About the Cover

Lawrence Livermore scientists and engineers are using their modeling expertise to help design more efficient engines and formulate cleaner fuels. Their work contributes to energy resource conservation and to abatement of carbon dioxide emissions that contribute to global warming. One of their projects involves the engine shown on the cover, a cross between a spark-ignition and diesel engine called the Homogeneous Charge Compression Ignition (HCCI) concept. The article beginning on p. 4 describes how modeling is being used to determine control of the HCCI's ignition timing, the key to its effectiveness, efficiency, and marketability.

Cover photos: Michael Anthony and George Kitrinos

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Prepared by **LLNL** under contract
No. W-7405-Eng-48

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the World Wide Web at www.llnl.gov/str/.

Printed in the United States of America

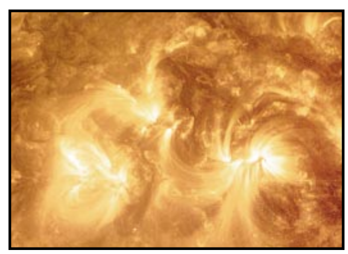
Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-52000-99-12
Distribution Category UC-0
December 1999

Science & Technology REVIEW

December 1999

Lawrence
Livermore
National
Laboratory



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Revealing images of Titan

Astrophysicists from Lawrence Livermore and the University of California campuses at Berkeley and Los Angeles have captured the best images ever of Titan, one of Saturn's moons. The images reveal what may be the only known liquid bodies in the solar system other than those on Earth, as well as bright regions that may be ice-and-rock continents or highlands. They hint of complex chemical processes that make Titan resemble the prebiotic Earth more closely than any other place in the solar system.

The astrophysicists took the images using the world's largest telescope, the 10-meter Keck I in Mauna Kea, Hawaii, and a special technique called speckle interferometry. The powerful Keck allowed them to "map surface features 240 kilometers in size on a moon that is more than 1,200 million kilometers from Earth," said Livermore astrophysicist Claire Max. With speckle interferometry, the scientists took hundreds of infrared snapshots so fast as to freeze the atmospheric turbulence that otherwise would blur the images. The snapshots were computer-processed together and then converted into a map of Titan's surface features.

Livermore scientists developed a version of speckle interferometry to image satellites during the Cold War. Laboratory engineer Don Gavel adapted it for astronomical use. "Speckle imaging is limited to bright, compact objects; Titan qualifies perfectly," said Gavel.

What astrophysicists have learned about Titan's surface will be useful for the mission of the Cassini spacecraft currently en route to Saturn. Cassini is scheduled to land the Huygens probe on Titan in 2004. Ground-based studies such as these Keck observations using speckle interferometry will help predict whether the probe will land on a solid surface or splash into an extraterrestrial sea.

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Another use for seismic sensors

Livermore seismologists Steve Myers and Kevin Mayeda are collaborating with Yosemite National Park's rockfall specialists and the U.S. Geological Survey to apply seismic tools and techniques, typically used to study earthquakes, to monitor rockfall. Myers and Mayeda proposed this study after hearing that a climber had been killed by falling rock in Yosemite Park.

In the vicinity of the deadly rockfall that occurred this summer, Livermore field technicians installed a network of seismic sensors to determine whether very small, subtle motions from rock cracking or shifting can be detected. Myers said, "This research will let us see how useful seismic monitoring may be for predicting rockfall."

The sensors, connected to a recording box so detections can be recorded and graphed, are rechecked periodically and their data downloaded every three weeks. The information provided may help experts better establish the patterns and mechanisms of crack development that precede rockfall, thereby providing a warning system for rockfall hazards.

The seismic monitoring data are being correlated with continuing visual observations made by Yosemite rockfall experts of the area below Glacier Point, where the fatal rockfall occurred.

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Groundwater cleanup goes over 1 billion gallons

The Laboratory's cleanup of contaminated groundwater at its Livermore site has proceeded so efficiently that cleanup is predicted to be completed almost 20 years earlier than expected. In mid-July, the Laboratory reached a milestone when it treated its billionth gallon of contaminated water.

Groundwater contamination dates from the 1940s when the site was a U.S. Naval Air Station and chemical solvents used to clean aircraft parts leaked into the soil. Laboratory operations in the 1950s and 1960s also contributed some contamination. The contamination is deep underground. Drinking water has not been affected, and there have been no threats to human health and the environment.

