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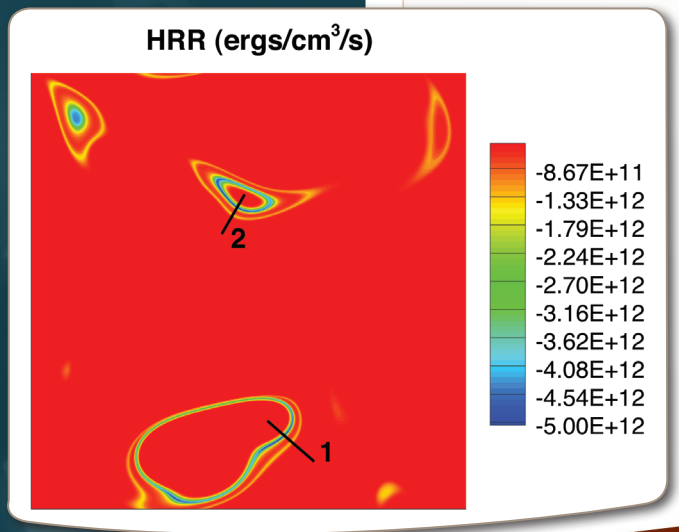
Petascale simulations of combustion phenomena in HCCI engine environments

Homogeneous charge compression ignition (HCCI) is a viable new concept for next-generation internal combustion engines. It has the potential for achieving ultra-low nitric oxides (NO_x) and soot emissions and at the same time offers higher fuel conversion efficiency. Strictly speaking, HCCI refers to combustion occurring in a nearly homogeneous charge of uniform temperature and mixture composition, whereby combustion occurs primarily volumetrically via autoignition. (Continued on page 4)

Figure 1. Twin-ringed structure of heat release rate (HRR). The outer combustion wave is due to second-stage ignition and the inner wave is due to third-stage ignition. Cut plots along lines 1 and 2 are shown in Figure 2(a) and 2(b), respectively.



Combustion properties of biomass lignin residues determined

Lignin, the organic "glue" of high-molecular-weight aromatic material that binds cellulose and hemicellulose components to make plant fibers, is a ubiquitous and undesirable component of plant material when trying to biochemically convert the plant into biofuel. In fact, not only is it chemically impossible to convert the lignin into ethanol, but the presence of lignin can inhibit the hydrolysis of the cellulose and hemicellulose polysaccharides into organic sugars (glucose and pentoses, for example) that can then be fermented into alcohols or biologically converted into advanced biofuels.

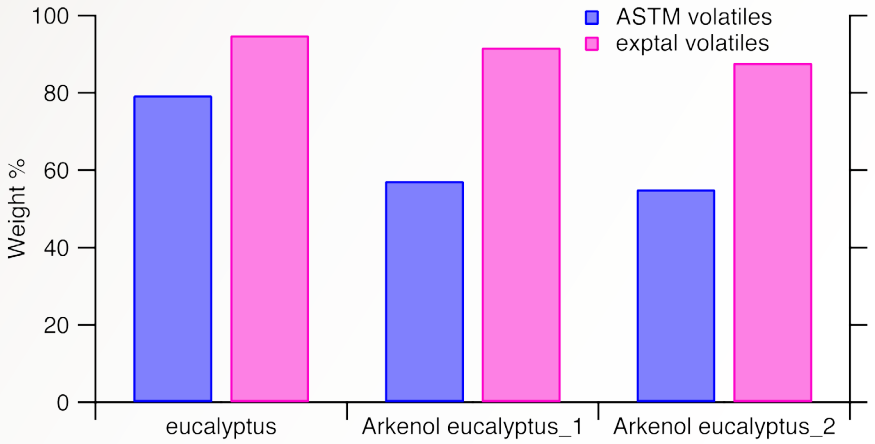


Figure 1. Comparison of ASTM volatiles content and experimental high-temperature, high-heating-rate volatiles yield of eucalyptus wood feedstock and lignin residues generated from two variations of the Arkenol biochemical process.

