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Soot Formation Avoided Through Use of Micro-Orifice Fuel Injectors

CRF researchers have demonstrated that soot formation in diesel fuel jets can be avoided with the use of very small orifices on fuel injector tips. The research, sponsored by DOE's Office of FreedomCAR and Vehicle Technologies in cooperation with automotive and heavy-duty diesel engine manufacturers, was motivated by the need to reduce engine soot and nitrogen oxide (NO_x) emissions.

Lyle Pickett and Dennis Siebers investigated the effects of injector tip orifice diameter on diesel combustion and emissions formation processes at the CRF. An electronically controlled common rail diesel fuel injector was fitted with single-orifice, mini-sac type injector tips with various size orifice diameters. The diameters considered ranged from 180 µm—the typical size used on current heavy-duty diesel fuel injectors—to "micro-orifices" as small as 50 µm.

The soot formation processes in these single, isolated fuel jets were studied in experimental conditions simulating the mixing-controlled phase of diesel combustion, the phase where soot formation rates are the highest. The researchers used reduced ambient oxygen concentration to simulate the use of exhaust gas recirculation (EGR) in engines, allowing them to investigate conditions where engine-out NO_x emissions are low, but particulate matter emissions are typically most problematic.

Using planar laser-induced incandescence (PLII), Pickett and Siebers found that soot levels decreased with decreasing orifice diameter. With a 50 µm orifice, no soot was detected despite much higher camera gain, as shown by the PLII images in Figure 1.

The decrease in soot that occurs within a fuel jet with a decreasing orifice diameter results from an increase in fuel-air mixing prior to the initial combustion zone in a fuel jet (i.e., upstream of the lift-off length). Soot disappeared when fuel-air mixing upstream of the lift-off length resulted in a cross-sectional average equivalence ratio at the lift-off length, $\bar{\phi}(H)$, with a value less than approximately two (see the values of $\bar{\phi}(H)$ in Figure 1). This trend of no soot within a fuel jet for $\bar{\phi}(H)$ less than two held over a wide range of operating conditions considered.

Micro-orifices, together with fuel-air mixing in the fuel jet prior to combustion, eliminate soot within the fuel jets.

Additional experiments were performed with ambient oxygen concentrations reduced to as low as 10% while other experimental conditions remained the same. Even with oxygen

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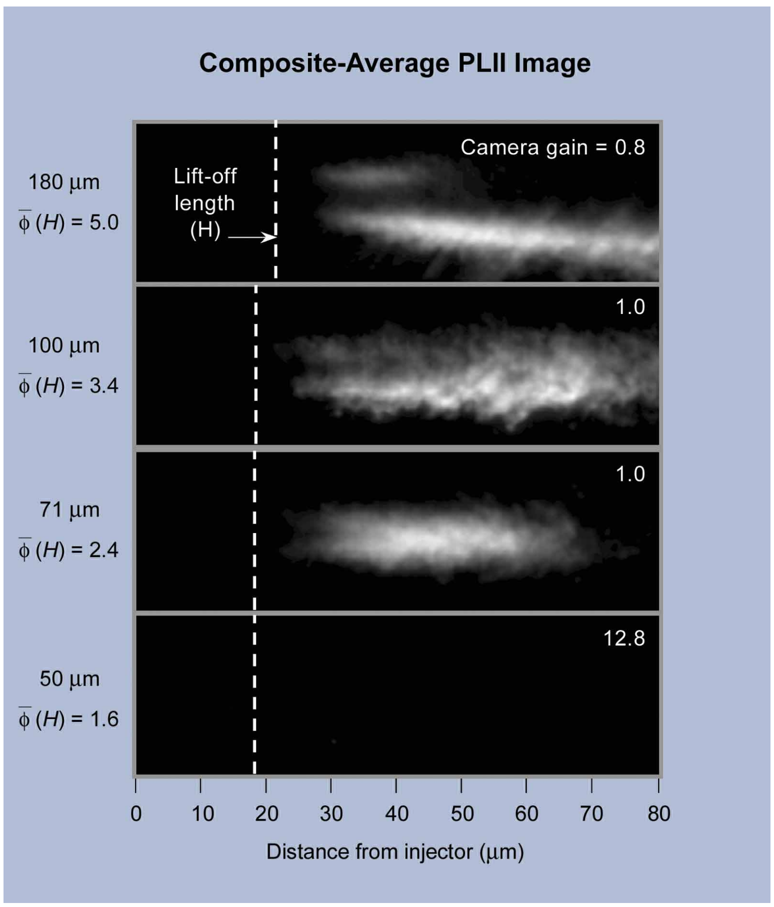


