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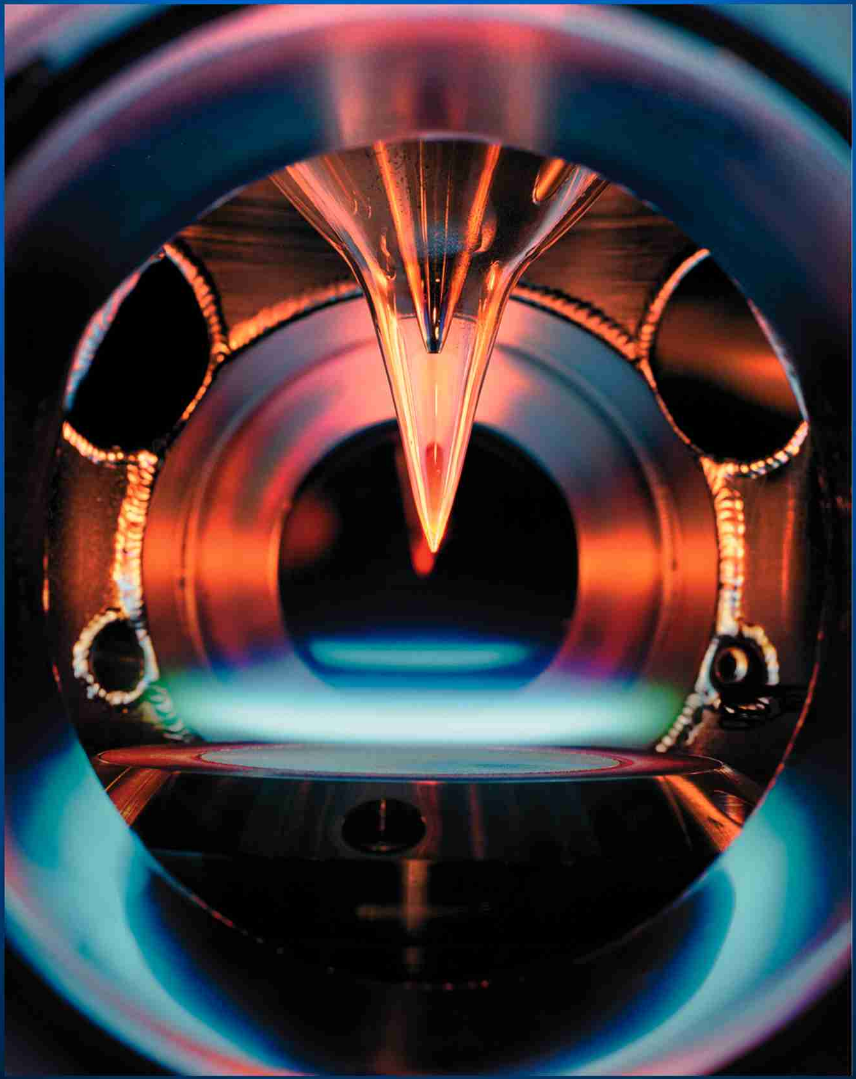
AN AGE-OLD PHENOMENON; A COMPLEX CHALLENGE
Sandia's Combustion Research Facility



ALSO:

Sandia Red Team Hacks All Computer Defenses

New Power Company Software Helps Keep Nation's Power On

Sandia National Laboratories

A Department of Energy National Laboratory

Elaine Raybourn, a member of Sandia National Laboratories' Advanced Concepts Group, pursues her interest in the virtual world by exploring new communication methods, including online collaborative virtual environments. The Advanced Concepts Group is made up of a dozen innovative Sandia researchers who analyze possible future needs of the nation and determine how Sandia can help meet them.

ON THE COVER:
For the cover: The combustion chemistry of a blue methane flame is studied using a molecular-beam mass spectrometer. The toothlike quartz probe provides input to the spectrometer.
(Photo by Randy Montoya)

Sandia Technology is a quarterly journal published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has broad-based research and development responsibilities for nuclear weapons, arms control, energy, the environment, economic competitiveness, and other areas of importance to the needs of the nation. The Laboratories' principal mission is to support national defense policies, by ensuring that the nuclear weapon stockpile meets the highest standards of safety, reliability, security, use control, and military performance. For more information on Sandia, see our Web site at *http://www.sandia.gov.*

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FROM THE *Editor*

Dear Readers:

Combustion accounts for about 90 percent of the world's energy usage. Besides power generation and transportation, it's also an important element in many critical technologies—glassmaking, steel production, wood and paper products manufacturing, to name a few. On the negative side, combustion is the major source of air pollutants and a major contributor to greenhouse gases, which are linked to global climate change. So it's no surprise that government, industry, and academia are interested in achieving a better understanding of how combustion works at its most fundamental level.

Sandia's Combustion Research Facility (CRF) plays a major role in creating a better understanding of combustion processes and the combustion environment. For more than 20 years, CRF researchers have been probing the complex chemical reactions and turbulent flows that occur during combustion with the help of a suite of state-of-the-art laser diagnostic equipment that can't be found all in one place anywhere else.

Their work is highly collaborative. CRF researchers work closely with representatives of industry and academia in labs that were constructed for collaborative research. Their "product" is greater knowledge, which quite often is turned into new technologies that industry can use.

As industries continue to seek cleaner, more energy-efficient, and fuel-flexible transportation, power generation, and manufacturing processes, and as the world seeks to reduce production of greenhouse gases, the CRF will increasingly become a valued resource for understanding the mysteries of combustion.

Julie Clausen
Guest Editor

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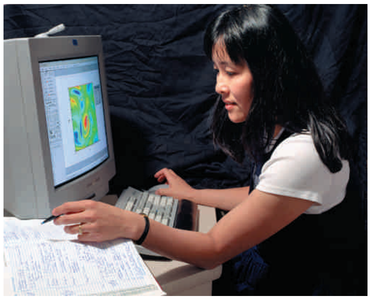


INSIGHTS

by *Vincent Henry, President, Henry Technology Solutions LLC and senior industrial advisor to the Department of Energy, Office of Industrial Technologies' glass program*

An Age-Old Phenomenon; A Complex Challenge

Plate glass. Steel. Diesel engines. Greenhouse gases.

Combustion processes play a significant role in all of these items. As complex as it is versatile, combustion has been used, pondered, and studied for eons. Its fundamental processes are still the subject of investigation today as scientists with increasingly sophisticated tools seek to unravel its complexities.

Researchers at Sandia National Laboratories' Combustion Research Facility (CRF) are attempting to understand, tame, and exploit combustion. From studying the behavior and chemistry of a simple flame to pinpointing when and where soot forms in a diesel engine, CRF scientists and engineers are probing the mysteries of age-old phenomena using modern tools and diagnostic methods. Their work is leading to knowledge and tools for improving the energy efficiency of combustion devices and industrial processes, and reducing the environmental impact of burning fossil and renewable fuels.

"For both of these goals, details at the molecular level are critically important," said Frank Tully, CRF deputy director for chemical sciences.

Basic Research is the Foundation

The CRF's basic research is the key to its success. Supported by the Department of Energy's Office of Basic Energy Sciences, this program includes work in fluid mechanics, chemical kinetics, chemical dynamics, and optical diagnostics. The work helps scientists understand, characterize, and fully model and simulate the combustion process and environment.

The Combustion Research Facility in Livermore, California

"Without the ground research that's been supported by the Office of Basic Energy Sciences, the CRF's applied research would not have been nearly as productive as it has been," said Bill Kirchhoff, DOE program manager for the Basic Energy Sciences Chemical Physics Program.

The CRF's work has helped many diverse industries that rely on combustion: steel, glass, oil refineries, and of course, power generation and engine and automobile manufacturers. Its strength is in using unique tools to achieve a fundamental understanding of critical processes such that improvements can be scientifically based.

"This is really a national treasure for anyone involved in combustion processes," said Fred Quan, manager of technology acquisition with Corning's Science & Technology Group. "The equipment and expertise located at Sandia is world-class with the capability to look at and analyze phenomena lesser facilities would miss."

> "The equipment and expertise located at Sandia is world-class with the capability to look at and analyze phenomena lesser facilities would miss."

Corning is collaborating with the CRF on a technology called laser-induced breakdown spectroscopy (LIBS). The company is interested in using the technology to increase its understanding of the combustion processes used in glass manufacturing. Among its many products, Corning provides high-performance glass for active matrix liquid crystal displays; cathode ray tubes for computers and television screens; and optical fiber, cable, and photonic products for the telecommunications industry and other technology applications.

"This often studied field still has its share of tradition, empirical black art, and trade secrets," Quan said. "A more basic understanding can increase manufacturing efficiencies and reduce waste byproducts so that less energy is used per unit made."