Consequently, the first step in converting general plant material (referred to as "lignocellulosic biomass") into biofuels is to attempt to separate the polysaccharides from the lignin via pretreatment processes that typically involve acid or base solutions. The lignin residues that are produced from the biofuel production processes have been assumed to be appropriate for use as a boiler fuel for generation of heat (in the form of steam) required in the process, but until a recent study at the CRF was conducted, no systematic evaluation of their combustion properties had been performed.

The research project, funded under Sandia's Laboratory Directed Research and Development (LDRD) program, evaluated the combustion properties of practical lignin residues produced by several alternative approaches to bio-ethanol production. Lignin residues were generated by Sandia biochemical engineers using two small-scale batch pretreatment processes and were also supplied by the National Renewable Energy Laboratory (NREL), which operates a pilot-scale weak acid enzymatic hydrolysis system for making bio-ethanol. Two promising biomass feedstock sources were investigated in the course of this study: corn stover—the

(Continued on page 2)

Combustion properties of biomass lignin residues determined (continued from page 1)

stalk, leaves, husk, and cob material that remains after harvesting corn—and eucalyptus, a fast-growing tree.

Two-step evaluation process

Evaluation of the combustion properties occurred in two discrete steps. First, Chris Shaddix, Ethan Hecht, and postdoctoral researcher Manfred Geier used an electrically heated entrained flow reactor to measure the high-temperature volatiles yield of the lignin residues. The volatiles yield under practical conditions is an important parameter for determining the ease of combusting or gasifying the material, as gaseous fuel inherently mixes and reacts more quickly than solid fuel. In contrast to the results for the standard American Society for Testing and Materials (ASTM) volatiles determination, which is performed at a low heating rate up to 950 °C, the experimental results show high volatiles loss upon rapid heating to 1,200 °C. In fact, as shown in Figure 1, the high-temperature volatiles loss exceeds 90 wt-%, and is only slightly lower for the lignin residues than for the original biomass feedstock. This result portends favorable combustion and gasification behavior of the lignin residue.

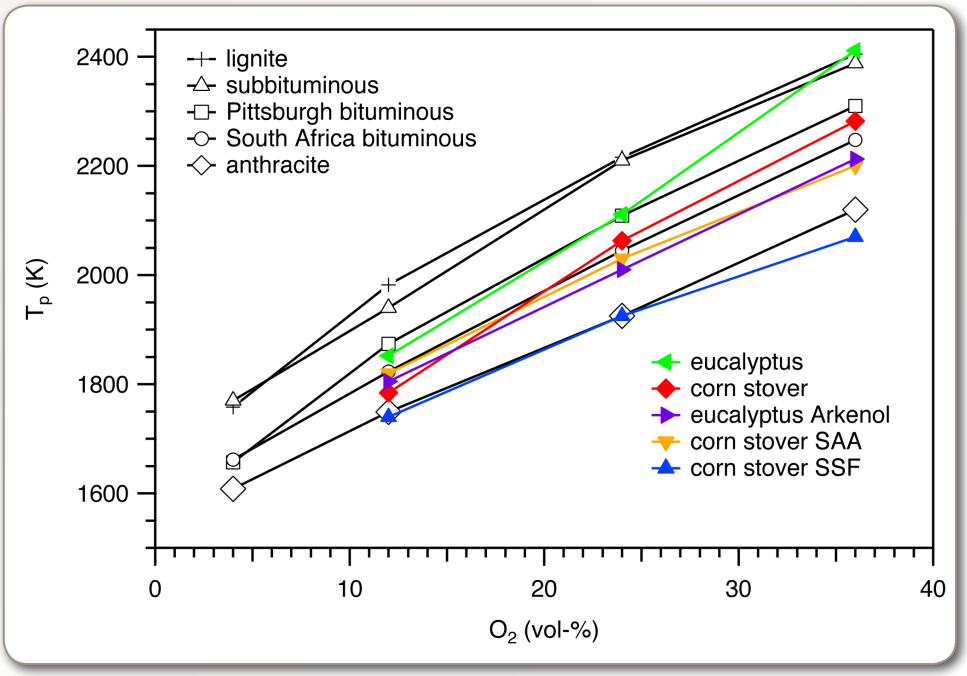


Figure 2. Measured mean char particle temperatures during combustion of 100-µm char particles in 1,650-K gas with the indicated oxygen content.

