions are self-similar and can be fully characterized by their integral time scales. The time-series statistics are compared to previous data for other jet flames and to numerical simulations of the time-series statistics. These numerical simulations utilize the laminar flamelet approximation and assumed values for the mixture fraction statistics.

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**MEASUREMENTS AND STOCHASTIC TIME AND SPACE SERIES SIMULATIONS  
OF SPECTRAL RADIATION IN A TURBULENT NON-PREMIXED FLAME**

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Abstract

Experimental data are essential for the validation of radiation sub-models, which have been found to be important for predicting pollutant formation in turbulent flames. Instantaneous radiation signals also provide fundamental information about scalar properties in turbulent combustion. Motivated by this, we report measurements of line-of-sight spectral radiation intensities from a non-premixed CH<sub>4</sub>/H<sub>2</sub>/N<sub>2</sub> turbulent jet flame. The burner and the operating conditions are selected to take advantage of extensive scalar property and velocity measurements available in the literature. At three axial locations in the flame, a fast IR array spectrometer was used to capture the instantaneous radiation intensities for diametric radiation paths. Radiation intensities for the chord-like paths along various radial positions at one of the axial locations were also measured. By using stochastic time and space series analysis (STASS), the instantaneous emission spectra were also simulated accounting for the turbulence/radiation interactions. In the simulations, the measurements of scalar statistics and mean velocity data were adopted to avoid uncertainties of a combustion model. The calculated mean and root mean square spectral radiation intensities are within 10% of the experimental data. Since the calculated root mean square values are strongly dependent on the integral length scales used in the STASS, these scales were estimated by fitting the calculation to the data. A tomographic technique was also adapted to simulate the radiation intensities for chord-like paths from the flame edge to the center to examine the radial variation of the integral length scale. The results show a factor of three variation in the integral length scale that has been ignored in the past work.

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**Passive-Active Control of Combustion Oscillations**

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*ABSTRACT*

Combustion oscillations (dynamics) have become a major challenge in the development of low-emission premix combustors. Numerous recent papers have considered the various mechanisms that drive oscillations, as well as acoustic features of the combustor and fuel system that participate in sustaining unwanted oscillations. In this paper, a technique to control these oscillations is demonstrated. The technique combines both passive and active elements. A variable impedance fuel system is used to modulate the phase and magnitude of the combustion response, similar to active control, but without high frequency fuel modulation. Tests carried out in an atmospheric 30 kW combustor demonstrate significant oscillation attenuation over a reasonably wide combustor operating map. In this paper, results of these tests will be presented, along with ongoing theoretical analysis needed for reliable scale-up.

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## Premixed Flames

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B4.1

### Effect of micro-jet injection on the nonpremixed flames

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#### Abstract

The injection of a high-velocity micro-jet along the centerline of a laminar non-premixed methane jet flame established in a quiescent environment has been investigated both numerically and experimentally. The flame height and shape change significantly as the central micro-jet containing either air or nitrogen is introduced. The flame heights are smaller and the flames are considerably less sooting. The flame also becomes free from the buoyancy-induced flickering. In the presence of the micro-jet, the flame shape contains two distinct regions, i.e., a diffusion-dominated round overventilated attached flame along the periphery, which surrounds a central trailing jet that is formed due to strong advection. We hypothesize that the narrow, strong central jet enhances the entrainment of the surrounding air that leads to a larger oxidizer influx, which reduces sooting. The effects of the micro-jet on the flame characteristics similar to those of partial premixing, but the former is free from the inherent hazards involved with the handling of a premixed fuel-air mixture.

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**Structure of a Reacting Wall Jet**

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Abstract

When a jet impinges on a wall, the structure of the jet after impingement may be close to that of a wall jet. The structure of the wall jet differs from that of a free jet. These differences will be discussed. In the case of a combusting jet, the wall interaction may affect the chemical kinetics and the structure of the flame. This paper describes the results from a computational study that shows the effects of wall interaction on the structure of a laminar flamelet. Computations are carried out for a laminar reacting methane jet that impinges on a wall. Chemical kinetics is modeled with two mechanisms: a reduced mechanism with 19 species and a detailed mechanism with 53 species. The structure of the flame is studied in both the free jet region and in the wall jet region. It is shown that heat loss to the wall has a noticeable effect on this structure. This difference would, in turn, affect NO and soot formation rates and soot oxidation rates in impinging jets.

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**Opposed Jet Flames of Lean Premixed Hydrocarbon-Air Reactants vs. Hot Products**

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Abstract

Since lean direct injection for internal combustion engines has the benefit of increased fuel efficiency, it is attracting wide research interest. At low power, lean direct injection of fuel may lead to stratified charge regions: lean, stoichiometric or rich areas in combustor. In the lean regions, incomplete combustion can lead to increased hydrocarbon emissions in the engine exhaust. In order to understand how to maintain lean-limit combustion occurring in a direct injection engine, several lean partially premixed methane-air flames versus hot products are investigated. A hydrogen-air flame that doesn't bear the carbon element is used to generate hot products to support lean the partially premixed flame. Different from previous studies with propane as fuel, some improvements for the experiment system have been made: an improved Raman optical collection system is used to give better discrimination against flame background; a flush exit screen is used instead of ring for opposed jet burner to avoid an anchored flame. The Raman scattering measurement of major species concentration and temperature will be compared to detailed numerical simulations using the Oppdif code with several chemical kinetic mechanisms.

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**On Laminar Flame Speeds of Fuel Blends: Ethylene, n-Butane, and Toluene Flames**

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Abstract

The atmospheric laminar flame speeds of mixtures of air with ethylene, n-butane, toluene, ethylene-n-butane, ethylene-toluene, and n-butane-toluene were experimentally and computationally investigated over an extended range of equivalence ratios. Binary fuel blends with 1-to-1, 1-to-2, and 2-to-1 molar ratios were examined. Experimentally, the laminar flame speeds were determined using Digital Particle Image Velocimetry (DPIV). Since the use of DPIV enables the mapping of the two-dimensional flow field ahead of the flame, the reference speed based on the minimum axial velocity point as well as the imposed strain rate can be identified simultaneously. The latter can now be unambiguously determined by the radial velocity gradient at the minimum velocity point. By systematically varying the imposed strain rate, the corresponding laminar flame speed was obtained through nonlinear extrapolation to zero strain rate. The associated experimental accuracy of the DPIV measurements is also assessed and discussed. Computationally, the laminar flame speeds were simulated for all single-component fuel/air and binary fuel blend/air mixtures with a detailed kinetic model. Comparison of experimental and computed flame speeds shows generally good agreement. A semi-empirical mixing rule was developed. The mixing rule, which requires only the knowledge of the flame speeds and flame temperatures of the individual fuel constituents, is shown to provide accurate estimates for the laminar flame speeds of binary fuel blends under the conditions tested.