Ten years ago, the Laboratory began operating its Treatment Facility A to pump and treat contaminated groundwater. Today, four fixed treatment facilities, eight portable units, three solar-powered units, and many special-purpose units have been developed and built by Livermore's environmental restoration specialists to speed the cleanup. Most of these special units are unique and also cost considerably less than a fixed facility.

Over 425 kilograms of contaminants have been removed to date. So, where once the contamination stretched almost a quarter of a mile to the west of the Laboratory, it now reaches only a few yards beyond the Laboratory's perimeter. And the concentration of the contamination that remains is close to the regulatory limit.

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Carbon Management in Today's Environment

BURNING coal polluted our skies well into this century. Then the burning of other carbon-based fuels continued the pollution. As a result, we face concerns today about possible climate change from emitting carbon into the atmosphere. In the Energy Directorate, where we join together the expertise of multiple disciplines from throughout Lawrence Livermore, we are addressing these concerns with innovative research in carbon management technologies.

There are three basic strategies for reducing carbon emissions into the atmosphere. First, we can use fuels that contain less carbon (for example, natural gas), find better ways to manufacture low-carbon fuels (methanol, liquefied natural gas, and hydrogen), and produce electricity with renewable resources and nuclear fission instead of coal. Second, we can improve energy efficiency in all use sectors—whether utility, transportation, industrial, residential, or commercial. And third, we can develop low-cost carbon separation and sequestration technologies.

The article beginning on p. 4 addresses part of the second strategy: improved efficiency for the transportation sector. By applying our fundamental understanding of combustion chemistry, nonthermal plasmas, and catalytic processes to the venerable piston engine, we are working to improve engine efficiency and thereby allow the public more engine choices.

Over the past 25 years, Livermore has developed chemical kinetic models for studying ever-more complex systems of hydrocarbon fuels. Livermore scientists have gained insight into the processes that produce pollutants—the hydrocarbons, oxides of nitrogen, carbon monoxide, and particulates—that now are regulated. Using the models, designers have modified engines to reduce emissions to the point that with after-treatment technologies (catalytic converters), the engines can meet ever-tightening regulatory limits.