Char particles measured via two-color pyrometry

Next, the combustion reactivity of the char particles that remain after lignin residue devolatilization was evaluated in Sandia's optical entrained flow reactor. In this reactor, the char particle temperatures are measured optically by performing two-color pyrometry on individual pulverized char particles as they are carried through the reactor and are burned. For a given reactor environment, the particle combustion temperature is a direct measure of the oxidative reactivity of the particle, and, when coupled with particle size information, can be used to derive overall combustion kinetic rate parameters.

Figure 2 shows the mean char particle combustion temperatures that were measured for several different lignin residues and corresponding raw biomass feedstocks, in comparison to previously measured data for a wide range of coal rank (i.e., spanning the range of coal reactivity). For all of the fuels, the char combustion temperature increases as the surrounding oxygen content increases because oxygen is the limiting reactant in the heterogeneous oxidation reaction. The figure shows that the raw biomass chars are more reactive than the lignin residues and, in fact, approach the reactivity of the most reactive coals (lignite). Most of the lignin residue chars have a reactivity corresponding to medium-rank coal chars (high-volatile bituminous coal char), and the residue from the most promising near-term candidate for bio-ethanol production, weak acid simultaneous saccharification and fermentation (SSF), shows the lowest reactivity, corresponding to a high-rank coal char (anthracite).

Overall, the results suggest that the lignin residues from both the Arkenol process and from the soaking in aqueous ammonia (SAA) process will be easily converted in conventional boilers and gasifier systems, whereas the SSF residues will likely experience carbon burnout difficulties. The SSF residue is collected at the end of the biofuels production process and has a high ash content, dominated by silica, which explains its low char reactivity. The results of this study were recently presented at the 7th U.S. National Combustion Meeting in Atlanta and are being submitted as a journal article.

Sandia and LLNL showcase hydrogen buses

What do two Ford shuttle buses, a 2006 Toyota Prius, and a mobile electric light stand have in common?

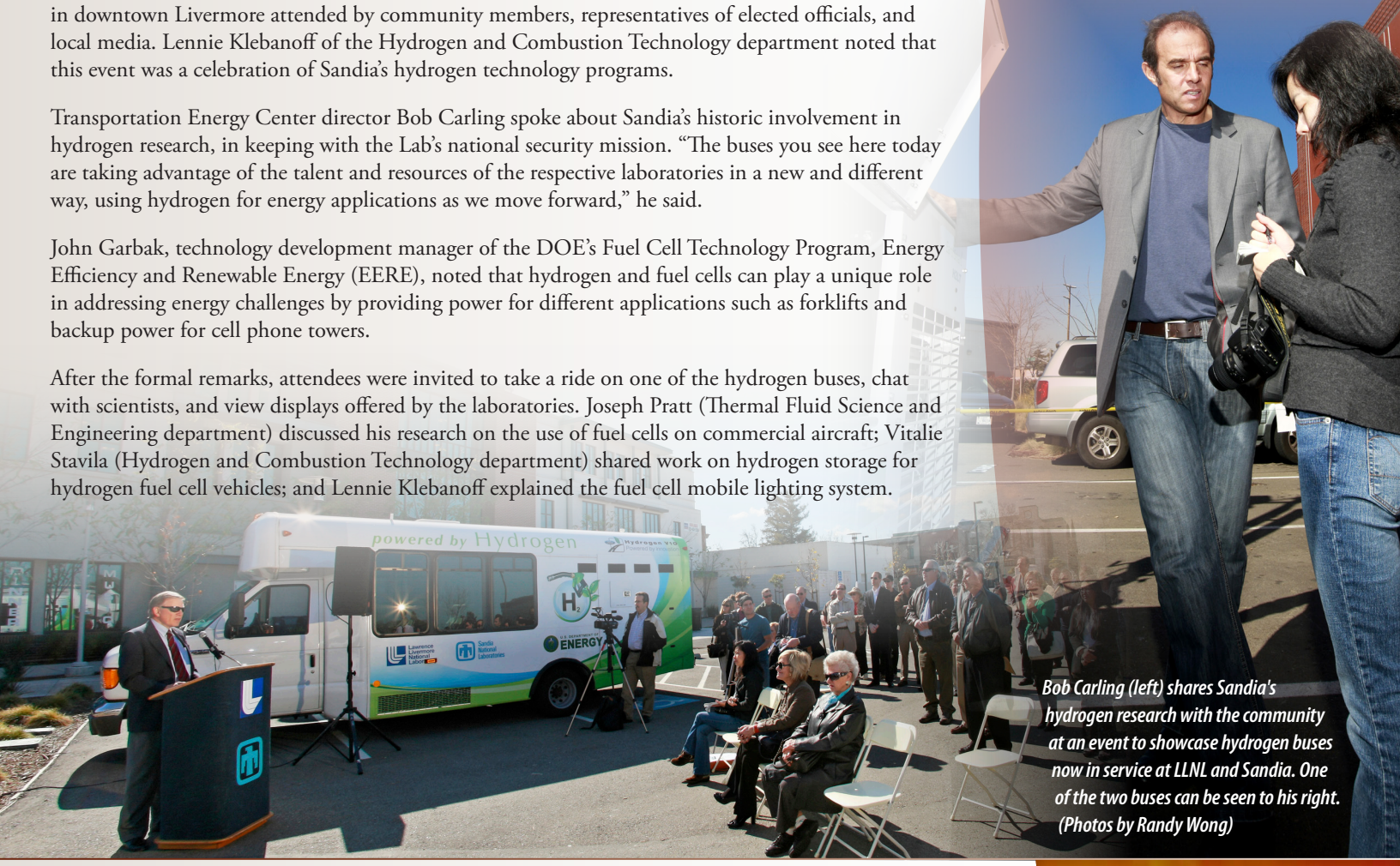
They are examples of hydrogen-powered technologies developed via collaborative programs between the U.S. Department of Energy (DOE), Sandia/California and Lawrence Livermore National Laboratories, and private corporations. On February 22, the buses made their formal debut at a public event in downtown Livermore attended by community members, representatives of elected officials, and local media. Lennie Klebanoff of the Hydrogen and Combustion Technology department noted that this event was a celebration of Sandia's hydrogen technology programs.

