JUNE 2007

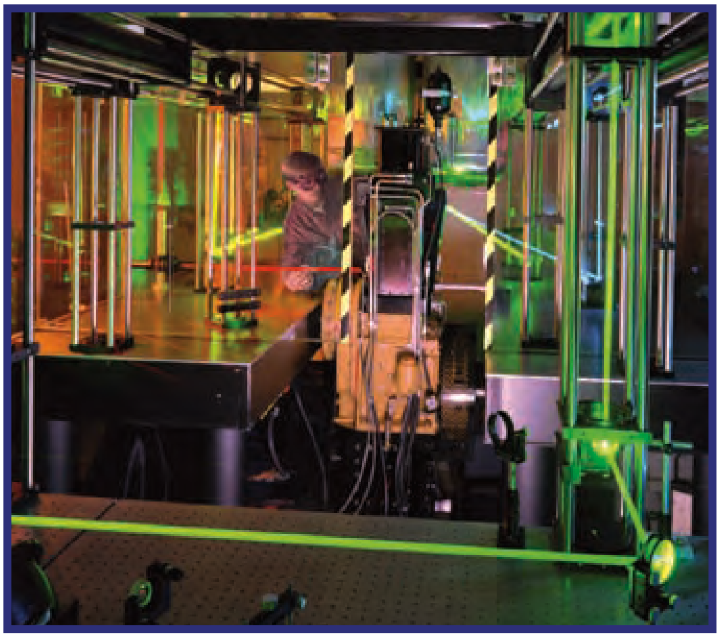
FOCAL POINT

SANDIA NATIONAL LABORATORIES

Extracting Clean Energy from Fuels

Many Californians can recall the years when their automobiles got less than 20 miles per gallon and thick smog blanketed the Los Angeles basin. Millions drove fuel-guzzling cars and trucks dozens of miles every day, spewing out noxious fumes wherever they went. But all that has changed, thanks to regulatory pressures and the pioneering work of the Combustion Research Facility (CRF) at the Sandia National Laboratories in Livermore, California.

Established in 1980, this world-famous laboratory uses powerful laser beams and computers to study how fuels actually burn—especially the complex reactions that occur within internal combustion engines and the exhaust gases and particulates that they emit. The resulting scientific understanding of combustion has helped car and truck makers to reduce these pollutants dramatically while improving the fuel efficiencies of their vehicles. What only three decades ago was largely educated guesswork is now science-based engineering technology. In short, Sandia's research has revolutionized how we think about combustion.



Laser beams are used to study a diesel engine designed for alternative fuels at Sandia's Combustion Research Facility.

This facility can trace its origins back to the mid-1970s "energy crisis," which followed the Arab oil embargo of 1973. As long lines of cars snaked toward gasoline stations, the U. S. Atomic Energy Commission and its successor agencies began seeking ways to apply the scientific and engineering expertise at national labs to looming energy problems. At Sandia's California laboratory, researchers led by Dan Hartley recognized that the laser-diagnostic techniques they had been developing to observe the hot, turbulent gases in nuclear weapons tests could be adapted to study combustion processes in exacting detail. They proposed to establish a national center for combustion research at Sandia, where scientists and engineers from academia and industry could combine state-of-the-art laser diagnostics with sophisticated combustion models using the lab's powerful supercomputers. Therefore the Combustion Research Facility finally took shape in the late 1970s under the auspices of the U.S. Department of Energy (DoE) and was completed in 1980.