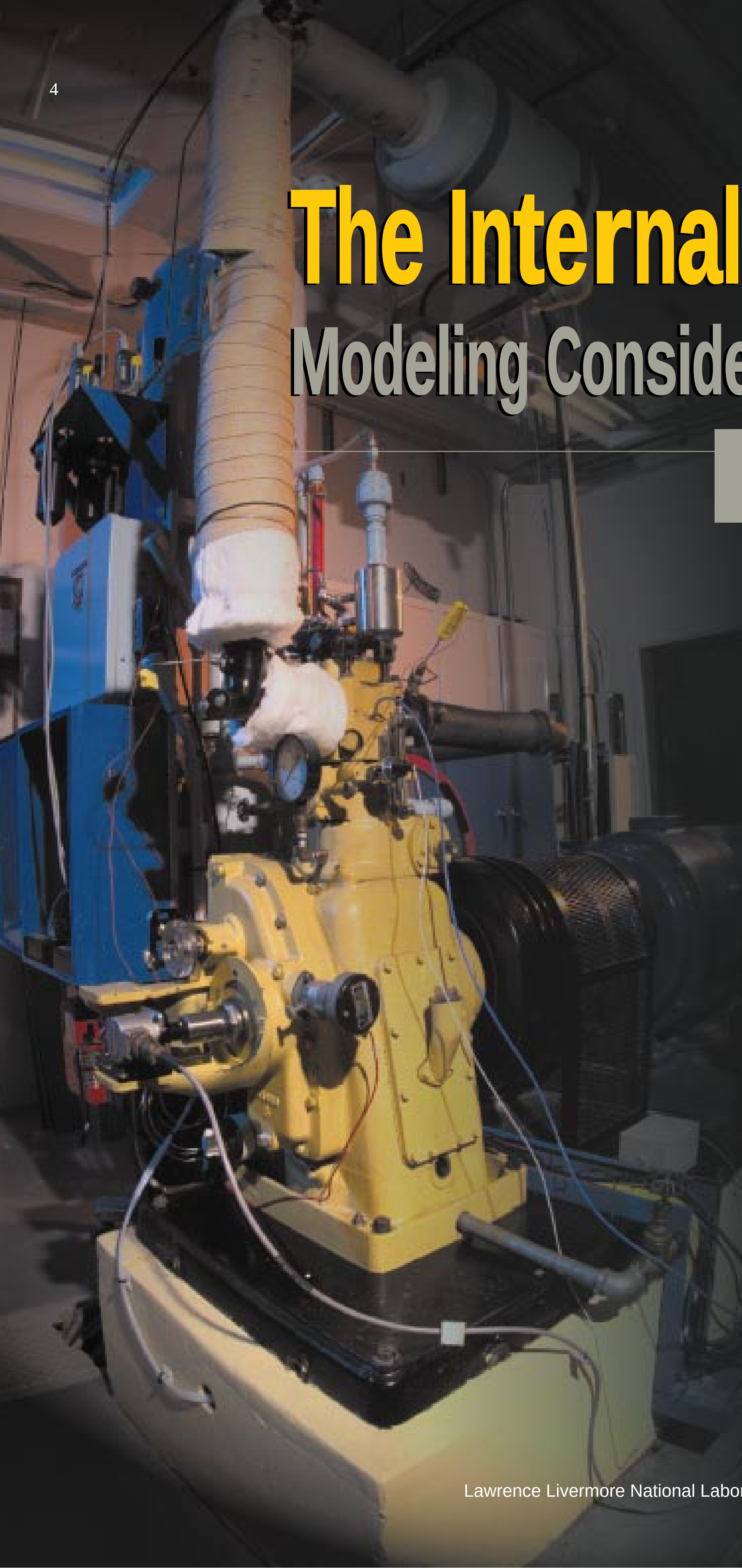
Now the challenge is to reduce the amount of carbon dioxide that automobiles and trucks emit per mile. Not yet regulated, these emissions are at the heart of carbon management for vehicles. The Partnership for a New Generation of Vehicles—a consortium of the three U.S. automakers, national laboratories, and industry for studying fuel–engine relationships—has concluded that the most viable technology for reducing the carbon dioxide emissions of lightweight vehicles is the diesel engine, probably in hybrid drivetrain configurations. Using lightweight materials, improved aerodynamics, and lower rolling resistance, we can build diesel cars that provide 60- to 70-mile-per-gallon efficiency with only a small increase to their cost. But the current diesel engine does not meet the regulatory standards that will be in place in the next decade, so we are researching after-treatment technologies for diesels.

We are also examining modified, or reformulated, diesel fuels. We are keenly aware of the recent history of MTBE contamination of water supplies and understand that the full environmental effects of fuel modifications must be carefully examined.

Another major project is a totally new engine combustion system known as Homogeneous Charge Compression Ignition. It does not produce significant emissions of oxides of nitrogen, thus making after-treatment of the hydrocarbons simple. If control mechanisms can be found for these engines, they may be as efficient as diesels and cost less.

Of course, none of this research will have any effect if it does not move into the marketplace. We are working closely with industry to understand the real-world constraints of all of these technologies. We want our work to result in viable options while also reducing industry's technical risk.

■ Ray Smith is Deputy Associate Director, Applied Energy Technologies.



The Internal Combustion

Modeling Considers All Factors

Increasing fuel efficiency in automotive engines while simultaneously reducing their exhaust emissions is a challenge. Modeling the combustion process is essential to meeting that challenge.

THE internal combustion engine—in particular the fuel that powers it—has been a powerful motivator for government decision-making and foreign policy in this century. Countries have been invaded and wars fought over petroleum. Germany lost World War II in part because it ran out of gasoline. Given the concerns over worldwide oil reserves and greenhouse gases, it is not surprising that considerable research is devoted to increasing the efficiency of the internal combustion engine, especially for the automobile, a major consumer of petroleum and source of carbon dioxide emissions.

But increasing efficiency, so that less fuel is used to produce the same amount of energy, is not a simple engineering task. Greater efficiency reduces carbon dioxide emissions but increases regulated exhaust emissions in the form of oxides of nitrogen (NO_x), which are a major source of photochemical smog. If the combustion process is modified to reduce NO_x emissions, these systems then emit large

Engine at Work

amounts of particulate matter and carbon monoxide.

In spark-ignited engines, which most automobiles today use, another problem arises when efficiency is increased. With an increase in the compression ratio comes a tendency for the engine to knock or ping unless the fuel includes an additive like tetraethyllead or MTBE (methyl tertiary-butyl ether).