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**Response of Flame Speed to Positively and Negatively Curved Premixed Flames**

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Abstract:

We address flame stretch effects on two-dimensional premixed *\_regular\_* (RF) and *\_inverted\_* (UF) flames burning methane-air and propane-air mixtures through an experimental investigation. The regular flames have a negative curvature and are concave to the unburned mixture, while the inverted flames have are positively curved and convex. The response to stretch (that addresses the influence of curvature) differs along the planar and curved regions of a premixed flamefront. A curved flame behaves as a lens that focuses (negative curvature) or defocuses heat from the burned to the unburned side depending upon its curvature, but defocuses (negative curvature) or focuses the concentration of the deficient reactant from the unburned side into the premixed reaction zone. The focusing of heat into the unburned side of the negatively curved RF raises the local temperature in the unburned region and increases the upstream velocity. The positive curvature of the UF induces a positive stretch rate, which decreases the flame propagation speed by lowering the local reaction and heat generation rates. However, the combined effects of stretch and curvature are more complex. The planar and curved regions have different responses to stretch. The planar regions behave in accord with the Markstein  $Su(k)$  linear relation and the unstretched flame speeds  $S_{uo}$  thus inferred are in accord with the literature. The flame speed, however, changes dramatically along the curved regions due to curvature effects. Although curvature effects are included in the definition of stretch, they are not fully accounted for by the  $Su(k)$  Markstein linear relation. Even after considering the effect of curvature in the definition of  $k$ , strong negative curvature raises the value of the flame speed above the prediction of the  $Su(k)$  expression, while strong positive curvature reduces its magnitude below that predicted by the relation.

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## Fires

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B5.1

### Large Eddy Simulation of Buoyant Turbulent Pool Fires

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#### Abstract

Three dimensional large eddy simulations (LES) of two buoyant flows were performed in conjunction with a Smagorisky turbulence model. The flows included a non-reacting helium plume previously simulated with two-dimensional simulations and a methane/air turbulent diffusion flame. In comparison with the previous two-dimensional simulation results, the three dimensional LES results for the helium plume show much better agreement with the available experimental data. A relatively simple combustion model involving Lagrangian thermal elements with a single empirical constant involving the time to burn out of notional fuel parcels was adequate for obtaining reasonable predictions of the mean velocity and vorticity fields. The model also captured the temperature distribution patterns in the methane/air diffusion flames reasonably well. The agreement between the measurements and predictions for these two flows establishes the basic capabilities of LES for buoyant fire applications.

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**Studies of Detailed Heat Transfer Processes in Flame Spread Over Thin Fuels in Microgravity**

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Abstract

Flame spread over cellulosic materials has received attention by researchers in the combustion community. We perform a numerical analysis of the heat transfer part of flame spread over a thermally thin fuel, whose physical and experimental aspects are discussed in the work of Oravec and Wichman (same conference). The numerical study is intended to indicate:

- (1) which heat transfer processes dominate the spread mechanism;
- (2) which heat transfer processes may cause instability mechanisms to arise;
- (3) the role of the backing or heat-loss substrate on the spread mechanism;
- (4) the influence of actual cellulose pyrolysis kinetics on the heat transfer, release of volatile combustibles, and formation of char from the original solid fuel.

The purpose of this study is to clarify some of the basic processes that occur in an environment in which it is difficult to make quantitative measurements, and to suggest the application of diagnostic methods to the actual tests. For example, the numerical methods suggest that the temperature traces at the back of the sample surface may in fact be more indicative of actual spread processes than those on the front surface underneath the flame. Other aspects of the overall heat transfer problem are also discussed, including analytical components.

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**Spreading Diffusion Flame Instabilities For Thin Solid Fuels in Reduced Buoyancy Conditions**

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Abstract

Diffusion flame instabilities for a flame traveling over a thin, wide cellulosic fuel were produced in a reduced gravity environment by varying the test section height in a Hele-Shaw apparatus. Aside from observing inviscid flow patterns, this type of wind tunnel may be employed to suppress buoyant motion and remove the effects of gravity by the close spacing of plates. The fuel sample was located in the middle of the test section between the ceiling of the tunnel made of quartz, and the floor of the test section, which was a polished copper heat sink. This enabled test section air velocities to be accurately calculated. The instabilities in low gravity were a function of the test section height and distance to the copper substrate, which were equivalent and varied between 3-7mm. An opposed flow oxidizer configuration was used, and air velocities were reduced for each test in situ to induce unstable flame behaviors. Depending on the change in flow conditions and the test section and substrate distances, the initial flat flame front that stretched across the fuel transformed into a corrugated front or broke apart into smaller cellular flames called flamelets. In some cases, flame pulses with definite frequencies traversed the front and flamelets, and flamelet oscillations in which the area increased and decreased periodically also occurred. A preliminary flammability map indicated observable regions of instabilities. Flamelet size was seen to increase with test section height, while pulsing frequencies decreased. Further analysis of results will be used for selecting proper conditions of tests in spaceflight onboard the International Space Station (ISS). Furthermore, the results will help to construct a theoretical model of low gravity diffusion flame instabilities, since many processes in the current tests have been seen in other studies using different geometries.

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**The Impact of Intumescent Coatings on Shipboard Fires**

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Abstract

Limitations of the intumescent class of paint have been documented with respect to shipboard fires. A series of full-scale fire tests were conducted at the Navy's Advanced Fire Research Laboratory ex-USS SHADWELL (LSD-15) in Mobile, Alabama. The goal of this testing was to determine whether the subject coatings could provide Passive Fire Protection (PFP) qualities for shipboard surfaces. These tests, using both ALPHA and BRAVO fuel sources, evaluated six different intumescent coatings from four separate manufacturers. The data collected indicate the subject coatings are incapable of meeting heat transfer restrictions of the existing passive fire safety performance criteria, MIL-PRF-XX381, mandated by the Naval Sea Systems Command. In addition data show the coatings will not provide the level of protection equivalent to Navy fire insulation. The trends observed from both physical observation and data show the six intumescent coatings can be defeated, forming no char layer, when the thermal insult is slow growing or at a distance from the coated surface. Additional failure mechanisms attributed to these coatings include, fragile char of non-uniform depth, inability of one coating to remain bonded to the test surface once exposed to fire and inability of the coatings to form a char layer when the flaming insult is on the far side of the test surface. The subject test fires produced a fire growth curve less severe than the targeted UL-1709 standard. The documented performance of these coatings seems to indicate they will be incapable of mitigating conditions favorable for fire spread when exposed to a more severe fire. While the fire retardant characteristics of the intumescent coating are both recognized and documented, the shipboard need to prevent fire spread beyond the initial point of origin requires attributes not currently ascribed to the intumescent class of paint. Data and photographic documentation are presented to illustrate how an intumescent coating may not be a suitable PFP material for shipboard applications.

