Combustion Research Facility News

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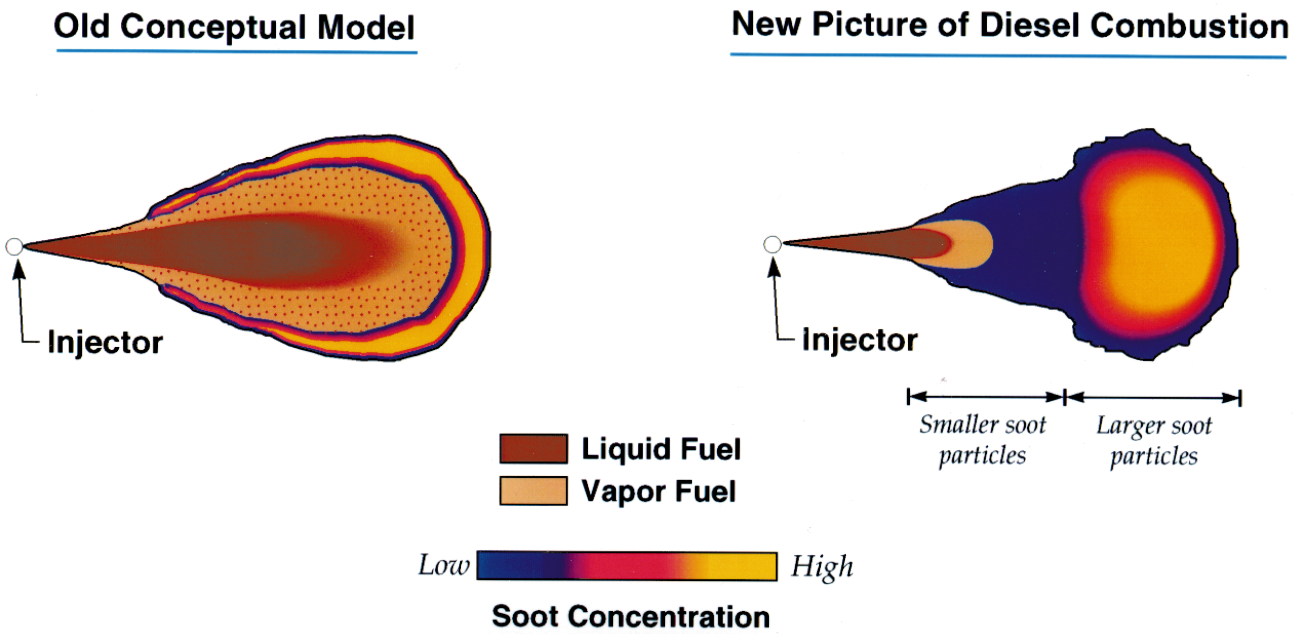
Team develops new description of diesel combustion

John Dec and Eldon Porter, along with visiting researcher Chris Espey, have developed a new description of the combustion inside a diesel engine. Using laser diagnostic techniques in conjunction with a special research engine with quartz windows, the team mapped out the way fuel in a heavy-duty diesel engine mixes with the in-cylinder air and where soot formation occurs. Their findings have permanently changed the picture of diesel engine combustion.

It had been thought that diesel combustion occurred as a simple diffusion flame and that soot formed only around the periphery of the fuel jet. In contrast, the new studies show that fuel-air mixing, combustion, and soot formation occur progressively as the fuel moves down the reacting jet (see figure). The entrainment of hot in-cylinder air vaporizes all the fuel by the time it travels about one inch from the injector. Then, in the vapor-fuel region of the jet, combustion and soot formation occur. Initially, soot particles are small; but, as the soot moves down the reacting jet toward the 'head vortex' at the leading edge, both soot concentration and particle size increase significantly.

John has worked for more than five years as principal investigator on the project with Eldon Porter and for four years with visiting researcher Christoph Espey, a Cummins-sponsored graduate student. The collaboration with Cummins, the world's largest producer of diesel engines over 200 horsepower, began in the mid-1980s and developed into a Cooperative Research and Development Agreement (CRADA) in 1993.