This interplay of efficiency and emissions—and to a lesser extent engine knock—is at the heart of almost all research today on the automotive engine and on other practical combustion systems such as gas turbines, industrial burners, boilers, and so on. Fixing engine knock with a fuel additive is easy. But recall that leaded fuel was a major air pollutant, and MTBE is currently polluting groundwater. Reducing exhaust emissions is equally challenging.

Trial-and-error research on the combustion engine produced results for many years, including the first solution to the problem of engine knock. However, by the middle 1970s, computers had advanced sufficiently for use in detailed, full-system modeling, a cheaper and more effective way to explore combustion problems.

A challenge for modeling automotive fuels is the enormous variation in their chemical makeup. On a day-to-day basis, refineries mix and match the hundreds of components in the fuel they produce to meet certain mandated specifications. But there are broad tolerances in those specifications, which largely dictate only that the fuel will make an engine run and that it meet a particular octane (antiknock) or cetane (diesel-ignition) rating. This variability is what makes modeling so challenging and so important. Modeling makes it possible to predict with confidence the effect of each of the ingredients on the overall fuel mixture.

At Livermore, modeling of the combustion process was an offshoot of nuclear weapons research. According to Livermore physicist Charlie Westbrook, an internationally recognized authority on combustion and combustion modeling, “Modeling the combustion process really isn’t very different from modeling what happens in a nuclear weapon. Instead of looking at the reactions of protons and neutrons in a weapon, we started looking at what was happening to hydrocarbon and oxygen molecules under combustion conditions.”

Livermore’s computational capabilities have always been among the best in the world. Add to that Livermore’s multidisciplinary staff and you have a powerful modeling team. Charlie Westbrook today leads the Chemistry and Chemical Engineering Division in the Chemistry and Materials Science Directorate, but for years he was in the trenches leading much of Livermore’s combustion modeling work. Working with computer experts, engineers, and others, his team produced some revolutionary results. That tradition continues today in work on a novel engine design, a new method for reducing NO_x emissions from diesel engines, and reformulated diesel fuels.

Early Results

Livermore brought its talents to three major cooperative research groups formed in the middle 1970s by the Department of Energy with Ford Motor Company, General Motors Corporation, and Unocal. Other participants in these groups included universities, private industrial firms, and the Los Alamos and Sandia national laboratories. While working in collaborations that lasted for almost 20 years, group members won about one-third of the Horning Memorial Awards given by the Society for Automotive Engineering for the best paper on engine–fuel relationships presented at the society's annual meeting.

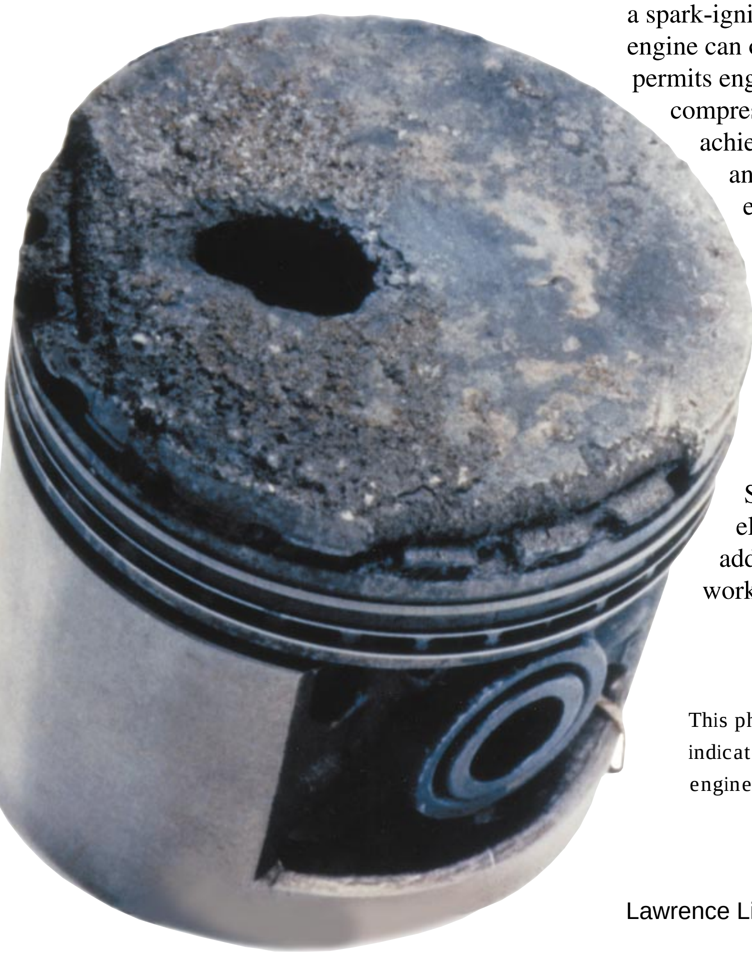
One major project of the research groups modeled flame quenching at engine walls. In the cylinder of an automobile engine, a flame ignited by a spark propagates through an air–fuel mixture and toward the cylinder walls and piston. Before this project began, engine researchers everywhere were certain that a major source of unburned hydrocarbon emissions was the extinguishing of the flame as it approaches the relatively cold walls of the cylinder. They thought the process left behind a thin layer of unreacted fuel.