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**Influence of Bubbles on In-Depth Structure of Surface Layers of Thermoplastics During Combustion**

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Abstract

A new experimental procedure for the determination of the thermal conductivity of polymer subjected to an incident heat flux under flaming conditions is presented. The procedure involves determining the number distribution and average size of voids formed in the burned polymer sheet. In reality, the layer in which bubbles form is liquidous, but such layers are difficult to examine. We therefore allow the heated polymer to cool, solidify, and freeze in place, then we examine the voids for their number and size distributions. The void distribution depends on both depth and heated location of the polymer layer, since the in-depth heating distribution varies with distance normal to the surface and with surface location under the flame, respectively. The thermal conductivity of the entire material can be calculated as a function of depth in the polymer sheet. These values are to be eventually compared with measured global values obtained using parameter estimation techniques.

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## Kinetics

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B6.1

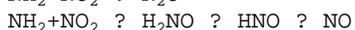
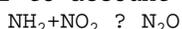
### Selective Non-Catalytic Removal of NO<sub>2</sub> by Ammonia: Experimental and Numerical Results

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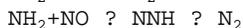
#### Abstract

The emission of pollutant gases (*e.g.*, NO, NO<sub>2</sub>, N<sub>2</sub>O, CO, and hydrocarbon species) from combustion devices is of concern due to their noxious roles to the local and global environment. Among the pollutants, nitric oxides (NO<sub>x</sub> = NO + NO<sub>2</sub>) are two of the major ones produced by combustion processes involving exothermic reactions with air. Of a number of available NO<sub>x</sub> removal processes, Selective Non-Catalytic Removal (SNCR) of NO<sub>x</sub> by the injection of ammonia (NH<sub>3</sub>) into the exhaust gas stream (Thermal DeNO<sub>x</sub>) has been reported to be effective for NO<sub>x</sub> control.

For further understandings of the exhaust gas chemistry related to both NO and NO<sub>2</sub>, a chemical kinetic model has been devised based on the latest works for corresponding experiments on the SNCR of NO<sub>2</sub> for temperatures of 800-1300 K using the injection of ammonia. The experimental results from the systems of NO<sub>2</sub>/O<sub>2</sub>, NO<sub>2</sub>/NH<sub>3</sub>/O<sub>2</sub> and NO<sub>2</sub>/NH<sub>3</sub>/O<sub>2</sub>/CO are compared to the corresponding results from the model predictions for the NO<sub>2</sub> removal pathways and for the effects of CO on the removal process. The NO<sub>2</sub> removal was found to be a strong function of temperature and gas composition. For the systems of NO<sub>2</sub>/O<sub>2</sub>/NH<sub>3</sub> and NO<sub>2</sub>/O<sub>2</sub>/NH<sub>3</sub>/CO, the NO<sub>2</sub> removal was significantly promoted by the injection of ammonia, in which the major products were NO and N<sub>2</sub>O. Two routes of chain sequence which appear to account for this observation are



The sequence for the conversion of the formed NO to N<sub>2</sub> exhibited the global characteristics similar to the conventional SNCR of NO using ammonia via



These conversions to N<sub>2</sub> from the initial NO<sub>2</sub>/NH<sub>3</sub> concentrations could be achieved up to 80-90% at the higher temperatures. The effect of CO on the magnitude of NO<sub>2</sub> removal was modest, but caused the temperature for the zero ammonia slip, minimum NO concentration and maximum N<sub>2</sub> formation to shift to lower values.

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**Radical Concentration Measurements in the Near-Substrate Region of  
Low-Pressure Diamond-Forming Flames**

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Abstract

Measurements of OH radical profiles in low-pressure diamond-forming flames are described. The measurements were performed in flames that have been characterized extensively using hydrogen CARS for temperature measurements. The experimental results are compared with the results of a numerical simulation of the flame. Attempts will also be made in the next few weeks to measure H-atom and C-atom profiles.

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### B6.3

#### Induction Time and Detonation Wave Structure of Acetylene, Ethylene and JP-10

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#### Abstract

Induction time and detonation wave structure are two important parameters used in shock tube combustion studies and other devices based on detonation. In the present study acetylene, ethylene and JP-10 were chosen for fuel because published experimental data are available and the heightened interest in JP-10 as a high energy density fuel. The flow properties of pressure, density, temperature, velocity, Mach number and species mole fractions were calculated as a function of downstream distance (or convective time) from the wave front. Ignition delay was approximated as the time to reach OH peak. Reduced mechanisms of medium length were chosen to avoid lengthy computations, while still preserving the necessary reaction steps to predict induction time. Select cases from published shock tube combustion studies were chosen for simulation and comparison to experimental ignition delay times, for wide ranges of temperature, pressure, equivalence ratio, and argon dilution. The results of the simulations show interesting features for lean and rich mixture conditions. Interestingly, under some conditions, very long ignition delays are observed. This undesirable behavior from a fuel property stand point, may provide insight into kinetic mechanisms and explosive characteristics. The full paper will include profiles of flow variables, mole fractions of major and minor species, effects of equivalence ratio and chemical kinetics on the detonation wave. The paper will discuss the suitability and advantages, if any, of using JP-10 for fuel.

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## Soot & Precursors I

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C1.1

### SOOT FORMATION AND EARLY OXIDATION IN LAMINAR DIFFUSION FLAMES AT ATMOSPHERIC PRESSURE

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#### ABSTRACT.

Soot formation (soot surface growth and primary soot particle nucleation) and early soot oxidation (soot surface oxidation) were studied in laminar jet diffusion flames at atmospheric pressure. Experimental conditions involved a variety of hydrocarbons (acetylene, ethylene, propylene, propane and benzene) burning in coflowing air. Measurements were limited to the axes of the flames to yield initiation of soot formation near the cool core of the flame, with soot particles subsequently passing in turn through regions dominated by soot formation and oxidation, typical of soot paths in practical nonbuoyant diffusion flames. Measurements included soot concentrations, soot temperatures, soot structure, major gas and radical (H,OH,O) species concentrations and gas velocities. The present soot surface growth rates in diffusion flames were independent of fuel type, were in good agreement with earlier measurements in premixed flames, and yielded encouraging agreement with existing Hydrogen-Abstraction/Carbon-Addition (HACA) soot surface growth mechanisms. Similarly, the present soot surface oxidation rates in diffusion flames were independent of fuel type, were in good agreement with earlier measurements in premixed flames, and yielded encouraging agreement with existing OH/O<sub>2</sub> soot surface oxidation mechanisms. Finally, the present soot primary particle nucleation rates were independent of fuel type, were in good agreement with earlier measurements in premixed flames, and yielded a crude correlation based on a simplified model that assumed that nucleation was controlled by the formation of large PAH molecules through the HACA mechanism.