Transportation Energy Center director Bob Carling spoke about Sandia's historic involvement in hydrogen research, in keeping with the Lab's national security mission. "The buses you see here today are taking advantage of the talent and resources of the respective laboratories in a new and different way, using hydrogen for energy applications as we move forward," he said.

John Garbak, technology development manager of the DOE's Fuel Cell Technology Program, Energy Efficiency and Renewable Energy (EERE), noted that hydrogen and fuel cells can play a unique role in addressing energy challenges by providing power for different applications such as forklifts and backup power for cell phone towers.

After the formal remarks, attendees were invited to take a ride on one of the hydrogen buses, chat with scientists, and view displays offered by the laboratories. Joseph Pratt (Thermal Fluid Science and Engineering department) discussed his research on the use of fuel cells on commercial aircraft; Vitalie Stavila (Hydrogen and Combustion Technology department) shared work on hydrogen storage for hydrogen fuel cell vehicles; and Lennie Klebanoff explained the fuel cell mobile lighting system.

The event showcased other hydrogen projects in addition to the buses. Below, Lennie Klebanoff discusses with a journalist the hydrogen fuel cell mobile lighting system.



Bob Carling (left) shares Sandia's hydrogen research with the community at an event to showcase hydrogen buses now in service at LLNL and Sandia. One of the two buses can be seen to his right. (Photos by Randy Wong)

Distinguished Papers chosen by the Combustion Institute

Two papers co-authored by CRF researchers were selected as Distinguished Papers by the Combustion Institute's 33rd International Symposium on Combustion. "Experimental study of flame-hole reignition mechanisms in a turbulent non-premixed jet flame using sustained multi-kHz PIV and crossed-plane OH PLIF, " co-authored by CRF researcher Jonathan Frank and A.M. Steinberg, I. Boxx, C.M. Arndt, and W. Meier, was chosen as the Distinguished Paper in the Turbulent Flames colloquium. "Picosecond time-resolved pure-rotational coherent anti-Stokes Raman spectroscopy in sooting flames," by Christopher Kliewer, Yi Gao Thomas Seeger, Johannes Kiefer, Brian Patterson, and Thomas Settersten was selected as the Distinguished Paper in the Diagnostics colloquium. The complete list of distinguished paper awards for the 33rd Symposium can be found at ***https://www.combustioninstitute.org/CIResources/awards.php***.