Figure 1. Composite-average PLII images for four different injector tip orifice diameters. PLII images were obtained by passing a laser sheet from the side through the centerline of the fuel jet during mixing-controlled diesel combustion. Measured lift-off lengths are indicated on the PLII images by the vertical dashed lines. The ambient gas temperature and density were 1000 K and 14.8 kg/m^3, the injector orifice pressure drop was 138 MPa, and the ambient oxygen concentration was 21%.

Laser-Based, Active-Illumination Technologies Show Greater Sensitivity Than Passive Methods for Airborne Detection of Gas Pipeline Leaks

Industry interest in the ability to detect leaks from gas transmission pipelines from aboard an aircraft has prompted Sandia researchers to explore the possibility of extending the range of remote gas detection using backscatter absorption gas imaging, or BAGI (*CRF News*, July/August 2000). Since the sensitivity of BAGI declines with standoff distance, researchers explored the possibility of using passive methods, which rely on detecting the thermal transfer between the gas and its surroundings.

In a recent theoretical and experimental analysis, a CRF team led by Tom Reichardt found that laser-based active illumination technologies have greater sensitivity than thermal-based passive methods for remotely detecting methane at distances up to 600 m (see Figure 1). Since the aircraft would be flown at an altitude of approximately 200 m, the laser-based approach would provide significantly improved sensitivity over the thermal approaches for this application, according to the team's findings.

The findings resulted from a thorough comparison of the relative merits of the two approaches, sponsored by the National Energy Technology Laboratory (Morgantown, WV). The team, which also included Sandians Sanjay Devdas, Tom Kulp and Wayne Einfeld, predicted leak concentrations and geometries, calculated detection sensitivities for the two approaches and experimentally confirmed performance predictions. For thermal detection, they examined the signal source term, measuring temperature differences between the ground and air that would drive the thermal transfer and define the detection limit.

Pioneering Laser-Based Leak Detection

For the past decade, Sandia's Remote Sensing Group has pioneered the development of these laser-based, active illumination leak detection systems. These systems transmit light that is absorbed by the gas to be detected. The transmitted light is then reflected by surfaces behind the gas, and collected by the instrument's receiving optics (see Figure 2). These laser-based instruments have been limited to relatively short distances appropriate for ground-portable systems (5-20 m).

Because the range of active illumination methods were limited, Sandia researchers considered passive methods to detect gas leaks. Such methods allow a nearly unlimited range with a simple instrumental configuration but rely upon a thermal flux between the gas plume and the ground's surface. However, for the distances needed for airborne deployment, experimental and modeling results indicate that active illumination methods maintain greater sensitivity in detecting the leaking gas, without having to rely on a thermal flux (see Figure 1).

Future work on this project involves the design and construction of a laser-based instrument that demonstrates the performance requirements suitable for airborne remote sensing of pipeline leaks.