With Hartley serving as its first director, the CRF produced twin laser beams, dubbed Diana and Orion, that could be directed into a variety of different test stands in order to study the detailed molecular dynamics of chemical reactions—particularly what occurs inside internal combustion engines. Specially built engine models with quartz windows allowed laser beams to enter their combustion chambers. Through other windows, researchers could observe what happened to these beams as they zipped through the turbulent fuel-air mixtures inside. That helped them discern what molecular species arose during successive stages of the combustion process, their concentrations, and the dynamics of the fluid flows within. Using the

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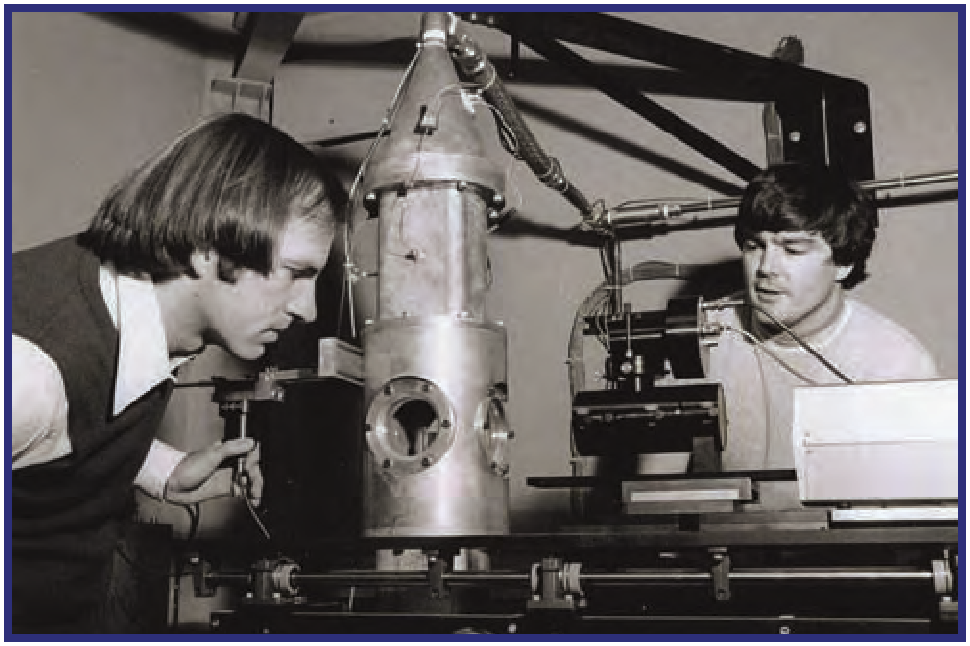


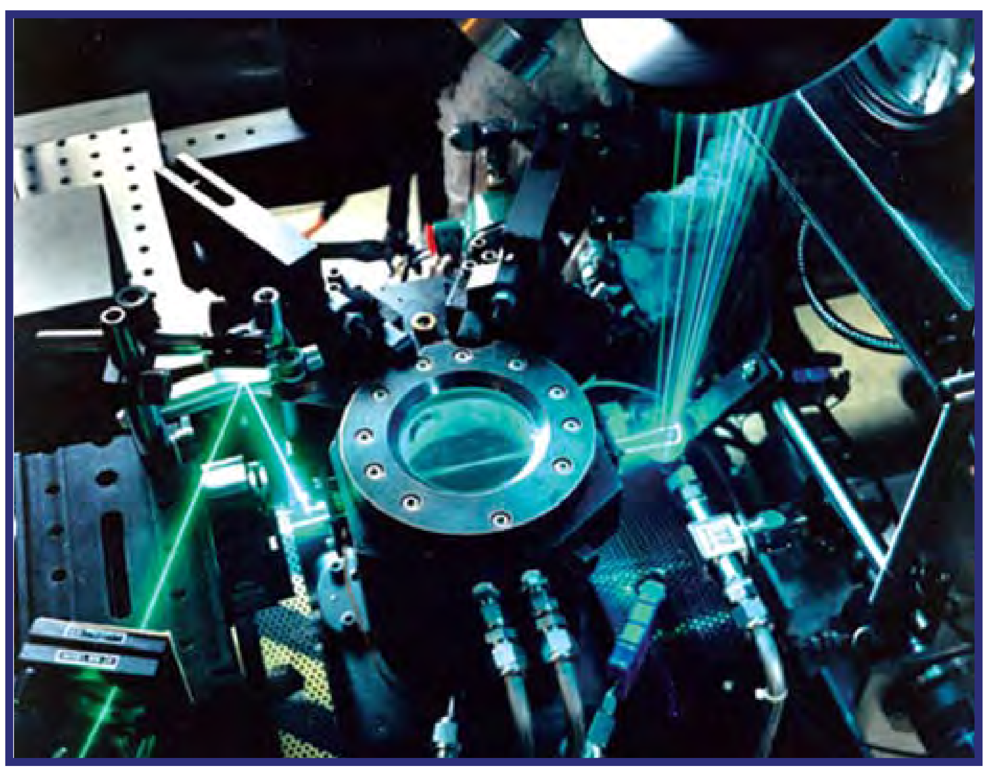
Founding CRF Director Dan Hartley (left) and research scientist Peter Witze adjust an experimental combustion setup in the late 1970s.