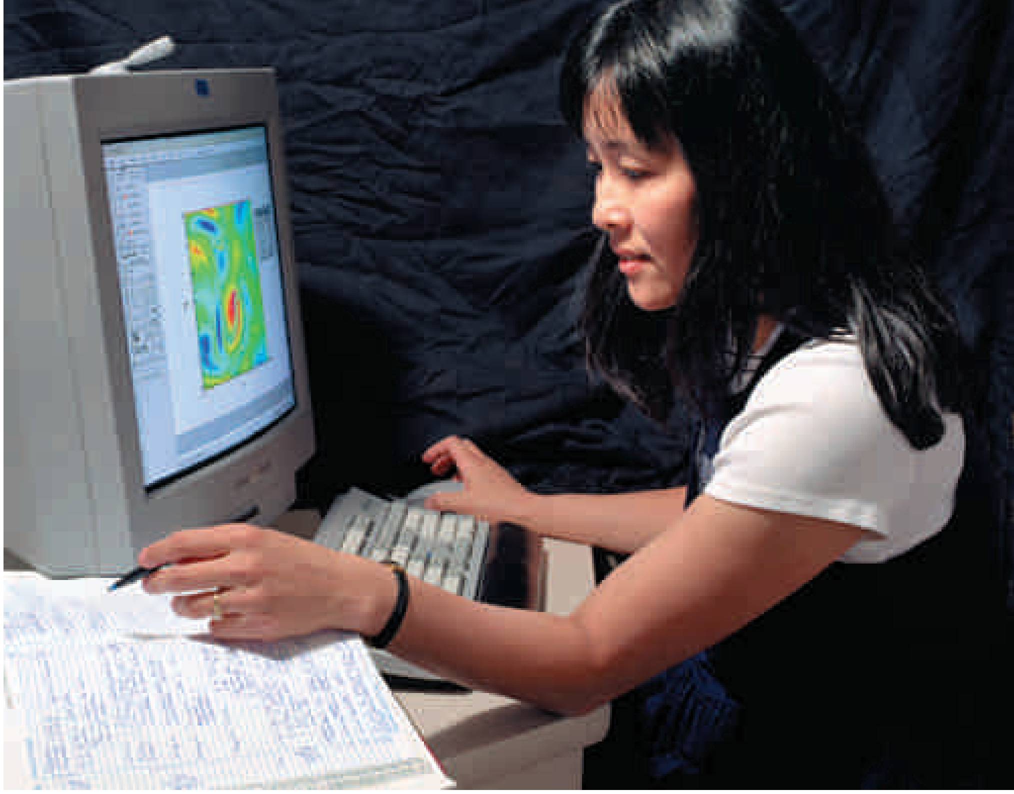
Developing and Using the Best Tools

Housed in recently expanded facilities at Sandia's Livermore, Calif., site, the CRF is a "one-stop shop" for those needing help in tackling complex combustion problems. As a DOE "user facility," industry and academia representatives collaborate with some 75 CRF researchers on problems of mutual interest for weeks to months to years through its User Program. Visitors have access to the CRF's cutting-edge laser diagnostics equipment, combustion experts, and 37 specialized laboratories. CRF staff members benefit from their exposure to new developments and unique knowledge from the visitors' home institutions.

The CRF's multiple, state-of-the-art, combustion science and technology equipment and facilities have provided for significant contributions over the past two decades to the advancement of combustion science and technology. The high-tech resources allow researchers to nonintrusively study and measure fleeting combustion events in a variety of environments. In internal combustion engines, industrial burners, furnaces for making steel or glass, and other hostile or inaccessible environments, lasers are needed to interrogate and measure the processes occurring inside.

Cummins Engine Company has used the CRF's laser expertise in multiple collaborations over the past 20 years.

"The most significant element of that cooperation has been the laser diagnostics of the combustion process inside an operating diesel engine," said Patrick Flynn, Cummins vice president of research. "This analysis allowed us to determine the process sequence for combustion and made us completely reevaluate how we diagnose and analyze that process."



CRF researchers use computational modeling and simulation to understand and predict complex combustion events.

The CRF has been a leader in the combustion community in the development of new optical diagnostic methods and computational tools for understanding fundamental combustion processes.

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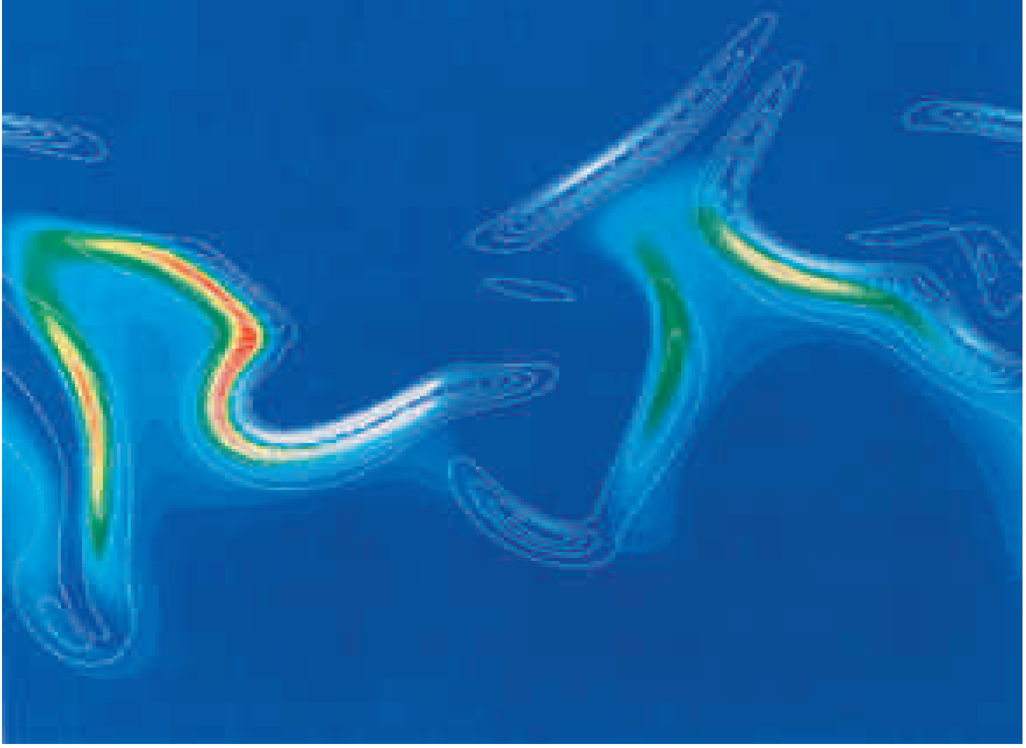
A new CRF laboratory equipped with subnanosecond lasers and fast detectors allows scientists to measure fundamental chemical processes such as collisional energy transfer and photoionization (ionization resulting from collision of a molecule or atom with a photon). Both of these are high-speed processes that occur on an atomic or molecular level. These laser sources are not commercially available. The facility's picosecond laser system is capable of providing pulses in the 100 picosecond range (a picosecond is one trillionth of a second) at the higest possible spectral resolution. Outside researchers collaborating with CRF staff members are able to use this capability.

CRF researchers also have developed a powerful, new experimental technique that allows them to study combustion events that typically occur in femtoseconds (one millionth of a billionth of a second). A pulse of laser light, a few femtoseconds in duration, is fired at the molecules, causing them to dissociate. In strobe-light fashion, subsequent pulses "freeze" and probe the reaction, providing a detailed, time-lapse picture of molecules splitting apart, rearranging, and combining with others. This information is particularly useful to scientists who model combustion reactions.

Researchers also use computational modeling and simulation to understand



This image—generated using a technique called direct numerical simulation—provides researchers with detailed information on reaction rates and regions of intense burning in a turbulent, nonpremixed flame.

and predict combustion events. Even simple combustion models typically involve a dozen or more chemical species as well as multiple, concurrent chemical reactions coupled with complex fluid transport processes. Working closely with experimentalists, theorists at the CRF are assessing how the combination of flow and chemistry in burning fuels affects the performance of combustion devices. The goal is to reliably predict factors that can guide design, operation, fuel design, and fuel selection.

The Future

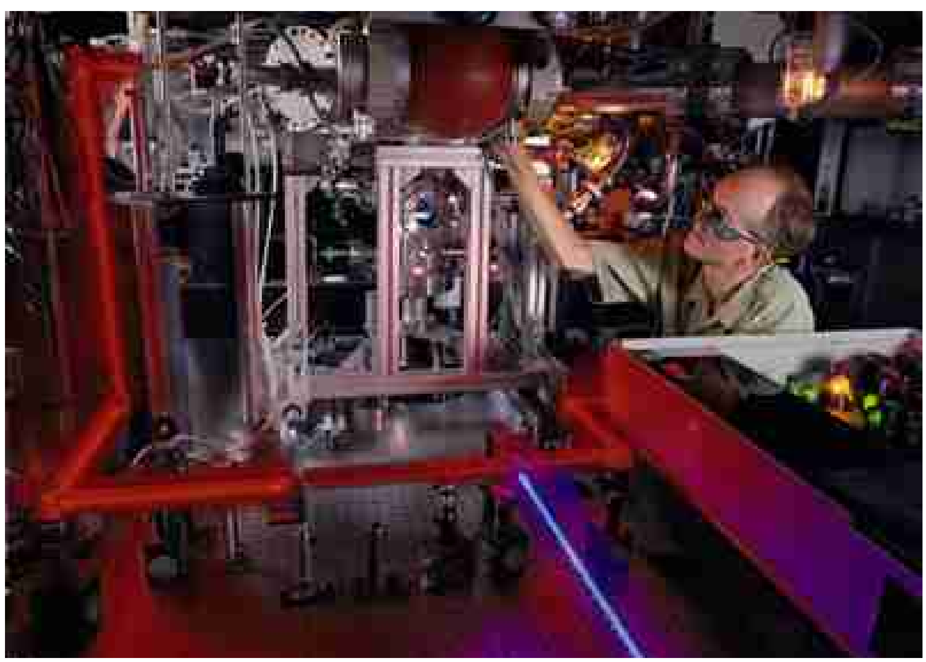
Continued investment in the CRF and its people will produce results that extend beyond the realm of combustion research and applications, said Mim John, California Laboratory Vice President. "We can expect to see research results that impact on a much broader array of important national security issues," she said.