With this selection, these papers have been nominated as candidates for the Silver Medal Award for the 33rd International Symposium on Combustion. Together with the Distinguished Papers from the other colloquia, the CRF papers will be reviewed by the Silver Medal Award Committee, and their decision will be announced to the membership at the 34th Symposium in Warsaw, Poland. The Combustion Institute was founded in 1954 to provide ways for combustion scientists and engineers to communicate with each other and the rest of the technical world. The biennial International Symposium on Combustion is the primary conference organized by the Institute.

Petascale simulations of combustion phenomena in HCCI engine environments

(Continued from page 1)

However, in real engines there are always some charge inhomegeneities due to naturally occurring thermal stratification resulting from wall heat transfer and convection by in-cylinder flows. This slows the heat release rates, allowing a higher load than would be possible for a truly homogeneous charge. Additionally, varying amounts of fuel stratification can be deliberately introduced at some operating conditions to reduce the pressure-rise rate to allow higher loads without engine knock. Therefore, it is essential to thoroughly investigate autoignition and subsequent combustion behavior in high-pressure stratified turbulent mixtures. A fundamental understanding of turbulence–mixing–autoignition interaction in high-pressure stratified systems will provide underlying physical insight to guide the optimal development of these engines.

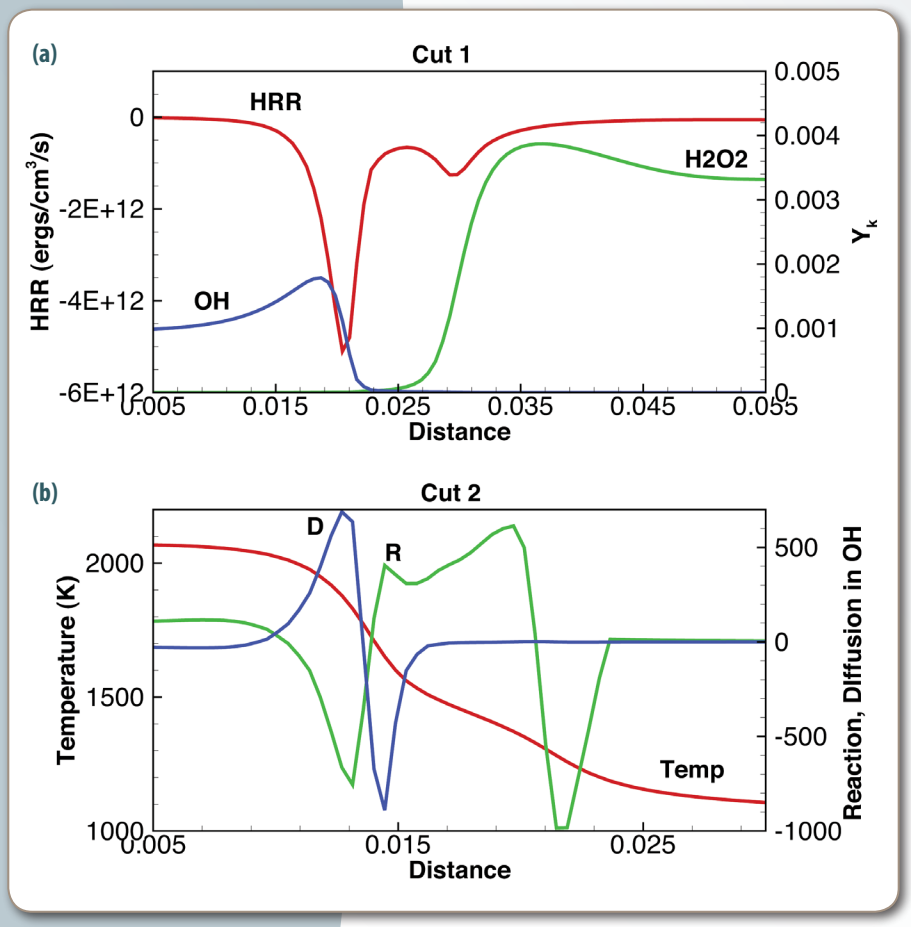


Figure 2. *These two graphs show cut plots along the lines indicated in Figure 1.*