Modeling results seemed to support that traditional view until near the end of the ignition process, when data indicated that fuel trapped in the cold boundary layer at the wall begins to diffuse back out toward the high-temperature region where it is rapidly consumed. Later research confirmed that unreacted fuel in the piston ring crevices is actually the primary source of unburned hydrocarbon emissions.

Equally revealing was a chemical kinetic study of fuel additives for engine knock in spark ignition engines, for which Westbrook and William Pitz, also of Livermore, received the Horning Award in 1991.[1] Knocking occurs when the flame from the spark plug does not consume the gases in the piston chamber fast enough. The remaining "end gases" spontaneously combust, sending a damaging shock wave across the chamber.

Engines operate most efficiently at the highest compression ratios, but that is precisely where knocking occurs. Engine knock therefore sets an upper limit to the compression ratio at which a spark-ignited internal combustion engine can operate. Suppressing knock permits engines to operate at higher compression ratios and thus to achieve higher fuel efficiency and lower carbon dioxide emissions.

In the 1920s, years before air pollution became a major issue, trial-and-error research produced an effective solution for engine knock that was used for decades: the additive tetraethyllead. Since leaded fuel was eliminated in the 1970s, other additives have been used that work in a variety of ways.



This photo of a badly damaged piston indicates the effects of long-term engine knock.

Today, MTBE is the oil refiners' additive of choice for suppressing knock. But MTBE leaking from underground storage tanks has been found to be contaminating groundwater (see *S&TR*, April 1999, pp. 21–23).

Westbrook and Pitz's award-winning paper was the culmination of a long-term study of the fundamental chemical factors that control knocking. Earlier work had resulted in models for different families of elementary reactions with varying dependencies on temperature, pressure, and fuel–air concentrations. Working up from simple to complex molecules, from single-component fuels to fuel mixtures, the research team simulated the ignition of fuels with a variety of ignition characteristics. They also examined an array of proknock and antiknock additives, including MTBE. The goal of this work was to provide chemical engineers with the ability to predict the knock behavior of arbitrary mixtures of hydrocarbons and additives.

Sleuthing Chemical Reactions

Livermore developed the chemical kinetics model known as HCT, for hydrodynamics, chemistry, and transport, for use in all of this early work. Because of limited computer capabilities early on, modeling of hydrocarbon oxidation and ignition could consider fuel molecules containing only one or two carbon atoms. But those simple models served as the basis for mechanistic studies of larger fuel molecules, which are made up of many smaller ones. The extensive research on engine knock, for example, would not have been possible without those smaller building blocks.

Mechanisms for hydrocarbon fuel reactions range from relatively simple to extremely complex. As shown in the table to the right, hydrogen–air combustion produces just 7 species, involving about 20 chemical reactions. Reactions involving cetane produce

1,200 species and are much more time-consuming to model. Each species requires a differential equation to explain its behavior in any reaction. Fortunately, with recent strides in advanced parallel computing, large, complex kinetics problems may be handled comparatively easily.

The HCT code permits the use of a variety of boundary and initial conditions for reactive systems, depending on the needs of the particular system being examined. Over the years, the code has been used to study the combustion properties of many hydrocarbons, including methane and other paraffin fuels; natural gas; alcohols such as methanol and ethanol; oxygenated fuels, including dimethyl ether and MTBE; aromatics such as benzene, toluene, and naphthalene; as well as blends of automotive fuels for particular octane ratings. HCT has also been applied to studies of various exhaust emission species such as NO_x, metals, and chlorinated, brominated, and fluorinated species.