In recent years, technologies originating in the CRF have found their way into other highly visible projects at Sandia. For example, the CRF's strength in laser-based diagnostics led to an ongoing effort in remote sensing, especially as it applies to the study of global climate change. Sandia researchers also drew on the CRF's laser diagnostics capabilities and chemical sciences capabilities to develop a device that can quickly detect and analyze minute concentrations of chemicals. Researchers believe the device could be used in a wide variety of applications including monitoring food and water quality and detecting chemical or biological hazards.

"We can expect to see research results that impact on a much broader array of important national security issues."

But combustion research will remain the CRF's focus. Combustion accounts for about 90 percent of the world's energy usage and it is a key element in our critical technologies. Although fossil fuels are relatively abundant and accessible, there will be a continued push to squeeze more energy and efficiency from them. More stringent emissions regulations also will dictate a need for more environmentally safe combustion systems.

"The challenge of the future is ultra clean, highly efficient, fuel-flexible combustion systems," said Bill McLean, CRF Director. "Using the capabilities that are in place here at the Combustion Research Facility—experimental capabilities, simulation capabilities—we will meet those challenges in concert with our partners from industry and academia."



This instrument is used to study the details of flame chemistry in model combustion systems.

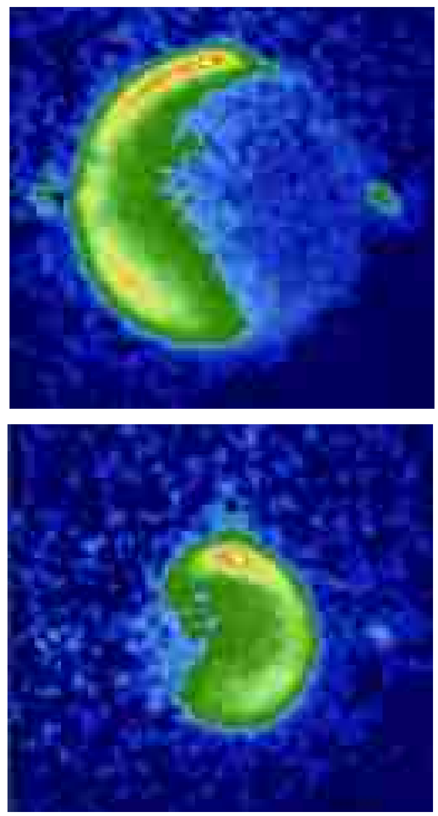
Witnessing A World of Violent Collisions

Researchers Build Knowledge Base Necessary for Applied Research

We think of lighting a candle as a soothing, often romantic act. But on a molecular level, this seemingly simple act unleashes unseen, violent collisions that tear molecules apart and send fragments spinning into space where they may collide and recombine with other molecules.

Understanding this invisible, frenetic world is the goal of physical chemist David Chandler. By exploiting the capability of lasers to selectively excite and break apart targeted molecules, he has created "snapshots" of molecules colliding and splitting during chemical reactions. The snapshots provide detailed information about bond strengths and velocities of the reaction products.

Chandler and other scientists at the Combustion Research Facility (CRF) study fundamental chemical reactions. This basic research is a core component of the CRF's work and forms the foundation for its applied research. By examining how molecules undergo chemical change, the researchers gain a better understanding of chemical processes that control combustion: mechanisms involved in individual chemical transformations, the rates at which reactions proceed, and the products they produce. This leads to better knowledge of how flames



Ion images taken after a collision of hydrogen chloride and argon molecules reveal how fast and in which direction the molecular fragments traveled.

The fundamental nature of this research makes it applicable to other fields as well. Chandler's ion imaging technique is not combustion-specific.

burn, why engines knock, and how to minimize pollution.

"The CRF's work in chemistry, optical diagnostics, and chemically reacting flows is very important in providing the information required to generate predictive models of combustion, and it provides the basis for much of the other applied work that's done here," said Frank Tully, CRF deputy director for chemical sciences.

The fundamental nature of this research makes it applicable to other fields as well. Chandler's ion imaging technique is not combustion-specific.

"It's a generic way of measuring the velocity of ionized particles," Chandler said. "It allows you to look at things you could never look at before."

Since the first paper was published in 1987, the technique and apparatus have been replicated in more than 40 laboratories worldwide. Many of the people who have built the systems have been post docs or visiting researchers at the CRF. "Cross-fertilization" occurs when they independently make improvements to the original technology, and Chandler incorporates them into Sandia's system, which is housed in the CRF's Chemical Dynamics Laboratory.

The ion imaging system works by ionizing the products of either a unimolecular photodissociation (using a photon to fragment a molecule) or a bimolecular collision and recording their velocity images. When studying unimolecular photodissociation, a laser is fired into a

A laser beam can penetrate a flame and detect, at a molecular level, the various chemical species present without disrupting the combustion process.

gas, breaking apart the molecules. The fragments are ionized with another laser of a different wavelength. The ions are captured on a detector, and a camera records the impacts from multiple angles at once. From the digital picture, researchers can extract information about the three-dimensional distribution of ion velocities. The data are so detailed that one can discern whether a molecule is spinning clockwise or counterclockwise.

In the past, such information was a lot harder to come by. Scientists were not able to simultaneously record multiple, angular impacts. Instead, they had to record impacts from one angle at a time.

"What we did was 'multiplex' previous measurements so we can measure all angles at once," Chandler said. "Now, in a month we can take measurements that would have taken a graduate student a lifetime."

CRF colleague Carl Hayden has developed a variation of the technique that allows researchers to study the dissociation of molecules a single molecule at a time. Such events typically occur in femtoseconds (one femtosecond is one millionth of a billionth of a second). A laser pulse lasting a few femtoseconds breaks the molecules apart. A second femtosecond laser pulse ionizes a molecular fragment. Using simultaneous measurements of the fragment and its electron, details of the dissociation process can be extracted. The new experimental technique and facility promises to be a powerful tool for the validation of predictive models and theories of chemical reactions.

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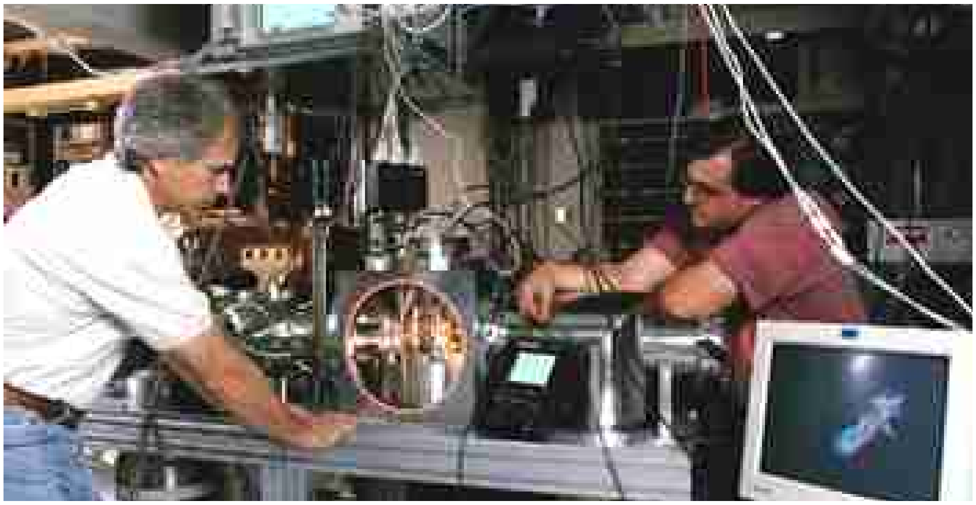
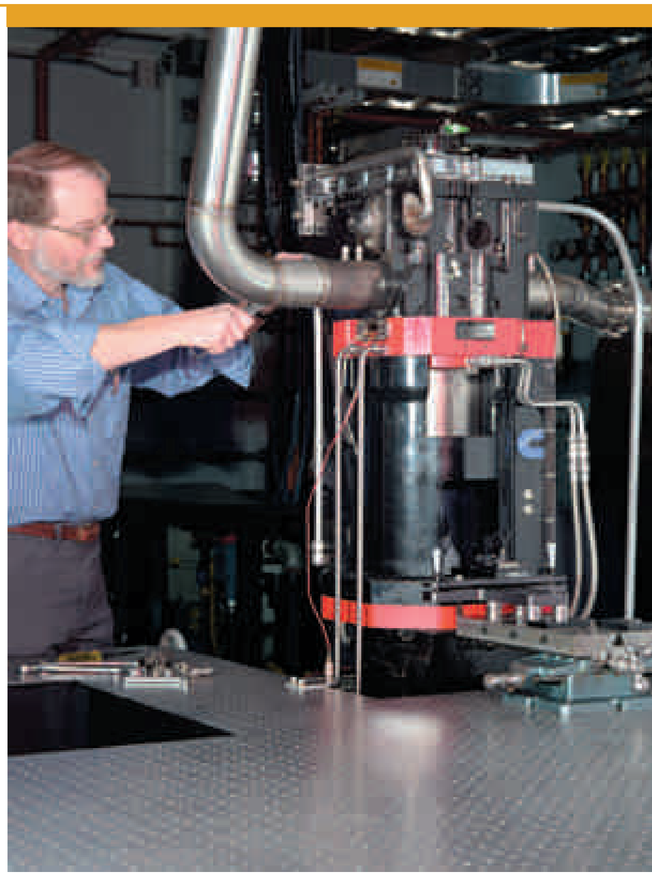


Researchers assemble a new photoelectron/imaging apparatus for use in femtosecond laser studies of fundamental chemical processes in isolated molecules.