The ultimate goal is to build a truly predictive computer model. The CRADA addresses this goal, and Ken Marx is working on computer submodels of the fuel spray and combustion. Previously, computer model developers knew little more than how fast the fuel burned and what exhaust emissions came out the tailpipe. With the new data from the optically accessible engine, the number of assumptions required for the computer models has dramatically decreased, and predictive capabilities of the newly refined models are continuing to improve.



Laser-sheet imaging shows the true cross-sectional distribution of soot and liquid- and vapor-phase fuel in a combusting diesel fuel jet (right). These distributions contrast markedly with the previous model of a simple diffusion flame (left).

Fine-scale structure imaged in a free shear flow

Phillip Paul and Ken Buch have undertaken an experimental study of mixing in a free shear flow. Fluid turbulence acts to bring reactants together (large scale stirring); however molecular mixing (diffusion at fine scales) is required for chemical reactions to proceed. This work is aimed at measuring the structure of a flow at the finest turbulence scales in order to better understand the progression from a stirred to a mixed fluid.

The study employs high resolution planar laser-induced fluorescence (PLIF) imaging. The technique uses a thin sheet of laser light (from a tunable pulsed laser) to excite fluorescence from specific molecules present in the flow. The resulting fluorescence is recorded with an intensified solid-state camera, which provides a spatially resolved snapshot of the distribution of molecules in the plane of the laser sheet. The high spatial resolution required for this study was attained using pin-hole spatial filtering of the laser beam and an aberration-corrected sheet-forming telescope, which gave a sheet thickness of 80 µm (measured full width at $1/e^2$).

The experiment was performed by seeding a trace of NO into a jet of N_2 exiting into a slow co-flow of pure N_2. NO and N_2 have similar diffusion rates, thus the signal can be taken as a direct measure of the local concentration of jet fluid. The fact that N_2 does not quench NO fluorescence provides the high signal levels required for measuring gradients. Resolution of the finest fluid scales was achieved by taking images of small regions in the far field of a round jet with Reynolds numbers (as based on nozzle diameter) of order $Re_D \approx 6000$.

Figure 1 shows a typical NO image. At this location all of the jet fluid has been stirred several times by the large scale structures. Stirring produces long convoluted interfaces that bound broad regions of differing concentration. Inside these regions the flow may be turbulent but mixing is complete, so the concentration is relatively constant. For chemical reactions an important aspect of the concentration field, ζ, is the scalar dissipation, $\chi \equiv \nabla\zeta \bullet \nabla\zeta$, which can be interpreted as the local rate of molecular mixing. Relatively simple kinematic arguments suggest that the concentration gradient across an interface is smooth, hence the scalar dissipation profiles should also be smooth.

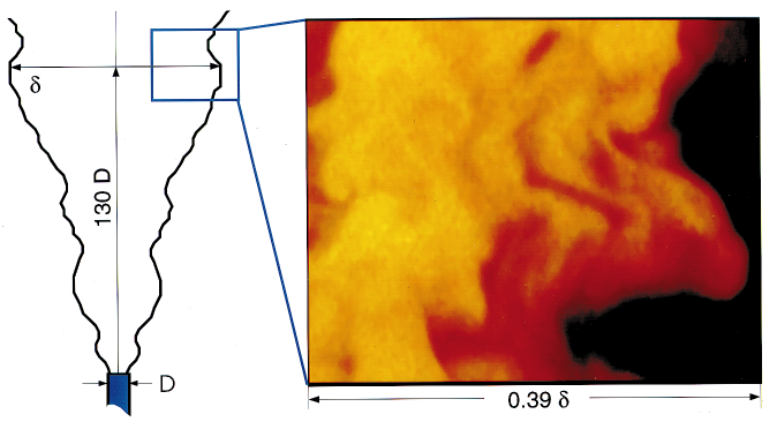


Figure 1: Schematic showing the region imaged (left). Concentration image of jet fluid taken 130 jet diameters downstream; $Re_D = 5000$ (right). The color table is continuous and linear from black for pure ambient fluid to bright yellow for jet fluid.