A more recent application of the HCT model has taken it far from the automotive industry. With HCT, researchers at Livermore are studying the kinetics of chemical warfare nerve agents to learn more about their reactions and how they evolve over time so that protection against them can be improved.

An Engine for the Future

Today, a version of HCT is proving indispensable for research on an innovative engine concept known as Homogeneous Charge Compression Ignition (HCCI). Combining features from both spark-ignition and diesel engines, the HCCI engine is promising the high efficiency of a diesel engine with virtually no NO_x or particulate emissions. The engine can operate using a variety of fuels. Given this mix of attributes, it is not surprising that considerable research is going on around the world on the HCCI engine. Much of Livermore's research on it has been done in conjunction with a major industrial partner.

In the HCCI engine, fuel is homogeneously premixed with air, as in a spark-ignited engine, but with a high proportion of air to fuel. When the piston reaches its highest point, this lean fuel autoignites (spontaneously combusts) from compression heating, as in a diesel engine. But remember that autoignition is what causes knock in a spark-ignited engine. Knock is undesirable in spark-ignited engines because it enhances heat transfer within the cylinder and may burn or damage the piston. But in an HCCI engine, with its high air-to-fuel ratio, knock does not damage the engine because the presence of excess air keeps the maximum temperature of the burned gases relatively low. When the danger of engine damage is eliminated, autoignition becomes a desirable mode of operation.

Engineer Ray Smith began working on HCCI at Livermore in the mid-1990s. He realized early on that understanding chemical kinetics was the key to controlling HCCI combustion. This realization, combined with Livermore's access to detailed chemical kinetics codes such as HCT, quickly made the Livermore team a leader in HCCI analysis at a time when others did only experimental work.

In 1996, the Livermore team modified HCT by incorporating models required for engine analysis, such as an engine heat-transfer model, a turbocharger model, and a model for exhaust gas recirculation. This version then analytically predicted for the first time the regions of best operation for HCCI engines running on methane and natural gas.

More recently, the Livermore team, now led by Salvador Aceves–Saborio, has developed a comprehensive model for predicting HCCI combustion, linking HCT with a fluid mechanics code to calculate the effect of temperature distribution on HCCI combustion. This methodology not only predicts experimental pressure traces with great accuracy but also has produced the first prediction of hydrocarbon and carbon monoxide emissions, including where those emissions originate within the cylinder. All of this information is important for determining a course of action for emissions control in HCCI engines.

Livermore is now working with mechanical engineers at the University of California at Berkeley to verify the modeling results experimentally. A

Chemical Kinetic Model

Large database contains:

- Thermodynamic properties of species
- Reaction rate parameters

Reaction mechanisms grow with molecular complexity:

Fuel	H_2 (hydrogen)	CH_4 (methane)	C_3H_8 (propane)	C_6H_{14} (hexane)	$C_{16}H_{34}$ (cetane)
Number of species	7	30	100	450	1,200
Number of reactions	25	200	400	1,500	7,000

More complex fuels make much greater demands on computing time during modeling. Until improvements were made in advanced parallel computing, only simple fuel molecules could be modeled.

single-cylinder HCCI engine has been operating at the Berkeley campus and producing data since April 1999. A four-cylinder diesel engine has recently been modified as an HCCI engine. Thus far, modeling data and experimental results tally very well.

Autoignition must occur almost exactly at the point where the piston reaches its maximum height within the cylinder. Timing of autoignition is thus critical, but the HCCI engine gives up two timing control mechanisms: The start of ignition is not directly controlled by an external event such as the beginning of injection in the standard diesel or the sparking of the spark plug; and the heat release rate is not controlled by either the rate and duration of the fuel-injection process, as in the diesel engine, or by the turbulent flame propagation time, as in the spark-ignited engine.

Detailed modeling of engines using a homogeneous charge of various fuels has shown that by knowing the precise conditions (fuel species, temperature, and density) at the start of compression, the beginning of combustion can be accurately predicted. But knowing in theory the initial conditions and controlling the timing are two different things.

Aceves–Saborio says, "The control problem is what keeps the HCCI out of the auto showroom, and we are studying various options." One is to inject recirculated exhaust gases into the fuel–air mixture to raise the fuel temperature quickly. Another option is to use small amounts of dimethyl ether to enhance ignition slightly. Aceves–Saborio notes, "Most of our future work will be directed at engine control. It will be a challenge."