'Supercar' Work Focuses on Reducing Emissions

Building a car that gets 80 miles per gallon without sacrificing affordability, performance, or safety is the challenge for the Partnership for a New Generation Vehicle (PNGV), a consortium of domestic automakers, federal agencies, and laboratories. The "Supercar" also must be environmentally friendly, complying with increasingly stringent emissions standards.

Combustion Research Facility (CRF) researchers are working on several emissions-related PNGV projects. The CRF's engine research focuses on building a better understanding of the science behind the emissions process so that engine manufacturers and auto companies can design efficient, low emissions engines. With support from the Department of Energy's Office of Transportation Technologies, CRF researchers are studying emissions formation in direct-injection diesel and gasoline engines and evaluating the quality of exhaust gas recirculation in a multicylinder, direct-injection diesel engine.



CRF researchers use an optically accessible diesel engine to investigate combustion and emissions formation.

A Cleaner Diesel

The CRF's largest PNGV project involves a high-efficiency engine that is the leading candidate for PNGV's Supercar. The small-bore, high-speed, direct-injection (HSDI) diesel engine is a champ at converting the chemical energy in fuel into mechanical energy that propels the vehicle. But, like other diesels, its Achilles' heel is exhaust emissions.

"Our job is to provide the science base necessary to develop a cleaner engine," said principal investigator Paul Miles. "Our 'product' is greater knowledge."

CRF researchers are seeking to better understand the unique characteristics of combustion in HSDI engines, one of which is the strong swirling motion of fuel and air in the piston bowl. "Swirl," as well as interactions of the piston bowl wall with the fuel spray, have a large influence on in-cylinder processes. Even small changes in the piston bowl shape can have a profound impact on emissions. CRF research is directed at understanding the intricacies of fuel and air mixing, how the fuel burns, and the processes that produce emissions.

To conduct cutting-edge research on HSDI engines, Miles sought a four-valve engine. At the start of the project in 1997, production four-valve, direct-injection engines were unavailable. Two-valve production engines with indirect fuel injection were the standard. But previous research had shown that direct injection and placement of the fuel injector in a central, vertical position allowed greater symmetry of the combustion chamber and a simultaneous reduction of emissions and increase in power. So Miles had a one-cylinder HSDI research engine with a four-valve head custom-built for the CRF.

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NEWS *Notes*

Sandian Marlene Brown looks over a photovoltaic unit identical to those she is troubleshooting on the Navajo reservation.

Sandia Engineers Help Bring Solar Electricity to Remote Navajo Homes

Some Navajo families living in remote areas of their reservation in the Southwest are getting electricity in their homes for the first time, thanks to the Navajo Tribal Utility Authority (NTUA) and Sandia engineers.

As part of a solar power initiative that is the largest of its type in the country, the NTUA is buying 200 photovoltaic systems and installing them at private residences. The systems collect energy from the sun and convert it to electricity for use in the homes. Sandia engineers ensure the units are properly installed and working as intended.

Jimmie Daniels, NTUA solar program manager, said the utility decided to offer the alternative power source to its customers because of the high cost of stringing wire over parts of the reservation's rural terrain. Between 10,000 and 30,000 Navajos are estimated to live without electricity on the Navajo Reservation, which covers approximately 16 million acres in the Four Corners area where Utah, Arizona, Colorado, and New Mexico meet.

"The only way for many of these people to have electricity is to provide each household its own photovoltaic unit," Daniels said.

The program follows a solar electric home experiment conducted by Sandia and the NTUA in the early 1990s. DOE provided $300,000 and other support that resulted in the installation of 72 individual systems. Sandia provided technical assistance in the earlier project.

Based on results of that effort, the new photovoltaic systems are somewhat bigger. "They will be able to convert about 3 kilowatt-hours per day on average in the winter," said Roger Hill, who coordinates Sandia's work with Native Americans. "That's enough electricity to power a single household for a day—if the family members are conservative in their use of electricity."

Sandia's photovoltaics laboratory houses one of the units where engineers test it for potential problems. Sandia also conducted a two-day course for NTUA technicians, showing them proper installation and maintenance techniques.

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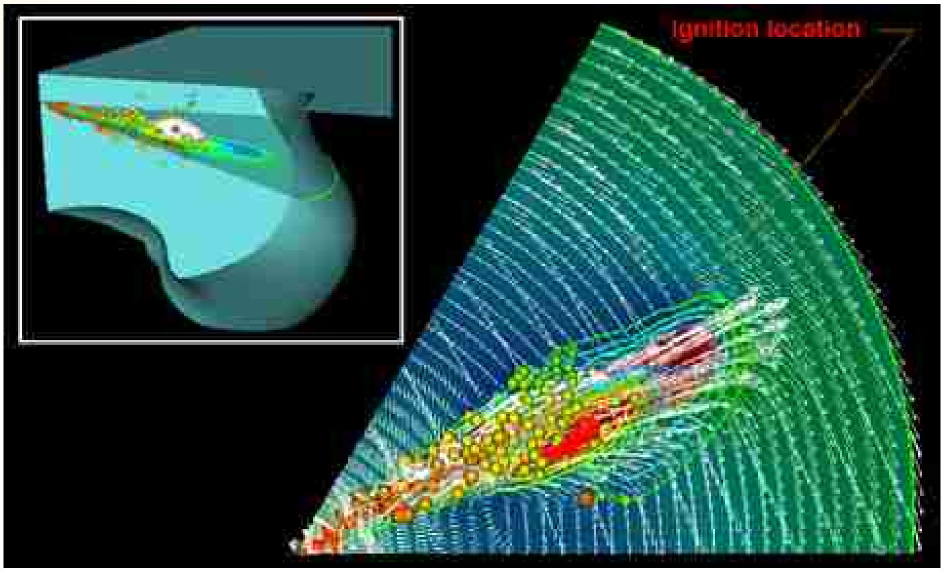

Computer simulations developed at the University of Wisconsin Engine Research Center provide a detailed picture of ignition in a high-speed, direct-injection engine. The simulations are compared with measurements taken in test engines.

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The engine has optical access through a quartz piston top as well as through access windows in the cylinder walls and in the head. An identical metal engine is located at Wayne State University in Detroit, Mich.—a collaborator on the project—where conventional emissions and performance testing is taking place. A second research partner, the University of Wisconsin Engine Research Center in Madison, Wis., is performing multi-dimensional computer simulations of the combustion process.

Comparisons of the computer models with data from the optical and metal engines give researchers the capability of refining and validating the models. The models, once perfected, could be used in engine design and development.

CRF researchers are applying some of the same methodology they used in studying what happens in the combustion chamber of a large-bore diesel engine during ignition. This work led to a fundamentally different understanding of how the diesel combustion process progresses, which engine manufacturers use in designing new engines to minimize emissions while maintaining efficiency.

"The CRF's engine research focuses on building a better understanding of the science behind the emissions process so that engine manufacturers and auto companies can design efficient, low-emissions engines."

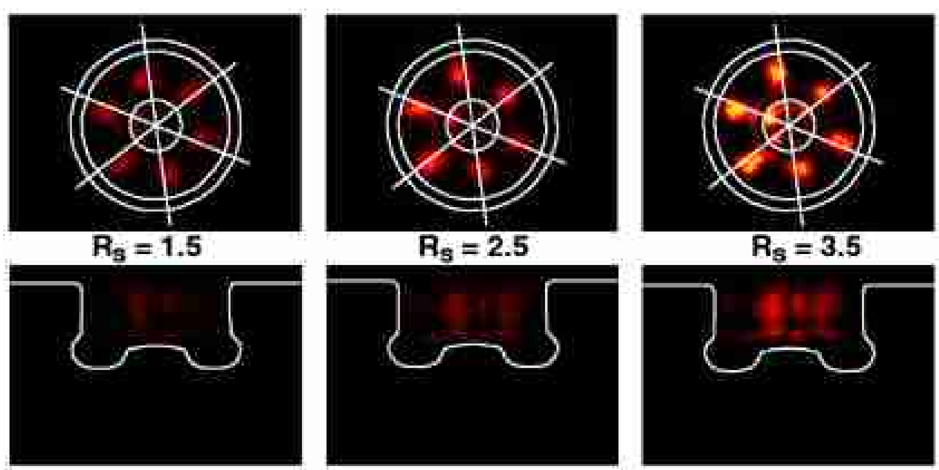
"We hope to accomplish this and more with small-bore diesels so researchers can more intelligently design injectors, combustion chamber shapes, and fuel-injection strategies that will minimize both soot and NO_X, two major emissions challenges," said Bob Carling, deputy director for combustion and industrial technologies.