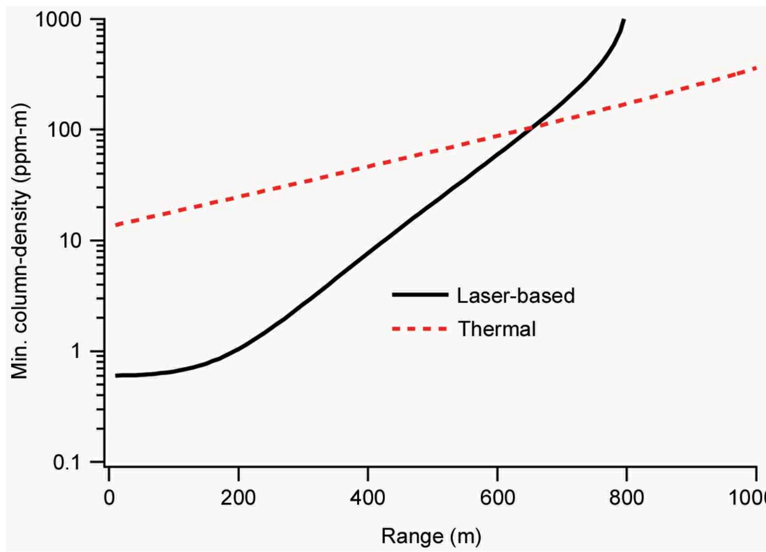


Figure 1. Experimentally confirmed modeling shows that a laser-based approach demonstrates superior sensitivity over a thermal approach at the ranges required for low flying aircraft.

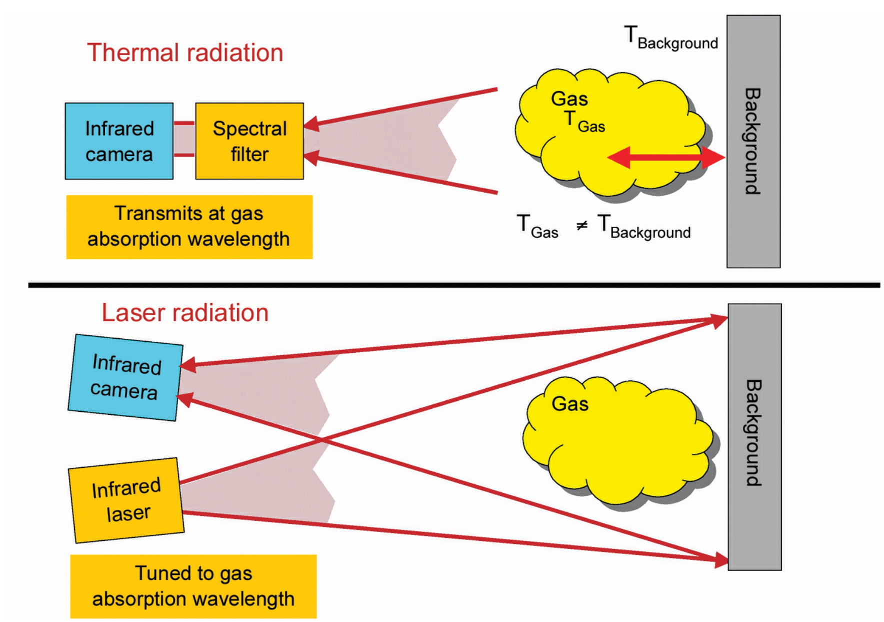


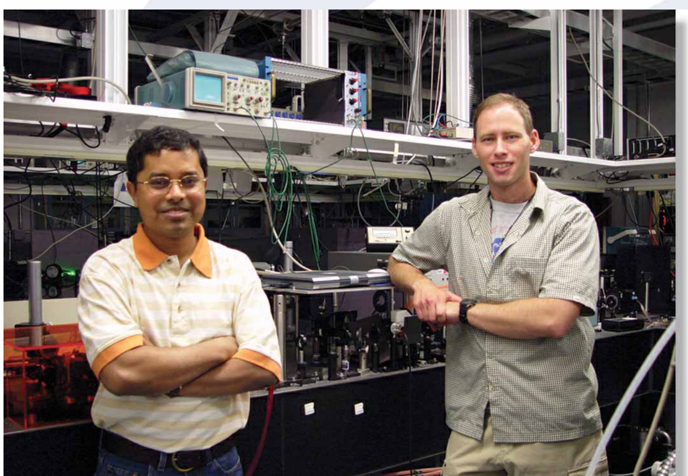
Figure 2. Sensing of gas plume by infrared radiation can be based on thermal exchange between the gas and the background, or illumination with an external source (e.g., laser radiation).