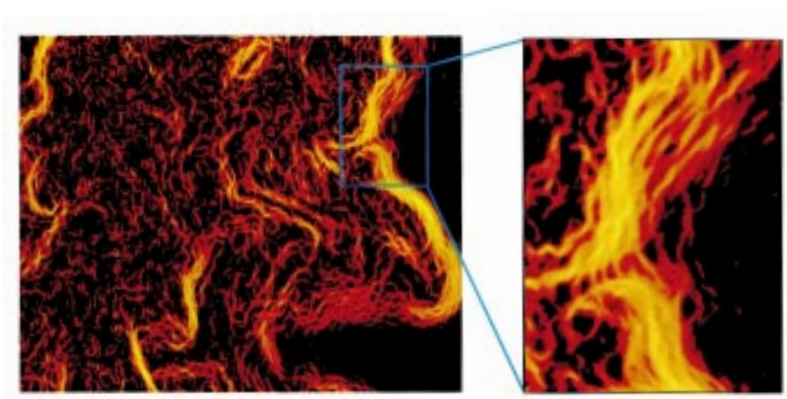


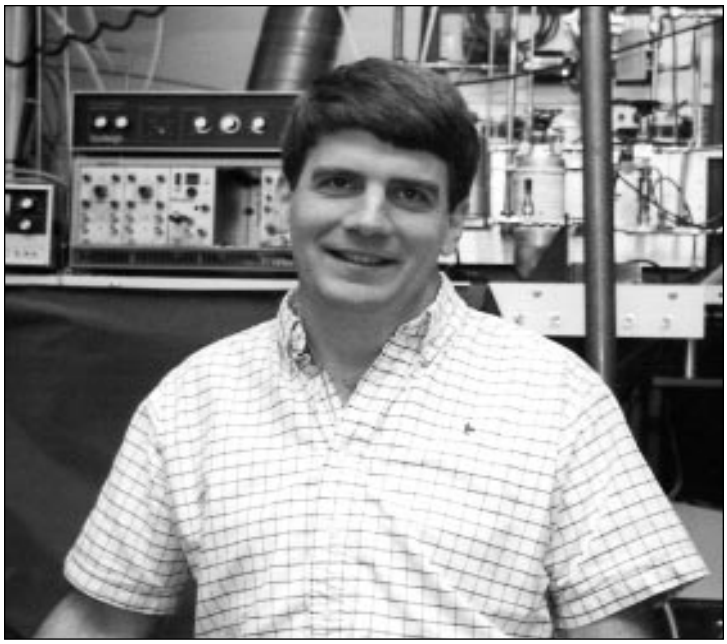
Figure 2: Scalar dissipation image derived from the data of Fig. 1 (left). Enlarged region of the dissipation image (right).

Figure 2 shows the logarithm of the scalar dissipation field derived from the data of Fig. 1. The most striking result of this experiment is that scalar dissipation at strong interfaces is not smooth; rather it appears to be composed of many fine 'filaments' lying side by side. Observing the large length-to-thickness ratio of the 'filaments' and remembering that PLIF takes a cut through the flow suggests a dissipation zone composed of layered sheet-like objects that conform to the surface shape of the larger structures.

The structure in the scalar dissipation layers was quite unexpected, and the initial response was to attribute it to some undesirable artifact in the imaging system. The technique was validated by acquiring images of a high contrast sine-wave pattern (at a signal level similar to that of the PLIF measurements). Processing these data did not yield 'filamented' dissipation structures.

Much of our understanding of the structure and characteristics of turbulent mixing in gases has been inferred from single point measurements and relatively simple particle-tracer flow visualization. High spatial resolution laser-based planar imaging provides a direct measurement of the spatial gradients in the molecular constituents of a flow.

PLIF imaging has shown that turbulent flows are highly unsteady at the large scale. The present work suggests that strong scalar dissipation layers bound the large (unsteady) structures in the flow and that these layers have far more internal structure than previously believed.