Reducing tailpipe emissions

To further minimize engine emissions, PNGV is attacking the emissions problem using a tried and true technology called exhaust-gas recirculation (EGR). EGR has been used in gasoline engines for 35 years and recently became available in diesel passenger car engines.

PNGV engine designs are incorporating EGR in large amounts to reduce the in-cylinder production of nitrogen oxides (NO_X), a major contributor to the formation of ozone-containing smog. By "recycling" some of an engine's exhaust, combustion temperatures are lowered and less NO_X is produced. However, large fluctuations of EGR can potentially lead to poor cylinder-to-cylinder distribution of recirculated exhaust, which in turn can result in both poor combustion performance and increased emissions.

Using a Volkswagen diesel engine, CRF researchers have developed a diagnostic that evaluates EGR distribution by measuring the concentration of exhaust gas in the intake flow



With the CRF's optically accessible high-speed, direct-injection diesel engine, researchers can take photographs of diesel spray ignition from two different angles.

entering the cylinders with a specialized laser optical technique. These measurements are conducted during transients in the operation of the engine (such as acceleration or deceleration), conditions that exacerbate the problems of EGR distribution.

The Volkswagen engine is equipped with a specially designed optical spacer between the head and the intake manifold that allows measurements and determination of the average concentration of EGR in the flow of fresh charge entering the intake port of each cylinder. Using the data obtained during the sequence of engine cycles that define a transient in the engine operation, principal investigator Bob Green can determine when poor EGR/air mixing occurs. The measurements can also be used to validate the accuracy of computer models that are an important tool in the engine development process.

An alternative to diesel

CRF researchers are also investigating the important fuel-air mixing process in a direct-injection, spark-ignited (DISI) gasoline engine. The project is part of a collaboration with DaimlerChrysler, Ford, and General Motors. Although PNGV is leaning heavily toward a diesel engine for the Supercar, DISI engines also have the potential for increased fuel efficiency and high performance compared with conventional gasoline engines.

"We thought it made sense to look at the possibility of another engine concept (other than diesel) for a number of reasons including public perception of diesel-powered vehicles, availability of diesel fuel, and relatively higher emissions from state-of-the-art diesel engines," said principal investigator Richard Steeper.

The research team started with a GM prototype DISI head and mated it to a transparent, fused-silica cylinder with a windowed piston, resulting in a geometrically correct engine with multidirectional optical access. Using an ultraviolet laser sheet to induce fluorescence in liquid- and vapor-phase gasoline, researchers are able to image the fuel-air mixing process in the cylinder. By comparing data on the fuel-air mixture quality with performance data from a twin research

Researchers can see inside the CRF's direct-injection, spark-ignited gasoline engine through the transparent quartz cylinder in the center of the photograph. A mirror provides a view of the valves, injector, and top of the combustion chamber.

Although PNGV is leaning heavily toward a diesel engine for the Supercar, DISI engines have the potential for increased fuel efficiency and high performance.

looking for insights into DISI engine design and control.

In a related project, researchers are investigating the physics of the combustion process in a DISI engine with an injector mounted between the intake valves targeting a piston with a bowl. This engine allows studies of the fuel spray and air mixture with the piston bowl, which can be seen through the engine's quartz viewing windows and transparent piston top. Researchers hope to determine the effect of these interactions on hydrocarbon emissions.

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NEWS
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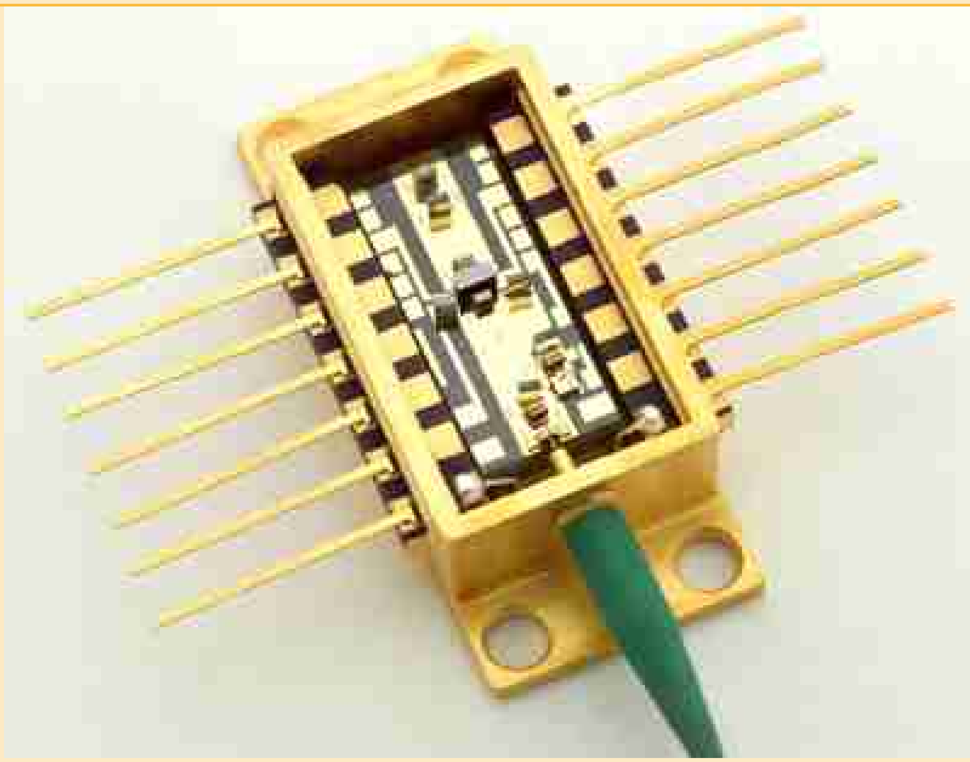

Alignment structures, less than a 10th of an inch in size in this optical module, make use of Sandia National Laboratories' expertise in the LIGA microfabrication process. This photonic subsystem, by Sandia's licensing partner Axsun Technologies of Billerica, Mass., sits on an electronic assembly that occupies about 60 percent of the area of a business card (2.5 inches long x 1.7 inches wide).

Microfabrication Technology Licensed to Massachusetts Firm

Sandia has licensed proprietary technology used to fabricate precision microcomponents to AXSUN Technologies, a telecommunications firm based in the Boston area. Called LIGA, the technology is an increasingly popular alternative to using semiconductor techniques for making microscopic parts because it allows the use of a variety of materials.

AXSUN's Agile Photonic Subsystems™ use micromechanical alignment structures that are fabricated using the LIGA process. The company plans to establish a LIGA foundry in the San Francisco Bay Area, providing what is believed to be the first LIGA commercial production in the United States. The foundry will supply components for the company's telecommunications products and for outside customers.

"Expertise in LIGA design and fabrication is not widely available," said James Lewis, AXSUN vice president of sales and marketing. "Sandia was a clear leader in this field, and an exceptional development partner for this key enabling technology."

Sandia's cutting-edge LIGA program grew out of a need to create small parts for defense applications. Until recently, fabricating microscopic parts has largely been based on semiconductor techniques. LIGA essentially is a technique to create a mold on a micron scale and uses this to mass-produce tiny, three-dimensional structures in a variety of materials including metals, polymers, and ceramics. The technology originated in Germany about 20 years ago and derives its name from the German acronym for the three-stage production process.

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Laser Technique Spots Refinery Leaks

A typical U.S. petroleum refinery spends about $1 million a year looking for invisible gas leaks in its vast array of high-pressure processing pipelines. The surveys are required by the Environmental Protection Agency (EPA) because emissions from refinery leaks contribute to greenhouse gases and smog.

Every three months, every valve, seal, and juncture throughout a refinery is scanned for leaks using a handheld "sniffer." The labor-intensive process can take weeks to complete.

Recently, a working group composed of members from the EPA, Department of Energy, and the American Petroleum Institute (API) began looking at ways to streamline the process. The group is evaluating technologies that can detect large leaks rapidly. An API study shows that the largest one percent of leaks produce more than 80 percent of refinery emissions.