People

Berlin University of Technology Professor Visits the CRF

Frank Behrendt (left), vice dean of the School of Process Sciences and Engineering at Berlin University of Technology, visited the Combustion Research Facility for three weeks in February 2003. A long time CRF collaborator, Behrendt worked with Sandian Bob Gallagher (right) to explore the possibility of initiating interactions between his Berlin research group and the CRF in the area of biomass combustion with particular emphasis on diagnostics development.

Sandians Work with Researchers



Sandians Tom Settersten and Brian Patterson (right) are working with visiting researchers Sukesh Roy (left) of Innovative Scientific Solutions, James Gord of Air Force Research Laboratory and Robert Lucht of Purdue University in the CRF's Picosecond Diagnostics Laboratory. The researchers are investigating two-color, two-photon, laser-induced polarization spectroscopy of atomic hydrogen using single-mode picosecond laser pulses.

Sandians Receive DOE Combustion Engine R&D Award

The DOE annual Advanced Combustion Engine R&D award for best project from 2002 was presented to Dennis Siebers (right) and Lyle Pickett (left) of Sandia, and Brian Higgins of California Polytechnic State University at this year's merit/peer review meeting. They received the award for providing fundamental new insight into the effects of diesel engine parameters on soot formation processes in diesel fuel sprays. The merit/peer review meeting for the DOE Office of FreedomCAR and Vehicle Technologies' CIDI (Compression-Ignition, Direction-Injection) Engine Combustion, Emission Control, and Fuels R&D Program was held May 13–15 at Argonne National Laboratory. Seven engine combustion research projects out of 28 projects reviewed were from Sandia. The review panel was composed of representatives from various universities and sectors of the automotive and heavy-duty engine industries.

New DOE Office Holds First Peer Review

Many Sandians attended the first peer review meeting under the new DOE Office of Hydrogen, Fuel Cells & Infrastructure Technologies, held May 19–22 at the Claremont Hotel in Berkeley, Calif. The meeting attracted 550 attendees, making it one of the largest peer review meetings held by DOE. Sandians giving presentations included Karl Gross on gas separations, Andy Lutz on power park systems analysis, Peter Van Blarigan on free-piston internal combustion engines and Bob Schefer on hydrogen-fueled gas turbines.

Pilot Project Facilitates Knowledge Sharing, Chemical Science Research

Researchers at the CRF have teamed with eight other institutions to create a knowledge management system on the Web that will allow scientists in various disciplines to collaboratively develop and share chemical information. This pilot project, called the Collaboratory for Multi-scale Chemical Science (CMCS), differs from earlier research projects in that it is dedicated to producing a production-quality service.

Spearheaded by Sandians Larry Rahn and David Leahy, the goal of CMCS is to enhance chemical science research by facilitating rapid sharing of validated information through a new environment designed to assist development of multi-scale research projects. To accomplish this, CMCS is developing a data-centric, adaptive informatics infrastructure that will provide researchers with a centralized information source, easily accessed through a Web-based portal. It works by publicly deploying an integrated set of key collaboration tools and chemistry-specific applications, data resources and services. This CMCS service becomes a problem-solving environment for scientists to share data and collaborate in diverse, geographically distributed teams.

Testing CMCS Capabilities

CMCS is piloting this new infrastructure among a multidisciplinary team of chemical scientists who are working to advance combustion science. The team is in the process of testing the capabilities of CMCS by using it to analyze and research different physical scales in various combustion problems. The use of the CMCS service by these scientists will prove that the CMCS project has initiated and facilitated collaboration. While this pilot collaboratory is focused on combustion, the underlying adaptive informatics infrastructure is broadly applicable to many other research areas, and has already received attention from other researchers in a variety of disciplines.