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**The Chemistry of Precursor Soot and Its Ramifications**

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Abstract

Precursor soot was generated in a flow tube reactor by acetylene pyrolysis. The reactor effluent was diluted by a factor of 100 with nitrogen immediately upon exiting the reactor. The particle and gas phase species were analyzed in real time with an ion trap mass spectrometer. Comparison of the particle and gas phase ion distributions reveal great differences and demonstrate the richness of the chemistry of precursor soot. The precursor soot particles show clear evidence of high-mass (>1000 Da) polymeric species when they are examined in real time. The effluent was collected on a filter and extracted with methylene chloride. The extracted material was then loaded on 5- $\mu$ m particles that are used as packing material in LC columns. Upon evaporation of the solvent, the particles were sampled into our aerosol mass spectrometer to provide an off-line comparison to our real-time work. The off-line mass spectra reveal a chemical alteration of the polymeric structure in the greater than 1000 Da mass distribution indicating that the polymeric species are metastable. Ramifications of these observations will be discussed.

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**PRELIMINARY EXPERIMENTS IN A SOOT-CONTAININGNON-PREMIXED TURBULENT FLAME**

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Abstract

Although turbulent conditions prevail in many engineering systems such as gas turbines and IC engines, there have been a relatively limited number of investigations of sooty non-premixed turbulent flames. Consequently, information obtained in laminar flames, which are experimentally and computationally more tractable, have been primarily used to describe the complex soot processes in turbulent flames, which are difficult to probe due to the inherent flow fluctuations, based on the laminar flamelet concept. Motivated by these observations, a systematic investigation on the properties of soot-containing turbulent flames has recently been initiated in this laboratory with the support of National Science Foundation. The ultimate objective of this broad effort is to understand the evolution of soot field in the fuel-rich conditions of hydrocarbon turbulent flames by undertaking various state-of-the-art experiments. The present paper reports our initial measurements of soot size, morphology, and volume fraction in an ethylene/air jet flame using the laser scattering/extinction and thermophoretic sampling techniques.

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**Sooting Limits of Microgravity Spherical Diffusion Flames**

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ABSTRACT

Limiting conditions for soot-particle inception were studied in microgravity spherical diffusion flames burning ethylene at atmospheric pressure. Nitrogen was supplied in the fuel and/or oxidizer to obtain the broadest range of stoichiometric mixture fraction. Both normal flames (oxygen in ambience) and inverted flames (fuel in ambience) were considered. Microgravity was obtained in the NASA Glenn 2.2-second drop tower. The flames were observed with a color video camera and sooting conditions were defined as conditions for which yellow emission was present throughout the duration of the drop. Sooting limit results were successfully correlated in terms of adiabatic flame temperature and stoichiometric mixture fraction. Soot free conditions were favored by increased stoichiometric mixture fractions. No statistically significant effect of convection direction on sooting limits was observed. The relationship between adiabatic flame temperature and stoichiometric mixture fraction at the sooting limits was found to be in qualitative agreement with a simple theory based on the assumption that soot inception can occur only where temperature and local C/O ratio exceed threshold values (circa 1250 K and 1, respectively).

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**Shock Tube Investigations of Hydrocarbon Oxidation and Pyrolysis  
Over Very Wide Pressure Ranges**

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Abstract

Accurately simulating the oxidation and pyrolysis of hydrocarbons is a crucial part of combustion science. A considerable amount of work by experimentalists, theoreticians and modelers has been devoted to developing accurate, reliable mechanisms to describe these processes. However it is normally only possible to test a model against experimental data that has been gathered at reaction pressures that do not exceed 10 bar. While this pressure is suitable for a large number of situations there are many devices that operate at considerably higher pressures e.g. 100 bar. Currently, if a high pressure process is to be simulated then it has to be assumed that a model that has been optimized for lower pressures is appropriate for high pressure use; a assumption that is not necessarily true.

Recent studies on the oxidation ( $\phi=1$  and  $\phi=5$ ) pyrolysis of ethane have been performed at reaction pressures of 40 bar, 340 bar and 613 bar over the temperature range 1050 K -1400 K in the high pressure single pulse shock tube at UIC. The results of these experiments and the ability of several well known combustion models to predict the experimental data will be discussed along with the implications for simulating high- pressure combustion. Additionally the results from the ethane experiments have prompted the examination of toluene oxidation and pyrolysis at elevated pressures and these results which by be important for modeling automotive fuels will be presented.

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**Effect of Partial Premixing on NO<sub>x</sub> and Soot Formation in Heptane-Air Flames**

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ABSTRACT

It is well known that NO<sub>x</sub> and soot are the main pollutants from diesel engines. The production of these pollutants is strongly related to the characteristics of the combustion that takes place in the engine. The fuel is introduced into the combustion chamber in the form of a spray of fuel droplets of different sizes. The smaller droplets evaporate at a faster rate. The non-uniform evaporation process gives rise to regions in which fuel and air form a rich mixture outside flammability limits that burns in a partially premixed mode. Partially premixed flames lead to a two stage combustion and help decreasing soot emissions by reducing soot precursors.

The purpose of this work is to study the structure and emissions of non-premixed and partially premixed flames of n-heptane and air. Heptane is considered as a surrogate for compression engine fuels. A very detailed reaction mechanism, composed of 174 chemical species and about 3500 reactions has been used in order to accurately model the formation of soot precursors. This reaction mechanism contains a set of 35 species and 500 reactions related to the N chemistry, which has been used to study NO<sub>x</sub> emissions. Since the objective of the present work is to study the formation of NO<sub>x</sub> and soot precursors using a very detailed reaction mechanism, a counterflow geometry has been adopted for the present work. The counterflow flames have been numerically simulated using the OPPDIF code, modified in order to handle very detailed reaction mechanisms and to take thermal radiation into account using the optically thin model. The reaction mechanism has been tested with experiments and simulations of n-heptane counterflow flames found in literature.

This investigation makes a parametrical study in order to find out the best degree of premixing at different strain rates and its influence on the flame structure and on pollutant emissions. A comparison of the results of the non-premixed flame with those of a representative partially premixed flame with a rich side equivalence ratio of 3.0 shows that the partially premixed flame gives a higher NO<sub>x</sub> emission but a lower emission index of heavier hydrocarbons, which are treated as soot precursors.

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**STRUCTURE OF SOOT AND SOOT PRECURSOR PARTICLES FORMED IN OPPOSED FLOW METHANE OXY-  
FLAMES**

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**Abstract**

Structure of soot and soot precursor particles formed in the opposed flow flames of methane and oxygen enriched air are studied experimentally. Soot samples were collected along the burner centerline using thermophoretic sampling technique and further analyzed using high-resolution transmission electron microscopy (TEM). The similar structure of soot layer was observed for all studied flames with oxygen content varied from 35 to 100%. Two distinctive layers of carbon particles are observed: layer of mature carbonaceous soot and layer of precursor particles. The layer of polydisperse precursor particles is located in the vicinity of the stagnation plane. The layer of agglomerated carbonaceous soot is located on the fuel side of the precursor layer. Agglomeration degree of mature soot increases in the direction of the fuel nozzle while the mean diameter of the primary particles remains practically constant. This suggests that soot growth occurs almost exclusively in the layer of precursor particles. The diameter of the primary particles reduces with increase of the oxygen content while primary particle concentration and agglomeration degree increases. High-resolution TEM imaging of young soot particles reveal presence of highly organized carbon nanostructures formed inside the amorphous condensate. These structures resemble shapes of carbon onions and carbon nanopolyhedral particles and can serve as precursors to the formation of multiwalled carbon nanotubes.