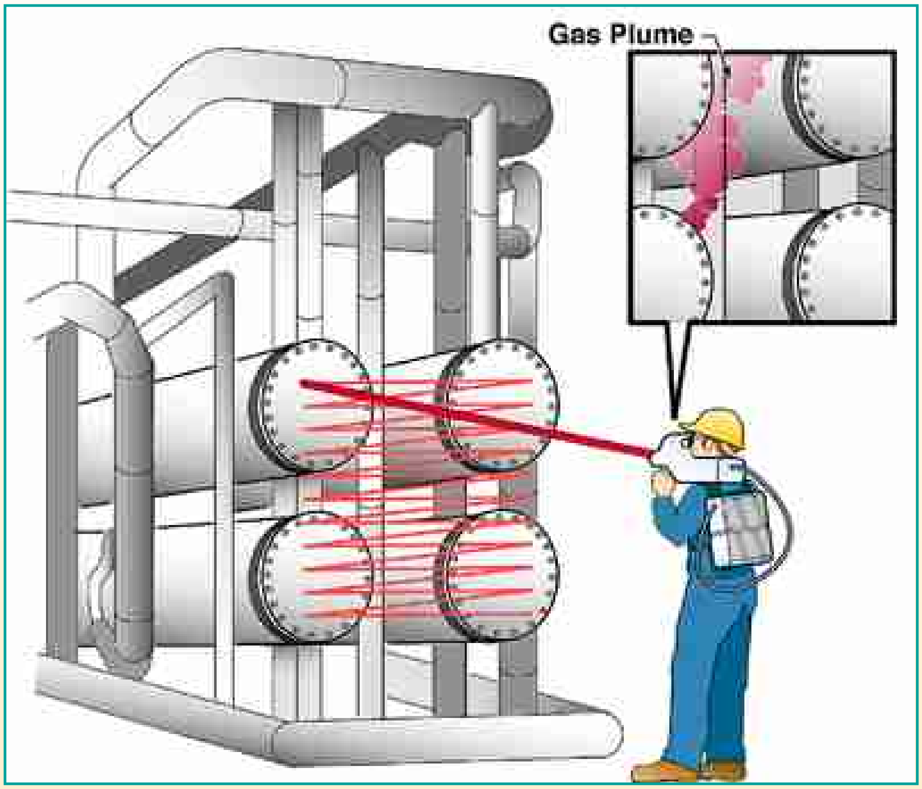
The group is focusing on an imaging technique developed by Combustion Research Facility researchers, which should provide for more efficient leak detection. The optical-imaging technology lets an operator "see" invisible leaking gases, which appear as a dark smoke cloud on a video screen. Imaging leaks is quicker because large areas can be viewed at once, and the technology focuses only on larger leaks.

"Their (the refineries') argument is that if we find the big ones we'll catch most of the emissions problem," said project leader Tom Kulp. The imaging technique would require EPA approval before it could be used as an alternative to the current monitoring process.

The Sandia technology uses a technique called Backscatter Absorption Gas Imaging (BAGI). Working in a manner similar to a television, a scene is illuminated by an infrared laser as it is imaged using an infrared video camera. The laser's wavelength is "tuned" so that its radiation will be absorbed by the hydrocarbons of concern. In April 1999 a test was conducted at a Gulf Coast oil refinery in collaboration with Laser Imaging Systems, Inc., of Punta Gordo, Fla., which has exclusive license of the BAGI technique.

In the test, a prototype, van-mounted gas imaging system demonstrated its ability to detect large hydrocarbon leaks 30 to 50 times faster than the federally mandated "sniffer" method. The data supported the view that most volatile organic compound emissions from a refinery come from a small percentage of valves and seals, and that the gas imaging system can efficiently identify those leaks. The technology also can be used for leak testing of containers and has proven effective for detecting natural gas leaks.

The Department of Energy Offices of Fossil Energy and Industrial Technologies are sponsoring development of the gas-imaging technology. Leaking gases present in the imaged area appear as a dark cloud in a real-time television picture. Researchers are working on a backpack-sized system, which is expected to undergo refinery tests in early 2001.



Sandia's gas imaging system illuminates an area with infrared light. A video-type camera scans and collects the reflected light and converts it to an electronic signal, which is displayed on a video monitor. Leaking gases appear as a dark smoke cloud (inset).

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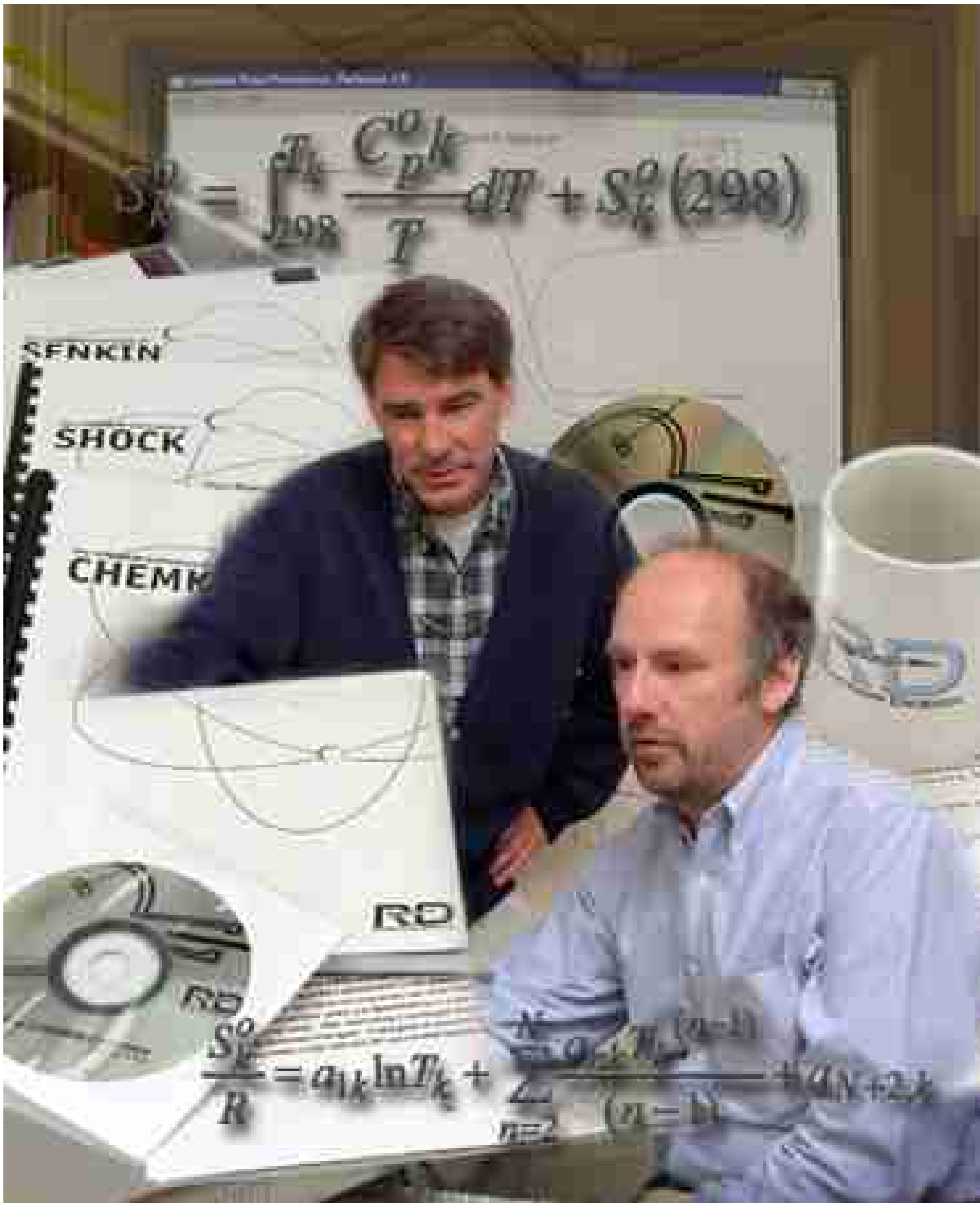
Software is Indispensable Tool for Chemistry Modelers

Whoever said "Necessity is the mother of invention" could have been talking about Sandia's CHEMKIN software.



Researchers use the CHEMKIN software collection to solve complex chemical kinetics problems.

Not only did it fulfill its developers' need for a more efficient way of solving problems involving complex series of chemical kinetics phenomena, but some 20 years later the software is still helping countless combustion modelers. The CHEMKIN collection, a software suite used worldwide in the microelectronics, combustion, and chemical processing industries, is one of Sandia's most successful and enduring products.

CHEMKIN is marketed by San Diego-based Reaction Design under license from Sandia. The company provides technical support and software upgrades to the approximately 200 CHEMKIN customers worldwide at research universities, national laboratories, and Fortune 500 companies. The product helps solve complex chemical kinetics problems and incorporates the information into simulations of reacting flows.

Sandia uses the software in the Combustion Research Facility's modeling work, in chemical vapor deposition studies for semiconductor research, and in fire simulations for nuclear weapons programs.

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The software's origins date to the mid-1970s when two Sandia researchers became frustrated with the time they were spending writing and rewriting computer code for models of chemical kinetics in different combustion situations. They needed a way to handle increasingly complex chemistry and transport in a general way, independent of the particular combustion situation. That would allow them to more efficiently develop new models.

CHEMKIN has greatly facilitated modeling of complex chemical processes such as combustion. It has become the standard for anyone conducting chemistry modeling and chemically reacting flow modeling. It also has become an important educational tool in chemical engineering, mechanical engineering, and chemistry curricula.

The researchers developed the first CHEMKIN prototypes by the late 1970s. The software got broad exposure among combustion researchers when the CRF opened in 1981.

Over time, researchers expanded the software's capabilities in molecular transport, chemistry at deposition surfaces, and plasma processes. Sandia licensed CHEMKIN to Reaction Design in February 1997. Founded in 1995, Reaction Design develops and markets software for simulation of chemical processes, including combustion and the manufacture of chemicals and materials.

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NEWS *Notes*

Summer Heat Spells Lights Out, But New Power Company Software Helps Keep Nation's Power On

Major power emergencies like the statewide conservation alerts in California this past summer might be averted if power companies adopt new command and control software, according to a recent Department of Energy (DOE) study headed by Sandia National Laboratories. Unlike software that power companies currently use, the new software predicts future energy demand rather than simply responding to it.