The adaptive informatics infrastructure uses a "portal" as the Web interface. The infrastructure takes advantage of a variety of open-source information technologies to share data, metadata and project information within groups and across communities. The portal, which can easily be enhanced and customized through the inclusion of new "portlets," includes real-time collaboration capabilities, search and notification tools, and a pedigree browser.

Using CMCS

Figure 1 shows how CMCS users interact primarily with the top layer: the CMCS portal and chemistry applications. These chemistry applications can appear within the portal or can provide their own user interfaces that interact directly with the underlying data store. The portal provides a straightforward way for data resources to be associated with automatic data translators. These translations are beneficial both for providing useful views for inspection of data and to transform data into application-ready input formats.

The capacity to record and display data pedigree (metadata) is at the heart of the CMCS project and a key capability for enabling new approaches to science. It allows researchers to categorize and trace scientific data across disciplines and scales and to identify both the origins and the context of scientific data. The metadata provides the handles for the CMCS data search engine. Researchers have developed a pedigree browser that provides a convenient visualization of pedigree data. This pedigree view can easily be traversed from dataset to dataset using embedded links in the pedigree.

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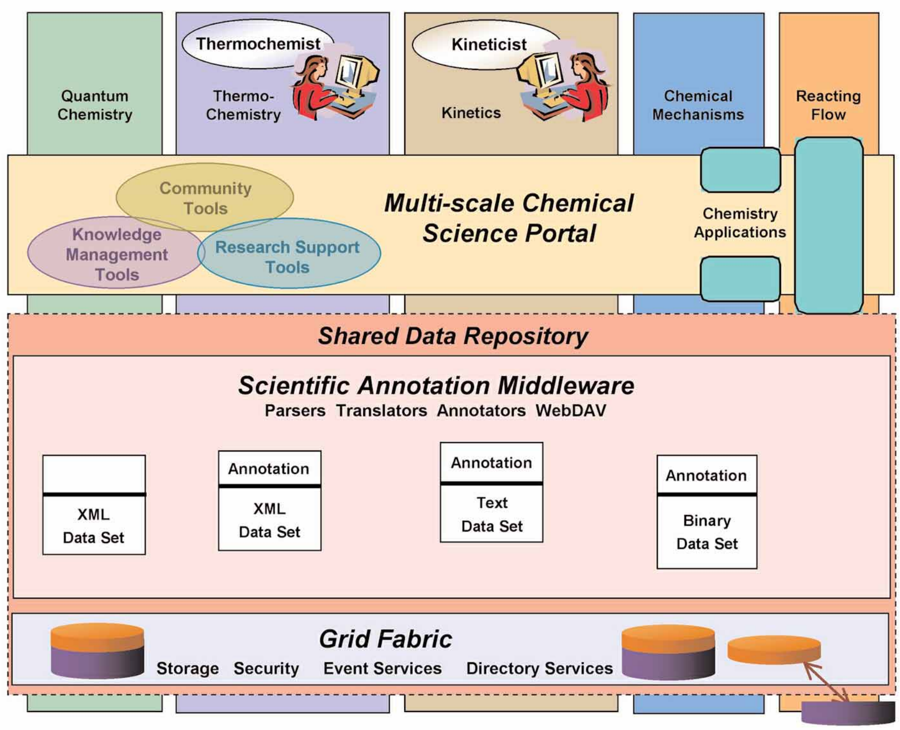

Figure 1. Architecture of the CMCS Data Service and portal: The large rectangle represents the Shared Data Repository. Contributors can use this to share chemistry data either privately or in groups. The Scientific Annotation Middleware wraps the repository, providing automatic ways to annotate data with pedigree information and performing translations of data to any format (ASCII, HTML, etc.). The yellow rectangle represents the CMCS portal, an easy-to-use Web interface that provides data searching, browsing and sharing capabilities. The portal has group management tools including discussion forums. Chemistry applications can connect from users' computers to the data store, or can be embedded in the portal for easy Web access.