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## Soot & Precursors II

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C2.1

### Nanoparticle Measurement Methods in Internal Combustion Engines

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#### ABSTRACT

Nanoparticles from combustion sources have been the subject of much recent research. Nanoparticles form in exhaust via many processes including condensation, homogenous nucleation, coagulation and adsorption. After being released from the exhaust into a dilution tunnel or dilution sampler, new nanoparticles also might be formed due to nucleation growth from low dilution ratio and long residence time. On the other hand, nanoparticles might be formed solely from the dilution process. Artifact formation in dilution tunnels occurs due to specific problems with the dilution process, such as dilution ratio, dilution air temperature, dilution air pressure, residence time and critical flow orifice.

This paper describes a variable residence time, micro dilution system for engine exhaust dilution. Particle detection instruments consisted of a scanning mobility particle sizer (SMPS), a condensation particle counter (CPC), and a NO<sub>x</sub> analyzer for determining dilution ratio. Particle size measurements were taken upstream and downstream of a diesel particulate filter (DPF) with residence time changing from 50 ms to 700 ms, which increased nanoparticle concentrations by up to two orders of magnitude. Size measurements of a spark-ignited, direct-injection gasoline engine were also determined. Results showed the effect of several dilution parameters on particle size distribution.

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**CARBON NANOTUBES AND CARBON NANOFIBERS FORMED ON CATALYTIC SUPPORT IN OPPOSED  
FLOW METHANE/OXYGEN FLAME**

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Abstract

Formation of carbon nanotubes and carbon nanofibers was studied experimentally using a Ni-based catalytic support positioned at the fuel side of opposed flow flame formed by streams of fuel ( $\text{CH}_4 + 4\% \text{C}_2\text{H}_2$ ) and oxidizer ( $50\% \text{O}_2 + 50\% \text{N}_2$ ). For constant flame parameters and the same catalytic material, a variety of carbon nanostructures were observed for variations of catalyst's position in flame. Observed carbon structures include: MWNTs and MWNT bundles, nanofibers with varying degree of crystallinity, helical regularly coiled tubular carbon nanofibers, ribbon-like coiled nanofibers with rectangular cross section, and, finally, long (~0.2 mm) uniform-diameter (~100 nm) tubular nanofibers with regular internal structure of carbon layers. Some of the above structures were synthesized only recently at carefully designed chemical vapor deposition experiments in other laboratories. The diversity of formed nanomaterials is attributed to the strong variation of flame properties along the flame axis including temperature, hydrocarbon and radical pool. This provides strong selectivity for formation of different nanoforms even if the single catalytic support is utilized.

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**The Application of Laser-Induced Incandescence to the Detection of  
Carbon Nanotubes and Carbon Nanofibers**

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Abstract

It is likely, based on previous studies of LII applied to metal aerosols, that catalyst particles contribute to the incandescence and/or plasma emission (the particular process depending upon the laser fluence). The super-elevated temperatures, derived from blackbody fits to spectrally resolved emission, observed using laser fluences of 0.8 J/cm<sup>2</sup> suggest continuum emission from a laser generated plasma. The absence of atomic, molecular and cluster electronic emission upon the "blackbody" (plasma) radiation is surprising but highlights the utility of 1064 nm excitation in order to avoid electronic excitation of plasma species. Unlike previous observations, LII from the metal nanoparticles does not produce distinct spectral signatures. Thus, their relative contribution to the emission signal is not readily extracted from that arising from the carbon nanotubes or nanofibers. It is also not readily rejected, spectrally nor temporally. The short temporal existence of the emission signal from Fe-SWNT system and Ni-nanofiber system confirms that vaporization occurs at high laser fluences, e.g. 0.8 J/cm<sup>2</sup>. In this case, there is no remaining solid incandescence. Fluence dependencies reveal the onset of laser induced vaporization as commensurate with that of pure carbonaceous material, approximately 0.6 J/cm<sup>2</sup>.

Two-pulse experiments highlight the differences observed in the temporal decay rates with variations in laser fluence, detection wavelength, and size of laser heated nanostructure, as well as uncovering laser induced material changes other than vaporization. An altered nanostructure would be consistent with the variation in LII peak intensity and different temporal decay rates produced by pulse 2, as compared to pulse 1. Apparently, laser induced coalescence of the heated nanostructure occurs, leading to different optical and thermal behavior for LII applied to SWNTs and nanofibers.

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**Synthesis of Multi-Walled, Well-Aligned Carbon Nanotubes From Hydrocarbon Diffusion  
Flames**

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Abstract

Synthesis of multi-walled carbon nanotubes was experimentally investigated using laminar diffusion flames. The entangled carbon nanotubes were grown on Ni-Cr wire substrates in a methane diffusion flame, having a diameter range of 20-60 nm. The diameters of nanotubes are influenced by temperature at sampling location in the flame. The well-aligned nanotubes were synthesized on silicon substrates in an ethylene flame using porous alumina film as a nano-template. They have a monodispersed diameter, approximately 60 nm, and their growing at the aluminum film surface is found to be stopped that makes it possible to readily control the length of nanotubes through geometry of aluminum film template. This unique character offers a potential of application in molecular electronic devices.

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**Premixed Flame Synthesis of Carbon Nanotubes Using Supported Catalysts**

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Abstract

A series of rich premixed flames are used to produce mixtures of CO, CO<sub>2</sub>, H<sub>2</sub> and H<sub>2</sub>O. Through variation of the hydrocarbon fuel (with different H/C ratios) and the flame fuel/air equivalence ratio, the post-flame mixture composition can be tailored over a broad range of compositions. Control of nanotube growth through adjustment of the post-flame reaction gas mixture is demonstrated. Both SEM and HRTEM imaging are used to correlate the nanotube overall morphology and internal structure to the reaction gas composition. The variations observed are understood in light of the gas composition and its interaction with both the deposited catalyst particles and supporting metal substrate. Further comparisons between flames producing the same CO or H<sub>2</sub> concentrations identify the roles of these gases in CNT synthesis. Optimum flame synthesis conditions, defined upon a H<sub>2</sub> and CO concentration map are gauged on the basis of CNT length, relative surface density and level of graphitic structure.