After last year's series of major regional power outages, DOE officials warned of the possibility of summertime power failures to large areas of the nation as power companies struggle to meet peak daytime electricity demands.

Traditionally, power companies use state-of-health software tools to monitor how power is flowing from place to place, watch for the telltale signs of imminent outages, and determine whether additional power should be purchased from other companies to bolster reserves.

The DOE report concludes that these "deterministic" grid-monitoring tools are becoming outdated and that new, more sophisticated software tools based on probabilistic risk assessment are needed. Such command-and--control software would include various mathematical models, including those that simulate load flow, dispatch options, weather factors, and contingencies, according to the report. They would, in a sense, help power plant operators predict the future—or at least quantify the likelihood of something happening and test the effects of responses hours or days in advance.

"The software tools power companies use to monitor and control the electric grid were not designed for the level of complexity and the number of transactions the system is experiencing today," said Sandia's Abbas Akhil, a member of a DOE-wide team looking at electric grid reliability issues. "They are not adequate for predicting and averting major outages of the future."

The report also suggests further study of a distributed power grid. Such a grid would consist of hundreds of traditional and nontraditional generation sources and storage devices, including wind turbines, solar collectors, and other generators.This would enable less reliance on large-scale power plants and give the grid a broader, more stable foundation.

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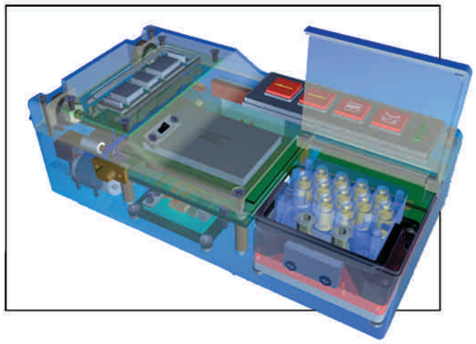
Not Just For Combustion Anymore

Chemical analysis is a complex challenge requiring specialized facilities, expensive equipment, and highly trained individuals. It's even more challenging to analyze chemicals quickly in the field without bulky lab equipment.

Sandia researchers have developed a handheld chemical-analysis system that can quickly detect and analyze minute concentrations of chemicals. The system, called µChemLab,™ uses miniaturized components to perform chromatographic separations. It draws on expertise in chemical sciences and laser diagnostics originally developed at the Combustion Research Facility (CRF). Researchers believe the device could be used in a wide variety of applications including monitoring food and water quality and detecting chemical or biological hazards.

"The portable chemistry lab is a good example of how technologies have broken out of the CRF and have really contributed to national security problems in addition to energy research," said Dave Rakestraw, a former CRF staff member who has recently left Sandia for a start-up company he helped form to commercialize some of the technologies.

While combustion is the primary focus at the CRF, the technologies, capabilities, and core competencies housed there are applicable to a wide range of national problems. Other CRF technologies include major programs in remote sensing and hydrogen energy, and a program for the destruction of a variety of hazardous materials.



A low-cost, hand-held chemical analysis system will provide rapid, accurate chemical analysis to meet both national security and commercial needs.

[While combustion is the primary focus, the technologies, capabilities, and core competencies housed at the CRF are applicable to a wide range of national problems.]

Having a balanced portfolio between basic and applied research also helps create an environment that's conducive to spinoff technologies, said CRF Director Bill McLean. "The breadth of our programs, and the multi-disciplinary expertise of our staff produce capabilities and results previously unavailable," he said.

For example, the CRF's expertise in fundamental spectroscopy and optical diagnostic methods makes it possible to carry out laser measurements of critical gaseous species in the hostile environment of a steel mill. In addition, the highly sophisticated quantitative imaging of trace species inside a practical diesel engine is made possible by the CRF's ability to analyze and understand the chemical physics of molecular fluorescence and collisional relaxation processes.

The remote sensing program is part of the Department of Energy's Atmospheric Radiation Measurement Program. Researchers use remotely piloted aircraft to measure water vapor in the atmosphere. The aircraft's payload contains a special laser-based detection system that probes the sky's ice and water content, both in clouds and in clear skies. The information helps scientists create more accurate computer models of global climate change.

In hydrogen energy, CRF and other Sandia capabilities are being used to conduct research concerning ultra-clean, high-efficiency energy systems involving combustion devices, fuel cells, fuel reformers, and hydrogen storage systems.

In the supercritical water oxidation (SCWO) program, CRF scientists are conducting experiments and theoretical modeling that improve our understanding of detailed chemical kinetics of SCWO processes. SCWO is a promising method for destroying hazardous materials ranging from unusual chemical munitions to municipal and industrial sludges.

NEWS *Notes*

Sandia-Developed Laser Promises to Reduce Cost of Fiber Optics Connections

Sandia researcher John Klem stands next to the molecular beam epitaxy system used to grow the crystal structure of the 1.3-micron communications vertical cavity surface emitting laser (VCSEL).

Sandia researchers have developed the first 1.3-micron electrically pumped vertical cavity surface emitting laser (VCSEL) grown on gallium arsenide, a breakthrough that promises to reduce the cost of high-speed fiber optics connections.

Sandia developed the gallium arsenide-based VCSEL, through a cooperative research and development agreement (CRADA) with Cielo Communications, Inc., of Broomfield, Colo. The laser will be cheaper and easier to build than standard edge-emitting lasers used in current high-speed communications.

"This VCSEL will meet the needs of high-speed fiber optics connections of the future," said Peter Esherick, manager of Sandia's Compound Semiconductor Materials and Processes Department. "We expect there to be great excitement over the device—fueled by the rapid expansion of Internet use and craving for faster Internet access."

Esherick says laboratories around the world have been racing to be the first with the 1.3-micron VCSEL on gallium arsenide substrates. Cielo teamed last year with Sandia through a CRADA to research several compound semiconductor alloys in an effort to find the one that achieved the 1.3-micron goal. In May, Sandia researchers came up with a materials combination and materials growth technique that hit the target. The research findings were submitted June 1 to *Electronic Letters* for publication.

The laser is the light source that transmits information down optical fibers. Two types of semiconductor lasers are used in high-speed data and telecommunications fiber optics—the edge emitter and the VCSEL. In the edge-emitter, which has traditionally dominated the semiconductor laser market, photons are emitted from one edge of the semiconductor wafer after rebounding off mirrors that have been literally cleaved out of a crystalline substrate.

In the VCSEL, laser photons bounce between mirrors grown into the structure and then emit vertically from the wafer surface. VCSELs, which are grown by the thousands on a single wafer, have significant advantages over edge-emitting lasers in the areas of lower manufacturing, packaging, alignment, testing costs, and lower power dissipation and higher reliability.

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Glassmaking Made Better

People have been making glass for more than 3,500 years. Although the basic recipe has changed little, the process is still not fully understood. The reason: it's technically difficult and very expensive to fully analyze the glassmaking process inside the super-heated temperatures of glass furnaces.

But that may soon change. In an attempt to help the industry be more energy-efficient, the Department of Energy (DOE) is sponsoring a new, advanced laboratory for the study of glassmaking at Sandia's Combustion Research Facility (CRF). Industry has long sought the CRF's expertise in combustion, high-temperature thermal processes, and optical diagnostic techniques and the new laboratory will facilitate that collaboration.

The Glass Melting Research Facility is being designed for glass furnace combustion and melting research, testing, and model validation. It will be open to all U.S. glass manufacturers for joint work with Sandia scientists and engineers.

"This facility will allow the industry to conduct R&D that will help them optimize their processes—reduce energy consumption as well as achieve higher outputs—without having to worry about down time at their own facility," said CRF chemist Peter Walsh.

The glass industry is one of nine industries participating in DOE's "Industries of the Future" program. These energy- and waste-intensive industries are involved in cost-sharing partnerships with DOE under the Office of Industrial Technologies to find ways to reduce their energy use and boost their bottom line.

The glass industry is an important contributor to the U.S. economy, employing more than 150,000 people and generating an estimated $22 billion worth of consumer products each year. The industry has set goals for itself that include reducing process energy use by 50 percent and reducing air and water emissions by 20 percent from 1995 levels.

Out of the industry's long-range planning process came the recommendation to construct a "user facility" for glass research. Companies typically cannot afford to use production furnaces for research nor to construct and operate separate R&D melters.

The DOE chose the CRF as the location for the test bed melter largely because of its expertise in combustion and high-temperature thermal issues. Users of the furnace will have access to the CRF's multidisciplinary talent, which includes chemists, engineers, and computer scientists.

The Glass Melting Research Facility will have the capability to gather data using optical techniques from inside the working furnace. This could then be used to test the validity of computer models of the glassmaking process for the first time, Walsh said.

Among the challenges and problems of glassmaking that may be studied are:

- Optimizing the melting of raw materials
- Increasing output
- Removing gas bubbles trapped in glass
- Reducing furnace corrosion and increasing furnace longevity
- Reducing gaseous and particulate emissions
- Developing end-to-end model-based digital control of production

The Glass Melting Research Facility will be able to produce several tons of glass a day. The furnace will be part of a larger Glass Research Facility designed to help industry address challenges spanning the full spectrum of manufacturing issues from the initial melting of raw materials through the creation of manufactured products.