Fundamental combustion processes revealed by DNS

To shed light on the fundamental processes associated with combustion in HCCI engine environments, researchers Gaurav Bansal and Jackie Chen of the Reacting Flow Research department at the CRF are conducting petascale direct numerical simulations (DNS) of these systems. Dimethyl-ether (DME), which has favorable autoignition characteristics and can also be bio-derived, is used as the fuel. A highly efficient, accurate, and reduced DME chemical kinetic mechanism with 26 chemical species, optimized and validated by Tianfeng Lu at the University of Connecticut and derived from a comprehensive mechanism by Zhao et al. 2008, is coupled with the DNS. The DNS configuration corresponds to a 3-D periodic cube initialized with homogeneous isotropic turbulence. A random temperature field is superimposed on the mean field using a scalar spectrum similar to the turbulence kinetic energy spectrum to specify the characteristic scales of the initial hot/cold spots. The turbulence integral time scale and chemical time scales are initialized such that they are of comparable magnitude to those existing in practical engines. Also, RMS values of initial temperature inhomogeneities are comparable to those found in realistic engines. As such, the turbulence–mixing–chemistry interactions observed in DNS are representative of those observed in real engines. To mimic isentropic compression due to piston motion, inert mass source terms are added to the governing equations in the DNS.

As a precursor to performing the 3-D DNS, a variety of 2-D DNS in a similar configuration are conducted to explore the parameter space in which to conduct the 3-D simulation. Various insights are gained from 2-D DNS. It is found that autoignition of DME occurs in three distinct stages, each corresponding to a distinct chemical pathway. Figure 1 shows the heat release rate (HRR) field during thermal runaway in a thermally and compositionally stratified case. A twin-ringed structure of heat release is observed; the outer ring corresponds to second-stage ignition while the inner ring corresponds to third-stage ignition. Two cut plots in Figures 2(a) and 2(b) reveal the structure of these waves. As observed in Figure 2(a), the second and third stages of ignition can occur in very close spatial proximity, which may lead to inter-diffusion of heat and radicals between these stages. Moreover, as revealed in Figure 2(b), the heat release mode in the second stage is predominantly a reaction-driven spontaneous ignition front, whereas the third stage is predominantly a premixed deflagration

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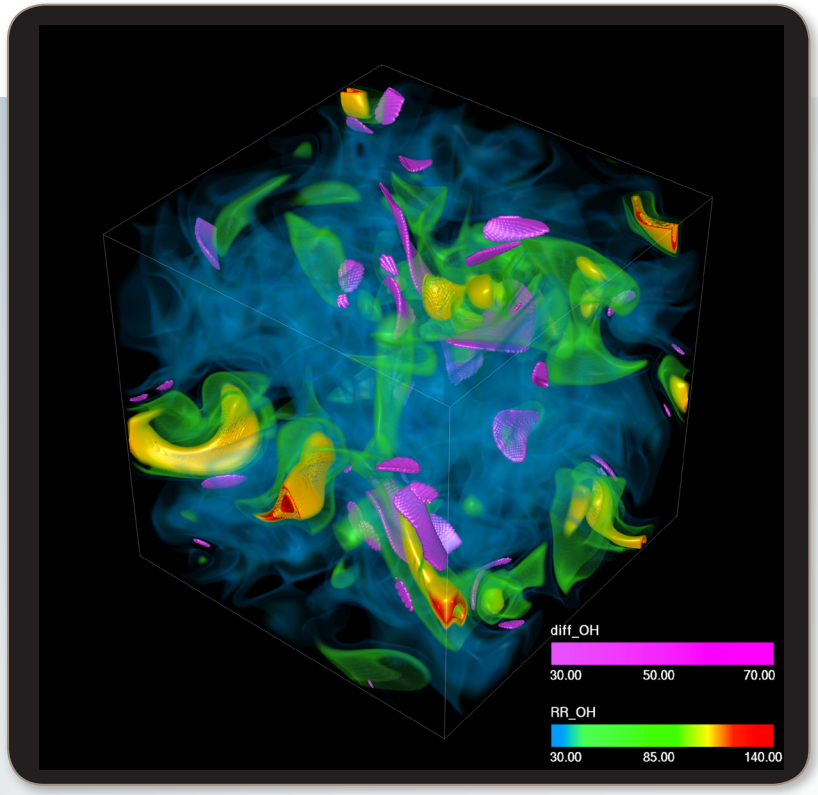