Rakestraw wins Coblentz Award

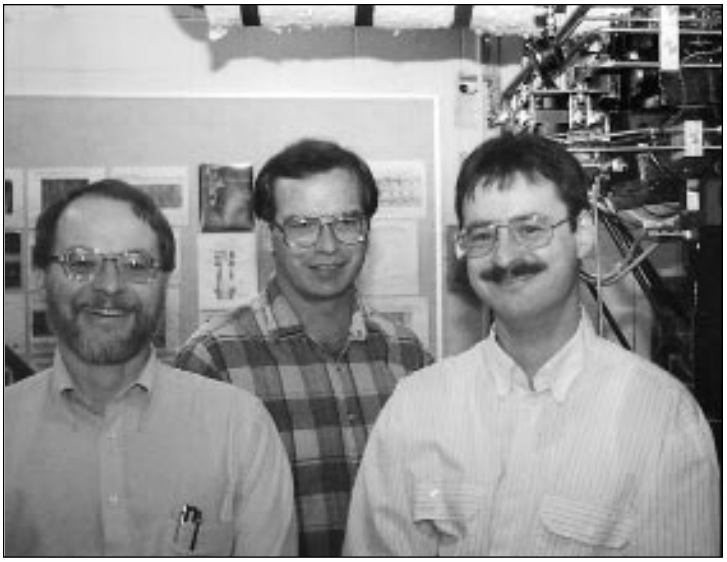
David J. Rakestraw, a Senior Member of the Technical Staff, has been awarded the 1995 Coblentz Award. This award, for outstanding accomplishments in the area of molecular spectroscopy by a scientist under the age of 36, was presented to David at the Ohio State Symposium on Molecular Spectroscopy in June. David was recognized for his pioneering efforts that enable use of nonlinear optical methods as quantitative diagnostic tools. Collaborating with several colleagues, David developed and applied degenerate four-wave mixing (DFWM) techniques to provide highly sensitive measurements of molecular concentration and temperature in gas-phase environments. Further, David extended DFWM applications to the infrared domain, wherein spectroscopic probes are advancing knowledge of molecular structure, energy transfer, and chemical reactivity. Most recently, David expanded his efforts to couple optical diagnostics with microseparation technologies for condensed-phase analysis.

Auto manufacturer liaison returns

Bob Carling, manager of the Engine Combustion Department, has just returned from a ten-month stay at Ford Motor Company Scientific Research Laboratory. While at Ford, Bob interacted with a broad range of Ford staff on issues relevant to the Partnership for a New Generation of Vehicles, the joint Big 3/Federal government initiative. His role was to develop a better understanding of issues within the auto companies and facilitate partnering opportunities between Ford and the national laboratories. While there he also served as a member ot the Engine Support System Technology (ESST) team. Bob's job was to help coordinate activities at several of the DOE labs for two ESST projects.

Forum on Vortex Methods held

Simulation of unsteady flow with the gridless vortex dynamics method is a growing area of research. Sandia sponsored a Forum on Vortex Methods for Engineering Applications that attracted 40 researchers from five countries to Albuquerque, NM, last February. Sandia's Engineering Sciences Center collaborated with the CRF in hosting the conference. Plenary lectures were delivered by Professor T. Sarpkaya (Naval Postgraduate School), J.M. Summa (Analytical Methods, Inc.), and W.T. Ashurst (CRF). the topics ranged from details of improving the vortex technique to using the method to describe premixed flame motion. Participants in the Vortex Forum plan to exchange ideas and samples of results over the Internet before holding the next gathering in 1997. For information contact William Ashurst (ashurst@ca.sandia.gov) or Steven Kempka (snkempk@engsci.sandia.gov).



Visiting researcher Christoph Espey (right) completed his Ph.D. thesis work using the Sandia/Cummins diesel engine (shown in back). He is pictured here with John Dec (left) and Eldon Porter (center); see article on front page. After his degree was awarded by Pennsylvania State University, Chris returned to Germany and a position at Daimler-Benz.