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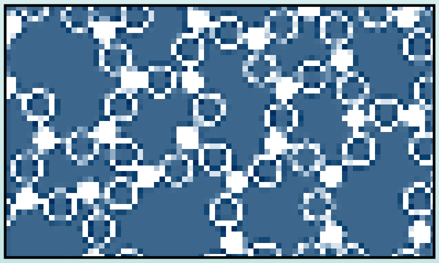

Glass has a random, non-crystalline molecular structure.

Sandia Red Team hacks all computer defenses

Sandia's Information Design Assurance Red Team seeks out weaknesses in computer systems.

Over the past two years, a group at Sandia National Laboratories known informally as the Red Team has, at customer invitation, either successfully invaded or devised successful mock attacks on 35 out of 35 information systems, along with their associated security technologies. This has occurred at a variety of sites.

Their work demonstrates that competent outsiders can hack into almost all networked computers no matter how well guarded, say spokespeople for the group, formally known as the Information Design Assurance Red Team, or IDART.

Networked computers might include e-commerce, transmitted or Net-stored financial data (from credit cards, money-machine cards, and bank accounts), as well as medical data.

Sites investigated by Sandia's self-described "bad guys" include information systems from two very large corporations and several key government agencies, said team leader Ruth Duggan from the Red Team lab in a restricted area of Sandia, a Department of Energy national security laboratory.

"We found specific weaknesses in every system," Duggan said.

The mindset of an adversary

While the Sandia group's actions are entirely legal, its adoption of an "outlaw" mindset combined with a willingness to do relatively deep analyses of ways an information system can be penetrated (whether through the Internet or by an insider) has helped test and develop concepts in security technology. Some of these concepts are so advanced they are not yet available in the marketplace.

The typical IDART group, which may consist of three to eight hackers, sometimes explains to clients in advance exactly how and when they will attack. System defenders have time to prepare specific, automatic, and even redundant defenses for their software, platforms, firewalls, and other system components. Yet results disconcert clients every time: their defenses are breached.

"Our goal is to improve the security of information systems to make the attacker's job difficult instead," Duggan said. But the group has a long way to go. "Fortified positions do take us longer to break in," she said, "but on the order of minutes, not hours."

The extraordinarily broad abilities of cyber attackers—from professional hackers to terrorists to state- and corporate-sponsored aggressors—to penetrate any system they desire can result in pilfered information, corrupted data, a change in the order of operations, or a flat denial of services. Any of these, to an individual, is an annoyance. To major corporations, they could result in billions of dollars misplaced or stolen, or in loss of reputation. In a medical or military emergency, an adversary who could intercept messages, corrupt data, and deny access to services could cause catastrophic damage.

To forestall such problems, the Red Team prefers to be called in on the design stage of a system, though it can attack a system already in place to ferret out weak points. "Our job is to understand how systems can be caused to fail, and then to help the customers improve the surety of their systems," said Sam Varnado, Energy and Critical Infrastructure Center Director.

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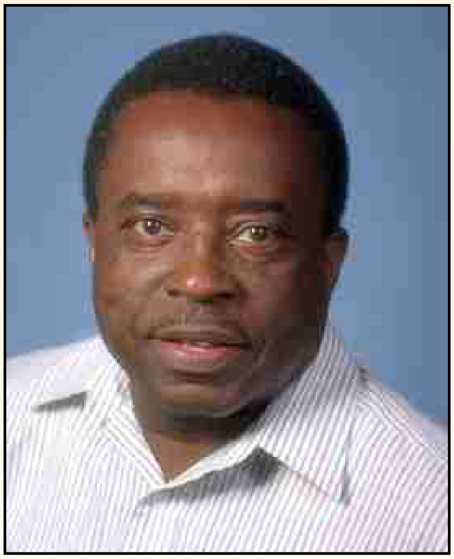
INSIGHTS

by Vincent Henry, President, Henry Technology Solutions LLC and senior industrial advisor to the Department of Energy, Office of Industrial Technologies' glass program



America's First Industry on Threshold of New Era of Development

Glass is an integral part of our everyday life. It insulates and lights our homes, brings us clear TV pictures, and provides containers for food, beverages, medicine, and a host of other products.

Glass is also an important component of the U.S. economy. The industry employs more than 150,000 people in skilled jobs and generates more than 21 million tons of consumer products annually with an estimated value of $22 billion.

American glass manufacturing traces its origins to Colonial times. In 1608, a small glass factory opened in Jamestown and became the Colonies' first industry. Since then, the glass industry has been continually evolving, with the most rapid change occurring in the last decade. Recent innovations such as injecting gas burners with pure oxygen instead of air, and new products such as fiberglass and fiber optics are transforming the industry and creating profitable new markets. At the same time, the industry has undergone restructuring brought about by rising labor costs, increasing energy and environmental costs, and excess capacity in some industry sectors.

Today, the industry is poised on the threshold of a new era, brought about by pressing competitive challenges and the industry's collective response to them. It promises to be a period of increased collaboration among industry members and between the industry, government, and academia, and, I hope, a period of unprecedented technological advancement and prosperity for the industry.

The two most pressing challenges facing the industry are competition from producers of alternative materials such as plastic and competition from manufacturers in other countries. New sensors and control technologies and breakthroughs in melter performance are expected to play a pivotal role.

The industry has made several significant steps in the past few years to increase its likelihood of successfully addressing those challenges. In 1996, it outlined its vision for maintaining and building its competitive market position in a document called *Glass: A Clear Vision for a Bright Future* (http://www.oit.doe.gov/glass/pdfs/glassvision.pdf). The vision focuses on developing technologies for reducing energy consumption, reducing environmental impacts, and enhancing economic competitiveness of the U.S. glass industry.

> Collaborative research is the key to addressing the challenges of the glass industry. Glass manufacturing requires significant capital outlays for equipment and facilities; no one company, or even the industry by itself, is capable of footing the bill for research on this scale.

Glassmaking is highly energy-intensive. In theory, about 2.2 million BTUs (British Thermal Units) of energy are required to melt a ton of glass. But in reality, it takes more than three times as much energy because of inefficiencies and losses.

The glass industry is one of nine energy-intensive industries partnering with the Department of Energy's Office of Industrial Technologies through its Industries of the Future Program. The goal of the partnership is to find ways to reduce the industries' energy use and boost their bottom line.

The industry took another significant step in 1997 when it developed a "technology roadmap" (http://www.oit.doe.gov/glass/pdfs/glassroadmap.pdf) Recognizing the value of cooperative technology planning, 38 experts from the glass industry, universities, and the national laboratories came together to identify key targets of opportunity, technology barriers, and research priorities in the entire glass industry. Workshop participants identified more than 130 process and product research priorities and conducted a risk/benefit analysis of each.

As the chairman of the Production Efficiency Subcommittee, I had a particular interest in this area. New research and development in production efficiency is essential to the industry's growth and survival. The subcommittee focused on strategies for improving the efficiency of glass production and new techniques that maximize glass strength and quality. In particular, production efficiency gains are expected to result from improvements in melting and refining processes that will increase product yield while lowering energy and other production costs.

The industry has identified the following goals to remain competitive:

- Reduce production costs at least 20 percent below 1995 levels
- Recycle 100 percent of all glass products in the manufacturing process (use of recycled glass lowers energy costs by an average of $3 to $8 per ton compared to solely using virgin raw materials)
- Reduce process energy use by 50 percent
- Reduce air/water emissions by at least 20 percent
- Recover, recycle, and minimize 100 percent of available post-consumer glass
- Achieve product quality at the "six sigma" level*
- Create innovative new products
- Increase supplier/customer partnerships

Overcoming these challenges will require increased collaboration with government, academia, and other industries to leverage scarce research dollars. It will also require partnerships between the industry, its suppliers, and customers to address issues concerning quality of raw materials, waste generation, and energy availability.

The glass industry participates in or has completed several cost-sharing R&D projects with the Department of Energy. Among the achievements and ongoing projects:

- Achievement of a 12-percent increase in energy to load in a high-efficiency burner
- Testing of new sensors that detect temperatures during manufacturing without contacting the glass
- Research into the feasibility of combining oxygen and preheated air to better control the states of combustion in side-port furnaces
- Development of computer models that examine the complex chemistry of combustion and how that process is affected by furnace configurations, burners, and other elements
- Construction of a pilot-scale glass furnace for combustion and melting research, testing, and model validation

Collaborative research is the key to addressing the challenges of the glass industry. Glass manufacturing requires significant capital outlays for equipment and facilities; no one company, or even the industry by itself, is capable of footing the bill for research on this scale. It also leverages investments in government-funded institutions, which provide both the facilities and brainpower needed to address these real-world challenges.

The glass industry faces exciting new opportunities and serious challenges. But the direction is clear, and together we are making progress toward securing a bright future.

■

**A term coined by Motorola in the 1980s, six sigma technically means a failure rate of 3.4 parts per million. It is used in more general terms as a total quality management approach.*

"Today, the industry is poised on the threshold of a new era. This new stage is brought about by pressing competitive challenges and the industry's collective response to them. It promises to be a period of increased collaboration among industry members and between the industry, government, and academia, and, I hope, a period of unprecedented technological advancement and prosperity for the industry."

Vincent Henry, President, Henry Technology Solutions LLC and senior industrial advisor to the Department of Energy, Office of Industrial Technologies' glass program

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000

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