Figure 3. Volume rendering of diffusion (diff_OH) and reaction (RR_OH) fields of OH mass fraction. (Image created by H. Yu)

wave with roughly equal contributions from reaction and molecular transport. The different heat release modes arise because during the third stage of ignition there are strong reaction-generated gradients in the reacting scalar fields, thus enhancing mixing and promoting the importance of molecular transport.

A 3-D DNS was subsequently performed to investigate the interaction of isotropic turbulence with ignition chemistry, representing the first 3-D DNS of multi-stage compression ignition with reduced chemistry. Although many of the insights gleaned from 2-D simulations also apply to 3-D simulations, it is well known that 3-D turbulence is fundamentally different from 2-D turbulence due to the presence of the vortex-stretching term. This may lead to anisotropic development of the initial hot spots. The researchers are collaborating with two computer scientists (also at the CRF's Reacting Flow Research department): Hongfeng Yu, on visualization of complex 3-D flow and reacting scalar structures, and Ajith Mascarenhas, on topological segmentation/tracking methods to isolate and temporally track local ignition kernels and perform conditional statistical analysis on the segmented kernels.

Figure 3 shows the reaction (RR_OH) and diffusion (diff_OH) fields of OH mass

Petascale simulations *(continued from page 4)*

fraction at a time when total heat release is dominated largely by third-stage ignition. Regions of high OH diffusion (or high OH dissipation) are denoted by pink surfaces. The figure shows that high dissipation of OH occurs in "pancake-like" structures scattered over the domain. By comparing the magnitudes of reaction and diffusion of OH mass fraction, the regions burning in a deflagration mode versus those burning in a reaction-driven spontaneous ignition front mode can be demarcated. In Figure 3, the regions of high dissipation (pink regions) close to green reaction rate fields are burning in deflagration mode, whereas those close to red reaction rate fields are burning in spontaneous ignition front mode. Figures 4(a) and 4(b) show close-up plots of Figure 3, again illustrating regions burning in different heat release modes.

In conclusion, combustion phenomena in these high-pressure stratified systems is found to be highly mixed-mode. This can pose a significant challenge in developing sub-grid closure models for large-eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) methods. The DNS conducted in this study not only provides unprecedented physical insights into the phenomena, but also provides high-fidelity benchmark data against which modelers can validate their sub-grid models.

Figure 4. These illustrations show close-ups of regions inside Figure 3. The colormap is same as that used in Figure 3. (Image created by H. Yu)

AEC/HCCI Working Group meetings held

The Advanced Engine Combustion (AEC) and the University Homogeneous Charge Compression Ignition (HCCI) Engine Combustion working group meetings, organized by Sandia National Laboratories, took place February 22–24 here at the CRF. Dennis Siebers, Paul Miles, Chuck Mueller, Mark Musculus, and Lyle Pickett served as chairs for the series of Working Group meetings, which explored topics ranging from combustion mode capabilities of Sandia's heavy-duty optical diesel engine, to the thermal characteristics of HCCI deposits, to RCCI combustion using high-speed chemiluminescence. These meetings reported on the latest progress from all DOE Office of Vehicle Technologies supported research on advanced, low-temperature combustion strategies for high-efficiency, clean engines and future fuels for these engines.

Approximately 80 representatives from the various AEC Memorandum of Understanding (MOU) industry and national lab partners attended the meetings. (The MOU partners include GM, Ford, Chrysler, Cummins, Detroit Diesel, Caterpillar, John Deere, General Electric, Chevron, ExxonMobil, ConocoPhillips, BP, SNL, LLNL, LANL, ORNL, and ANL). University attendees from MIT, U.C. Berkeley, and the Universities of Wisconsin and Michigan joined the group for the University HCCI working group portion of the meetings.

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