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## Turbulent-Combustion Modeling

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### C3.1

#### Group spray modeling of gas turbine combustion flows

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#### Abstract

Fuel droplets at low power conditions reside long time and thereby accumulate a large amount in gas turbine combustors. This requires huge computer memory and long computation time in procedure of numerical solutions. In this study, a group spray model was developed to make more efficient computations and to give more realistic descriptions of droplet sprays. The group model uses droplet groups to represent the spray, employs the Lagrangian approach to trace the motion of groups, and considers the turbulent dispersion of droplets within each spray group for the group growing. A group number, which is dependent of the droplet number density, size and Sherwood number, and the group size, was derived from the conservation equations of species and energy with Stefan flows. A group evaporation correction factor based on the group number was introduced to consider the effect of spray parameters on evaporation of droplets in the group. Both the stochastic separated flow (SSF) and the group spray models were validated with experimental data in reasonable agreements. It is found that the group model needs only about 1/10 of droplet groups required by the SSF model, and saves 40% computation time. Finally, the group model was applied for three-dimensional simulation of gas turbine combustion, and promising results were achieved. The group model and results will be presented in the paper in details.

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**The Premixed Conditional Moment Closure Method**

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## Abstract

The premixed Conditional Moment Closure (CMC) method is developed and coupled to a commercial CFD program to model an idealized lean premixed gas turbine combustor, namely a 2-D backward facing step burning premixed methane at an equivalence ratio of 0.9. Using the full GRI mechanism, temperature, velocity and major species are compared to data with good agreement. Intermediate species that contribute to the three NO<sub>x</sub> formation pathways are also presented. The CMC method is a new theory that has been applied to non-premixed combustion with good success (Klimenko and Bilger 1999). The application of the CMC method to premixed systems has recently been done. The premixed CMC method replaces the species mass fractions as independent variables with the species mass fractions that are conditioned on a reaction progress variable (RPV). Conservation equations for these new variables are then derived and solved. The general idea behind the premixed CMC method is that the behavior of the chemical species is closely coupled to the reaction progress variable. Thus, species conservation equations that are conditioned on the RPV will have terms involving the fluctuating quantities that are much more likely to be negligible. In essence, knowledge of the statistics of the RPV contains most of the information needed to calculate species mass fractions. In return for this better conditioned problem, an increase in dimensionality occurs and a new conservation equation (for the RPV) must be solved, along with a conservation equation for the variance of the RPV. The CMC method accounts for the interaction between scalar dissipation (micromixing) and the kinetics, while de-coupling the kinetics from the bulk flow (macromixing). The conditioned averages reduce the variability of the fluctuating variables allowing them to be neglected with less error, hence improving the accuracy of the chemical kinetic rates. The RPV and its variance are used to generate a beta function PDF that is used to integrate the conditioned mass fractions to obtain the species mass fractions in physical space. In certain cases the conditioned mass fractions are uniform over the computational domain, reducing the dimensionality of the problem. The test problem used is an experiment by El Banhawy et al. (1983) that consists of a flame stabilized by a backward facing step. Premixed natural gas (94% CH<sub>4</sub>) and air are flowed across the backward facing step, which establishes a recirculation zone that stabilizes the flame.

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**A Low-Order Discrete Dynamical System Model of Turbulent Fluctuations in a Reduced Mechanism for H<sub>2</sub>-O<sub>2</sub> Combustion**

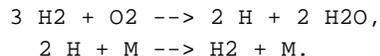
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ABSTRACT

In McDonough & Huang (3rd Int. Symp. Scale Modelling, 2000) and McDonough & Zhang (submitted to 29th International Combustion Symposium, 2002), we have recently demonstrated use of discrete dynamical systems as the (temporal) fluctuating factor in a large-eddy simulation subgrid-scale model formalism described in detail for simple incompressible flows in Hylin & McDonough (Int. J. Fluid Mech. Res. 26, 539, 1999). This consists of applying a Galerkin procedure to all governing differential equations (fluid flow, thermal energy and species concentration in the present case) and decimating the result to a single (arbitrary) mode for each dependent variable. In McDonough & Zhang this was applied to a 10-step reduced mechanism for hydrogen-air combustion, and good agreement of results with experiment was found.

In the present paper we will apply this technique to a simple two-step mechanism for a hydrogen-oxygen reaction given by Mauss et al. (in Reduced Kinetic Mechanisms for Application in Combustion Systems, Peters & Rogg (eds.), 1993):



We will provide details of deriving the DDS for this mechanism, time series of species mass fractions obtained from the calculations and comparisons with experiment.

We observe that success of such models depends on locality of their application. In particular, since only a single mode is retained in the Fourier representations it is necessary that the spatial domain be small. But, in fact, most combustion measurements are made at a single point, and are thus consistent with this representation, as suggested by our earlier studies. We also observe that, somewhat coincidentally, such a modeling approach may be appropriate in the study of micro-combustors, possibly even in real-time control applications because of the minimal calculation needed to evaluate the models.

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**A 'Synthetic Scalar' Subgrid-Scale Model for Large-Eddy Simulation of Turbulent Combustion**

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## ABSTRACT

It is widely believed that large-eddy simulation (LES) in some form holds the most promise of currently studied methods for accurate prediction of turbulent flows. But LES exhibits well-known deficiencies that are especially difficult to handle in the context of practical problems in combustion. These are associated with filtering the governing equations, and the form of subgrid-scale (SGS) models. In the present paper we will introduce a LES formalism intended to address both of these, based on three key ideas:

- i) filter solutions rather than equations;
- ii) model primitive variables (temperature, species concentrations, etc., hence, 'synthetic scalar') instead of their correlations, and
- iii) utilize the formal LES decomposition, directly incorporating SGS model results, to enhance the under-resolved large-scale results, as opposed to using the SGS model only indirectly (e.g., to compute an eddy viscosity, or in a source term in the filtered equations).

In the work to be reported we will emphasize ii) above, namely, the SGS models, themselves. We note that Kerstein and co-workers have investigated similar approaches (the linear-eddy model, and more recently, the one-dimensional turbulence models), and the present author and students have previously studied the proposed approach in the context of simple incompressible flows (e.g., ylin & McDonough, Int. J. Fluid Mech. Res. 26, 539, 1999). Furthermore, although considerable effort has already been expended on constructing the temporally fluctuating parts of such models in the context of reduced-mechanism finite-rate chemistry by McDonough & Huang and McDonough & Zhang (submitted to the 29<sup>th</sup> International Combustion Symposium), the scaling of the SGS model for this case has not yet been presented elsewhere. Such scaling is crucial; it is accomplished with structure functions from the Kolmogorov theories of turbulence, which lead to the magnitude of the SGS energy. This scaling plus the fluctuations alluded to above comprise the complete SGS model.

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**Comparisons of Combustion Models for Wave Rotor Combustion Simulation**

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Abstract

An internal combustor wave rotor machine utilizes non-steady wave motion to exchange energy by direct work action between chemically reacting fluids. It consists a large number of straight channels arranged about the axis of a rotor. By rotation the channel ends are periodically ported to steady-flow components.