David Yang (left), a postdoctoral fellow since 1993, worked with Joe Durant (right). David carried out experimental studies of the important NH_2 + NO reaction and theoretical studies of the NH_2 + O reaction. He is currently employed at Beckman Instruments in Fullerton, CA.

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Trace pollutants analyzed in aqueous environments

Recently, Deon Anex, Gary Hux and David Rakestraw exploited the CRF's strong technical base in lasers, spectroscopy and chemistry to analyze trace chemicals in aqueous environments. The work was conducted in collaboration with Chao Yan, Rajeev Dadoo and Richard Zare of Stanford University. Initial phases of this work were supported by Beckman Instruments under a Cooperative Research and Development Agreement.

In contrast to combustion environments, where it is possible to optically probe many gas-phase chemical species using their distinct spectral features, identification of compounds in condensed phases often requires an initial separation step. This is due the need to analyze larger molecules that have broad featureless spectra.

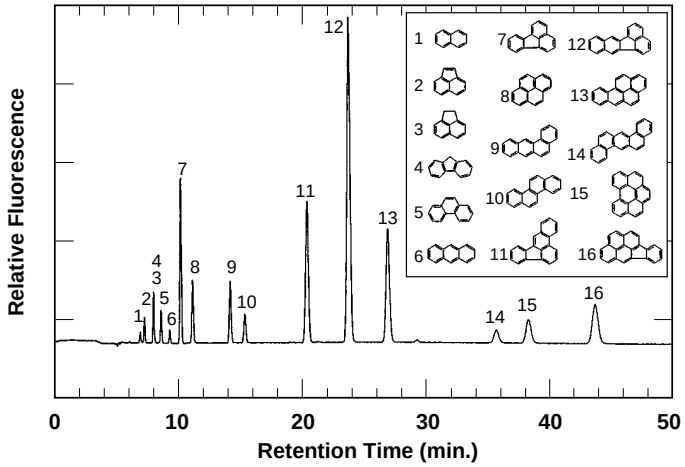
To separate a sample into its components, researchers use high-performance techniques based on electrokinetic flow and electrophoresis. One such method is capillary electrochromatography (CEC), a state-of-the-art technique for separating neutral species with high resolution. Currently CEC is being evaluated as a technology to rival pressure-driven, high-performance liquid chromatography (HPLC), which accounted for $1.4 billion of the world-wide analytical instrumentation market in 1994.

In the current experiments, the fluid flows through a fused-silica capillary (25-cm length, 50-150 µm i.d.) packed with hydrocarbon-coated 3 µm silica spheres. The driving force for transport is the electrokinetic flow induced by a high-voltage (5-50 kV) applied across the capillary column; neutral-molecule separation results from varying interactions with the stationary phase. In contrast to HPLC methods, CEC flow profiles are nearly flat and result in very high-resolution separations.

Although micro-separation techniques are very efficient, they also create detection problems. Typical injection volumes are a few nanoliters, which may contain only a few thousand molecules of any particular species. Lasers focused into the small capillaries and techniques such as laser-induced fluorescence (LIF) provide the necessary sensitivity to detect such small quantities.

An example of trace-species analysis in water using CEC/LIF with ultraviolet excitation is shown in the figure. The sample is a chemical standard containing sixteen polycyclic aromatic hydrocarbons (PAHs). These results demonstrate high separation efficiency and detection limits of 10^{-11} moles/liter.

Ongoing projects use CEC and the related technique, capillary gel electrophoresis, to examine a variety of chemical-analysis problems such as the characterization of environmental pollutants and the sequencing of DNA. It is clear that the coupling of laser-based detection with microcapillary separation technologies will enable the collection of chemical information of critical importance in many diverse applications.



Electrochromatogram showing the separation of the sixteen PAHs identified by the EPA as priority pollutants. These species were present at concentrations of 10^{-6} to 10^{-8} moles/liter, and their fluorescence was detected in the wavelength range 280 to 600 nm after laser excitation at 257 nm.

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For more information please contact:

William J. McLean
Combustion Research Facility
Sandia National Laboratories
P.O. Box 969
Livermore, California 94551-0969
(510) 294-2687

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