resulting detailed scientific understanding of internal combustion, engineers at the principal automobile- and truck-manufacturers could redesign gasoline and diesel engines to curtail the formation of nitrogen oxides, unburned hydrocarbons, and particulates while simultaneously improving their overall fuel economy.

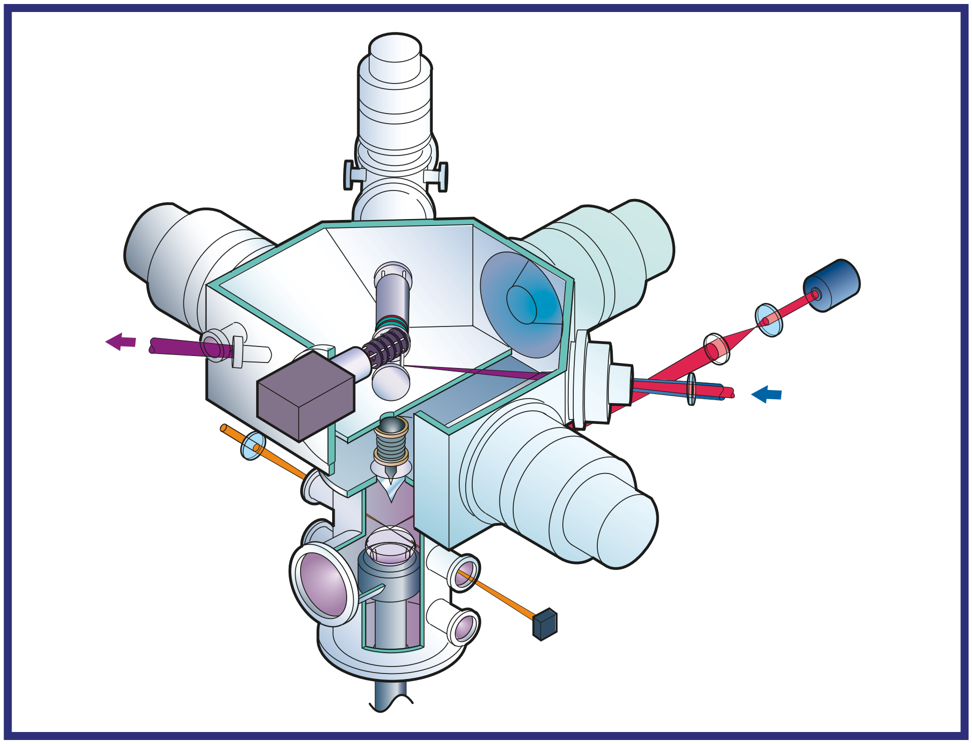
Also critical to these efforts was Sandia's ability to model internal-combustion engines and processes in finer and finer detail using powerful supercomputers. Both the kinetics of chemical interactions and the dynamics of fluid flows were included in these simulations. By combining these computer simulations with laser-diagnostic experiments, CRF researchers could check and validate their models against reliable data. These improved computer models gave automobile engineers much-needed design tools they could then use to evaluate the energy and pollution consequences of various possible design choices.