Hot Gas Injection, Constant Volume Combustion and Turbine Exhaust phases of a typical Internal Combustion Wave rotor cycle are studied. The base geometry involves fuel injection partitions [1] that allow stratification of fuel/oxidizer mixtures in the wave rotor channel radially thus enabling pilot ignition of overall lean mixture for low NO<sub>x</sub> combustion. Available turbulent combustion models are applied and compared to simulate approximately constant volume combustion of propane and resulting compressible flow. Transient, premixed/diffusive Eddy break up and Non adiabatic PPDF models are considered. Modeling effects on fuel consumption rate, two-dimensional flow and emission levels are evaluated. The second part of this study contains the validation of the PPDF based turbulent NO<sub>x</sub> model of the STAR-CD code, which will enable us to include turbulence and extend our previous [2] thermal NO prediction studies.

References:

- [1] Nalim M. R., 2000, Longitudinally Stratified Combustion in Wave Rotors, AIAA Journal of Propulsion and Power, 16, No 3.
- [2] Nalim R., Pekkan K., Two-Dimensional Flow and NO<sub>x</sub> Emissions in Deflagrative Internal Combustion Wave Rotor Configurations, NAG3-2207, NASA Glenn Research Center Grant Report. Also to appear in ASME Turbo Expo 2002, Paper No: GT-2002-30085.

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## Converters and Reformers

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C4.1

### THE EFFECT OF TEMPERATURE SLIP IN COMBUSTION SYNTHESIS AND CATALYTIC COMBUSTION SYSTEMS

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#### Abstract

Calculations have recently suggested that the magnitude of temperature slip in some combustion systems, most notably low pressure combustion synthesis and micro-combustion reactors, may be non-negligible in current and future reactor designs. Temperature slip occurs due to incomplete thermal accommodation of a gas that impinges upon a surface. The resultant effect of this incomplete accommodation is a steady-state temperature discontinuity ('temperature jump') at a gas-surface interface. Under these conditions, the temperature of the gas impinging upon the surface is different than that of the solid surface itself. Temperature slip appears in systems where the Knudsen number (Kn) is large (i.e. the mean free path is large compared to the relevant flow length scale). Both low pressure combustion synthesis, where mean free path is large, and micro-combustion, where system length scales are small, meet these criteria.

Addition of a temperature slip term to the model of a system where heterogeneous reactions are occurring affects the problem in several ways. Both heat transfer and flux of gas species to the surface are significantly altered over the case in which there is no slip. In addition, gas composition immediately above the surface is similarly changed. Lastly, gas-surface reactions that are sensitive to the translational energy of the impinging species, are characterized by rates that differ substantially from the no-slip case. All of these effects combine to change either the surface growth rates (in materials synthesis) or the surface combustion rates (in catalytic combustion).

Our study uses the SPIN code to model stagnation flows of low pressure diamond film synthesis and methane/air catalytic combustion under high Kn conditions. Explicit gas and surface chemical mechanisms are employed, and the results from cases with and without temperature slip are compared. In general, the effects of temperature slip are large enough to be experimentally observed and can be significant under a wide range of conditions. Recent experimental results from our group at UIUC and our collaborators at Texas A&M are also reviewed, and the implications are discussed.

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**Efficient Modeling of Full-Scale Catalytic Converters Using a Novel Sub-Grid Scale Approach**

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Abstract

To date, macroscopic modeling of catalytic conversion processes has been limited to single channel of a catalyst monolith primarily due to prohibitively large computational resources required to model the entire monolith using traditional computational fluid dynamic (CFD) techniques. While such modeling is invaluable for understanding the reaction kinetics and its coupling to local transport processes, it is by no means adequate for design and optimization of full-scale catalytic converters, which have inherent non-uniformities in flow and temperature distributions. Catalyst monoliths used in the industry contain several hundred channels per square inch of the monolith's cross-section. With state-of-the-art CFD techniques, it is necessary to generate computational grids within each monolith channel to couple mass transfer within the channels with heterogeneous reactions at the channel surfaces. This approach typically leads to several million grid cells even for relatively simple catalytic converter geometries. Thus, modeling of industrial full-scale catalytic converters is not feasible with currently available CFD techniques. In this article, a novel approach is presented to treat the disparity of length scales between the monolith channel dimensions and the overall size of the catalytic converter. The entire catalytic converter is treated as an anisotropic porous medium, and sub-grid scale models are used to couple transport with heterogeneous chemical reactions occurring at imaginary solid-fluid interfaces within the porous media. The mathematical formulation allows any number of reaction steps and species, including effects of site coverage and catalyst loading. The model was validated for catalytic ignition of hydrogen-methane-air mixtures over a platinum catalyst. Both steady state and transient characteristics of the ignition process were predicted very accurately. The computational requirements were found to be orders of magnitude lower than state-of-the-art approaches.

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**Review of Partial Oxidation for 'On-Board' Hydrogen Generation**

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Abstract

This paper summarizes a review of fuel processing options of hydrogen generation for fuel cell application, focusing on partial oxidation of hydrocarbon fuels. Thermodynamic equilibrium calculation of partial oxidation of methane, propane and iso-octane are performed using NASA equilibrium code. Temperature requirements of different fuel processing processes or options such as catalytic partial oxidation, steam reformation and water-gas shift reaction are reviewed and importance of thermal management of these processes for optimal performance is discussed. Initial results of experiments and CFD calculation of combustion of premixed flames "supported" by a honeycomb ceramic matrix are presented.

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**Effects of n-Butane Addition on Reformer Gas Combustion**

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Abstract

A major reason for the increased hydrocarbon (HC) emissions during the cold-start phase of the Federal Test Procedure is that the engine must be operated fuel rich in order to obtain suitable idle quality and driveability. Significant reductions in HC emissions would be obtained if the engine could be operated at the stoichiometric air/fuel ratio, or preferably lean of stoichiometric. In this work we investigate the possibility of starting an engine on reformer gas/air mixtures during the cold-start and then adding increasing amounts of hydrocarbon fuel to transition into fully warmed-up operation on gasoline. The laminar flame speeds and lean flammability limits of reformer gas/air mixtures with different amounts of n-butane addition are investigated numerically. The results indicate that the flame speeds are dramatically reduced with even as little as 10% n-butane addition. Although the flame temperature is increased with n-butane addition, the fact that the H and O radicals react preferentially with n-butane leads to a reduction in the radical pool and a consequent flame speed reduction. While the lean flammability limit of reformer gas/air mixtures is leaner than n-butane/air mixtures at 1atm, at 10atm the trend reverses and the flammability limit of pure reformer gas/air mixtures is richer than that of n-butane/air mixtures.