Workshop Focuses On Need for Improved Mesh Adaptation Ability

In computational fluid dynamics, researchers have worked to be able to computationally analyze and track the unsteady features of combustion. Current methods for tracking and computing the unsteady features place a mesh-based numerical "cover" over the features. However, this process poses its own problems, for meshes must be adaptable to account for the constantly changing features of the elements. If the mesh cannot adapt, essential flow features would be missed, causing the numerical results to be inaccurate.

Several automatic mesh-generation approaches are available, but they focus on adaptivity with respect to numerical solution, or on mesh geometry modification. None have yet proposed a general framework that could cover all variability with mesh adaptation.

About two dozen researchers working on issues of mesh adaptation gathered at the CRF Jan. 16–17 for the Workshop on Mesh Quality and Dynamic Meshing (WMQDM). Organized by Philippe Pébay, the workshop gathered researchers together to develop the general framework needed to account for the many different variables associated with mesh adaptation. The proceedings of the workshop can be found at **http://www.ca.sandia.gov/CRF/mqdm**.

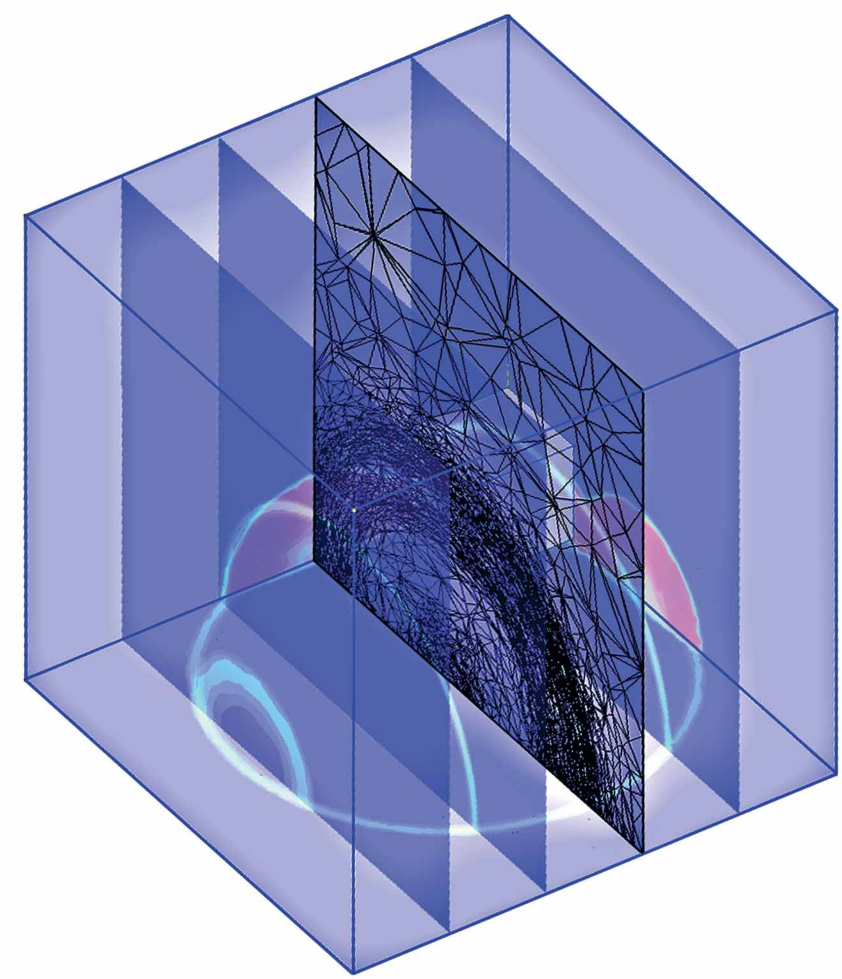

Figure 1. This Sedov explosion compares the present experimental determination of the $HCO+O_2$ rate constant to previously published measurements. This is an example of Jean-François Remacle's (Catholic University of Louvain, Belgium) work with mesh adaptivity. Remacle presented a remarkable discontinuous Galerkin scheme combined with dynamic anistotropic mesh adaptation at the workshop.