Hartley and other CRF managers wisely promoted the laboratory as an open user facility in which both academic and industry researchers were welcome to come and work—frequently in collaboration. This was no easy feat, because the two cultures are often at odds; academics pursue free and open publication of their results, while the propriety needs of industry usually require greater secrecy. But the two cultures had to be deeply involved—together with scientists from other government labs—if their results were to have a major impact on the automotive market. So leaders of these communities were included in all planning and oversight activities.

Several specific engine working groups soon arose that included members from the Big Three automakers and oil companies such as Chevron and Unocal working alongside researchers from UC Berkeley, MIT, Princeton, and other universities and national labs. As Ford, General Motors and Chrysler, plus diesel-engine manufacturers Caterpillar, Cummins Engine and John Deere, began implementing related design improvements during the 1980s and 1990s, air pollution began to fall dramatically in major urban areas. Automobiles getting better than 20—and sometimes over 30—miles per gallon became the norm rather than the exception.



Laser beam passes through a test engine via quartz windows on either side, permitting researchers to study the combustion reactions and fluid flows occurring within.

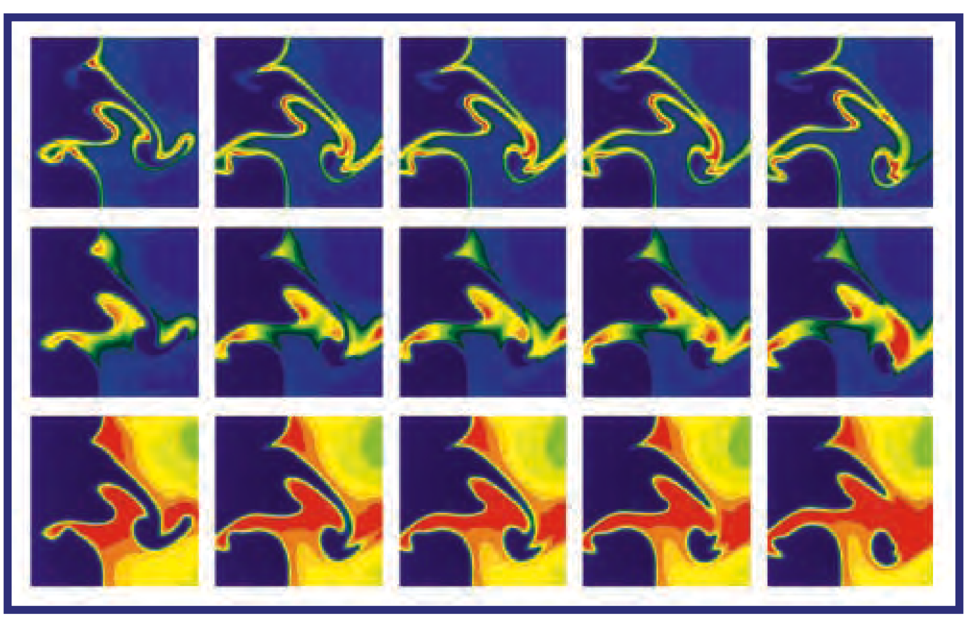


Cut-away drawing of a test facility in which lasers are used to study the dynamical structure and chemical composition of flames.

Of course, fuels are burned to produce useful power and heat throughout the economy, not just for transportation but also in buildings and industry. Here, too, CRF research has led to impressive improvements in the efficiencies of burning coal, oil, natural gas and even wood—thereby boosting economic returns while helping limit or reduce the emissions of pollutants or greenhouse gases, and especially carbon dioxide. For example, researchers from Toshiba, Lennox Industries and UC Berkeley have examined the use of pulsating jets of natural gas in furnaces for home heating. These studies showed that energy-conversion and heat-transfer efficiencies can be more than *doubled* by such a simple modification, which has since been incorporated in many residential, commercial and industrial heating applications.