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## Diagnostics I

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C5.1

### **Fluorescence lifetime measurements in 1-atm flames using nanosecond-pulsed lasers**

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#### Abstract

Measurements of fluorescence lifetimes are needed to quantify concentration measurements when using linear laser-induced fluorescence. A technique is described for experimentally determining the fluorescence lifetime in atmospheric pressure flames using a nanosecond-pulsed laser; that is, measurement of a lifetime an order-of-magnitude faster than the laser pulse itself. This technique relies on an observable temporal shift in the fluorescence signal as a function of lifetime. Simulations show the efficacy of this approach, and data in liquid samples and in an atmosphere-pressure flame show excellent agreement with prior picosecond measurements. This technique is successful because only the temporal shift is examined and details of the fluorescence profile shape are ignored.

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**MULTILINE HYDROXYL TAGGING VELOCIMETRY IN REACTING AND NONREACTING EXPERIMENTAL FLOWS**

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## Abstract.

The new nonintrusive instantaneous molecular flow tagging method, Hydroxyl Tagging Velocimetry (HTV), previously demonstrated only for a limited number of molecular gridlines, is now demonstrated in both low-temperature (non-reacting) and high-temperature (reacting) flows with multiple gridlines produced by compact micro lens optics. Single-photon photodissociation of ground state H<sub>2</sub>O by a ~193-nm ArF excimer laser "writes" a 7 x 7 beam molecular grid with very long gridlines (>50 mm) of superequilibrium OH and H photoproducts in either room air flowfields or in H<sub>2</sub>-Air flames due to the presence of H<sub>2</sub>O vapor. The new optical grid produces 49 unambiguous reference points in the experimental flow. After displacement, the positions of the OH tag lines are revealed through fluorescence caused by A<sub>2</sub><sup>+</sup> (v = 0) X<sub>2</sub>i (v = 0) OH excitation using a pulsed frequency-doubled dye laser with an operating output wavelength of ~308 nm. The dye "read" laser accesses the strong Q<sub>1</sub>(1) line, compensating for the relatively weak 193 nm absorption of room temperature H<sub>2</sub>O. The weak absorption of ground vibrational state H<sub>2</sub>O has previously precluded the use of HTV at low temperatures, since previous HTV systems relied on a KrF excimer "read" laser that could only access the weak and highly predissociative (30) OH transition. The DaVis time-of-flight analysis software from LaVision determines the instantaneous velocity field. HTV tag lifetime comparisons between experimental results and theoretical predictions (for low temperature flowfields) are discussed. Multiple line tag grids are now shown displaced due to experimental flowfields, thus providing 2-D multipoint velocity information. The instantaneous nature of the HTV tag formation makes it particularly suitable for, but not limited to, a variety of fast flowfield applications including either non-reacting base flows for high-speed projectiles and low temperature hypersonic external or internal flows, or high-temperature reacting flows.

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**Demonstration of Triple-Pump Coherent Anti-Stokes Raman Scattering  
Measurements in Hydrogen-Air Diffusion Flame for Simultaneous Temperature  
and Species Concentration Measurements**

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Abstract

Characterization of advanced propulsion systems requires careful measurement of performance and combustion efficiency. Careful evaluation of efficiency requires measurements of temperature and species concentrations in the exhaust stream with spatial and temporal resolution. Typically, this kind of data is collected via implementation of several independent techniques that are often executed serially. Ideally, these measurements would be accomplished simultaneously with a minimum number of diagnostics. Triple-pump coherent anti-Stokes Raman scattering (CARS) offers the possibility of monitoring the local temperature plus concentration of two target species using a single measurement instrument with both spatial and temporal resolution. We present here the first demonstration of a triple-pump CARS system for temperature and concentration measurements in reacting flows. Demonstration measurements of triple-pump CARS made in a laboratory hydrogen/air diffusion flame are discussed along with their implications for measurements in test rigs at Wright-Patterson AFB.

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## Diagnosics II

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C6.1

### Cross-sections for CH Quenching by N<sub>2</sub> and H<sub>2</sub>O from 1740 to 2160 K

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#### ABSTRACT

Measurements of time-resolved CH fluorescence are reported for 77 methane-based counterflow diffusion flames at atmospheric pressure. A procedure for extracting single collider cross-sections for nitrogen is developed, which utilizes the linear relationships between nitrogen and other collider mole fractions in these flames. The results show that N<sub>2</sub> quenching of CH at flame temperatures is less efficient by a factor of three than the correlation of Tamura et al. [Combust. Flame, 114:502], which relies on extrapolation from a single measurement at 1300 K. The data, spanning T=1740-2160 K, suggest an improved nitrogen cross-section correlation of  $s_{Q,N_2} = 3.153 \times 10^{-4} T^{1.23} \exp(-522.1/T)$  and are consistent with a constant H<sub>2</sub>O cross-section of  $s_{Q,H_2O} = 9.6 \times 10^{-5}$ .

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**Digital Recording and Numerical Reconstruction of Holograms: A New Optical Diagnostic  
for Combustion**

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Abstract

Holographic interferometry (HI) has proven to be a useful tool for nonintrusive temperature measurements in flames (and to thereafter infer the local composition based on the state relationship approach) with high spatial and temporal resolution. Digital holographic interferometry (DHI) is a relatively newer imaging and measurement technique that electronically records a hologram (e.g., on a CCD) and reconstructs it using a numerical method. Cumbersome chemical processing of the hologram is avoided in DHI, thereby providing greater flexibility, speed, and the potential for real time processing. In conventional holography fringes that are neither bright nor dark on a hologram cannot be accurately resolved. The DHI technique reported so far has not yet been used for combustion applications. Herein, we will evaluate its efficacy for making temperature measurements in flames and assess its applicability through a simulation. The double exposures associated with the holographic technique are each considered recorded by a hypothetical CCD sensor at separate times. We have applied the principles of Fourier optics to develop two numerical methods for hologram reconstruction and show that both methods provide an accurate reconstruction of the phase image associated with a flame. Due to the periodic nature of the wave function, the reconstructed phase values are limited to the interval  $[-\pi/2, \pi/2]$ . Thus an unwrapping algorithm is provided to get a continuous phase distribution based on the condition that the reconstructed phase is jumped by a value of  $-\pi$  or  $\pi$ . We have also developed an iterative calculation method to adjust the value of the digital reference wave parameters that determines the phase imaging reconstruction in DHI.

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**Diode-Laser-Based Ultraviolet Absorption Sensor for NO**

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ABSTRACT

We describe the development and demonstration of an all-solid-state continuous-wave (cw) laser system for optical absorption measurements of the NO molecule. The single-mode, tunable output of a 10 mW, 395-nm external-cavity diode laser (ECDL) is sum-frequency-mixed with the output of a 110 mW, frequency-doubled cw Nd:YAG laser in a beta-barium borate crystal to produce approximately 10 nW of tunable cw radiation at 226 nm. The wavelength of the 395-nm ECDL is then scanned over an isolated NO absorption line to produce a fully resolved absorption spectrum. The sensitivity of the system is well below 1 ppm per meter of path length.

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