Issues in Improving Mesh Quality

Numerical simulations, based on finite volume (FV) or finite element (FE) methods, require the prior construction of a mesh (T_Ω) of the domain of interest (Ω). This mesh (T_Ω) must form a polygonal (2-D) or polyhedric (3-D) cover of Ω (see Figure 1). However, it becomes much harder to create this mesh for a nonsimplicial, that is, nontetrahedral element. In addition, making the mesh adaptable for a nonsimplicial element is even more difficult.

Current mesh generation is inadequate for anisotropic or unsteady problems. For example, some essential features, such as fronts or vortices, within a reduced sub-domain of Ω, require local mesh refinement to improve accuracy. Conversely, zones where the considered variables are relatively smooth and slow-varying require mesh coarsening in order to save processing time.

Another issue is that the unfolding of the physical process itself may cause the geometry and/or the topology of Ω to be modified. All of these phenomena vary in time, essentially requiring a new assessment of the mesh at each step because the quality of the mesh must be maintained, or the numerical results of the mesh will be compromised. Not only is maintaining the quality of the mesh a concern, but in turn, the quality of the mesh affects the ability to adapt the mesh, creating an even greater challenge.

Limitations of Adaptivity Approaches

In recent years, a wide variety of approaches have been proposed to deal with these issues. Recent methods based on Riemannian metrics take into account the "weighted" geometry that results from numerical error estimates. These methods have been proposed and sucessfully tested in the case of anisotropic adaptivity. Nevertheless, the number of available results providing comparisons between these various mesh quality estimates, and in particular how they relate to the subsequent mesh adaptivity process, is still very limited.

2003 International Symposium
American Flame Research Committee

Sandia to Host American Flame Research Committee Symposium

Sandia will host the 2003 American Flame Research Committee International Symposium Oct. 16–17. The symposium will be held at the CRF and will focus on bridging the gap between combustion research and industrial practice in a more cost-effective manner. Presentations will also cover research, development and commercialization of technology for improvements related to combustion, pollution abatement and energy utilization.

Registration is $350 for members, $450 for nonmembers and is due Sept. 5.

Of interest will be papers identifying key combustion research and development activities that have produced significant advances in abatement of particulate and toxic combustion by-products; burners, boilers, furnaces, and industrial processes; flaring, incineration or recovery of waste by-products or process off gases; industrial energy utilization and reduction of greenhouse gas emissions; sensors and combustion control strategies.

For more information please visit **http://www.ca.sandia.gov/afrc/geninfo.html**.

Soot

(Continued from page 1)

concentrations as low as 10%, no detectable soot was found when using the micro-orifice. The results indicate that lift-off length increases with decreasing oxygen concentration, allowing more ambient gas entrainment into the fuel jet prior to the lift-off length, the net effect being that $\bar{\phi}$ (H) does not change significantly with oxygen concentration.

The reduced oxygen concentration results are significant because a decreasing oxygen concentration decreases flame temperature, which in turn decreases NO_x formation. The lack of soot formation even at low ambient oxygen concentrations suggests that soot and NO_x could be reduced simultaneously in an engine through the use of small orifices and EGR.

Although these single-jet results are useful in understanding limiting-case behavior of single-jet mixing and combustion during a diesel injection event, the investigation did not address the effects of jet-jet interactions as well as other "real" engine effects. If proven feasible, the use of micro-orifice injectors would likely require a significant redesign of the typical in-cylinder geometry in a diesel engine to promote efficient air utilization.

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