But the principal thrust of CRF research remains in transportation, which accounts for over 40 percent of California's energy use. A group of Sandia researchers, working with their academic and industry counterparts, has been studying and developing a new generation of low-temperature internal-combustion engines. By operating with lean fuel-air mixtures and at temperatures less than 2000°C, these advanced diesel and spark-ignition engines should virtually eliminate formation of soot and nitrogen oxides. At the same time, their fuel-burning efficiencies can be improved by up to 50 percent over existing engines, with consequent reductions in the emissions of carbon dioxide. Using the twin CRF techniques of laser diagnostics and computer modeling, researchers have been gaining a much better scientific understanding of the microscopic details—on a molecule-by-molecule basis—of the combustion process in these advanced engines, which ultimately will lead to better designs. These efforts have been a crucial part of Sandia's contribution to the DoE's Partnership for a New Generation of Vehicles and its successor, the FreedomCAR collaboration.

Hydrogen, ethanol and other bio-fuels have also been gaining major interest and attention recently as the potential impacts of global warming loom larger. These "carbon-neutral" fuels have their own particular problems—for example, storing hydrogen in sufficient quantities for it to compete with gasoline and diesel fuels. While Sandia is addressing the hydrogen-storage problem in other research groups (see sidebar), the



Supercomputers can simulate how pollutants form during combustion.

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1130 K Street, Suite 280, Sacramento, CA 95814-3965 • Phone: (916) 492-0996 • Fax (916) 492-0999 • E-mail: ccst@ccst.us • Web: www.ccst.us

CCST's Focal Point highlights innovative science and technology research at the Federal Laboratory Affiliate Labs that benefit California's economy and the well-being of its citizens. Focal Point is written by Michael Riordan.

Aerial view of Sandia National Laboratories buildings in Livermore, California, with the Combustion Research Facility at lower right.

issues of combustion efficiency and limiting pollutants from the burning of bio-fuels and hydrogen are ideal subjects for CRF research. In particular, hydrogen-fueled engines promise to attain high energy-conversion efficiencies while emitting extremely low levels of nitrogen oxides. And the scientific understanding of engines that can burn ethanol, bio-diesel and flexible fuels is still in its infancy. They will inevitably have their own issues of combustion efficiency and exhaust emissions to be dealt with.

Something like 90 percent of our nation's energy supply comes from burning fuels—a number that is unlikely to fall much over the next few decades. And with its heavy reliance on automobile and truck transportation, involving about a billion vehicle-miles and using over 50 million gallons of fuel per day, California is much the same. The scientific understanding of combustion and its impact on air quality will thus continue to play an important role in efforts to cope with energy shortages and global warming. Sandia's Combustion Research Facility will remain a focus of these activities, a center where people from government, industry and academe can combine their expertise and work together on innovative solutions.

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Toward a Hydrogen Economy

Sandia has assumed a leadership role in the DoE's R&D efforts to move the United States toward a new energy economy based on hydrogen. This work spans a broad range of activities that include hydrogen production, storage, distribution and combustion, as well as fuel-cell power systems. In particular, storing sufficiently large quantities of hydrogen safely and economically in vehicles is a major hurdle to be surmounted before it can become a widespread, commercially successful fuel.

Sandia was recently named as a DoE Center of Excellence for research and development activities on storing hydrogen in complex metal hydrides. These alloys act like sponges, reversibly accepting hydrogen into spaces between their individual atoms and then releasing it as required. Certain metallic hydrides are considered to be especially promising materials for use in onboard storage applications. The ultimate goal of this five-year R&D project is to store enough hydrogen in vehicles to enable them to travel 300 miles without refueling. Sandia's California partners in these pioneering efforts include the California Institute of Technology, Jet Propulsion Laboratory, Intematix Corporation, and Stanford University.