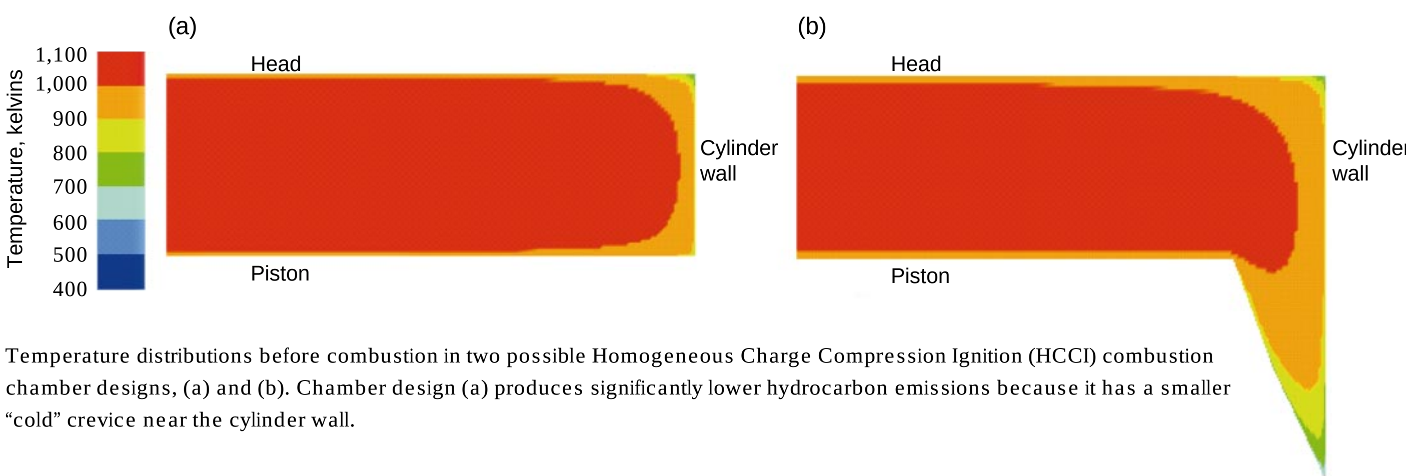
Cleaning Up Diesel Emissions

The catalytic converters used today in spark-ignited gasoline automobiles are responsible for major reductions in tailpipe emissions of carbon monoxide, hydrocarbons, and NO_x. But that kind of catalysis does not work well on diesel engines, which operate on lean fuel-to-air mixtures. Exhausts from these engines contain an excessive amount of oxygen that inhibits the chemical reduction of NO_x to nitrogen (N_2), rendering catalytic converters useless for NO_x removal.

Lean-burn engines such as the diesel are the focus of most engine research today because they offer fuel economy unmatched by any other commercially viable engine. But they must run cleaner and produce fewer emissions if they are to gain more widespread use. While diesel engines can rather easily be optimized to reduce either NO_x or particulate matter, cutting one usually causes an increase in the other. With a new process developed at Livermore, it appears that both emissions can be reduced. The engine can be optimized for low particulate matter and high NO_x, and Livermore's technique then reduces the NO_x to harmless molecules such as N_2.

Building on Livermore's years of experience in plasma physics, a team led by physicist Bernie Penetrante has developed a process to reduce NO_x in lean-burn engine exhausts. Known as Plasma-Assisted Catalytic Reduction (PACR), the process combines a nonthermal plasma with a catalyst. One application of this process involves a nonthermal plasma produced by short pulses of high voltage on a metal wire inside a metal cylinder (see schematic on p. 9 at top right). The plasma serves to oxidize the nitric oxide (NO) and hydrocarbons to nitrogen dioxide (NO_2) and partially oxidized hydrocarbon products, respectively. These plasma-conversion products are then reduced over a catalyst to nitrogen, carbon dioxide, and water.

The PACR process would not be where it is today without modeling early on to determine what the plasma can and cannot do. Generation of the plasma, by itself, does not guarantee a means for efficient oxidation of NO to NO_2, which is necessary for enhancing the reduction of NO_x to N_2 over the catalyst. Lean-burn engine exhausts contain large amounts of water vapor in

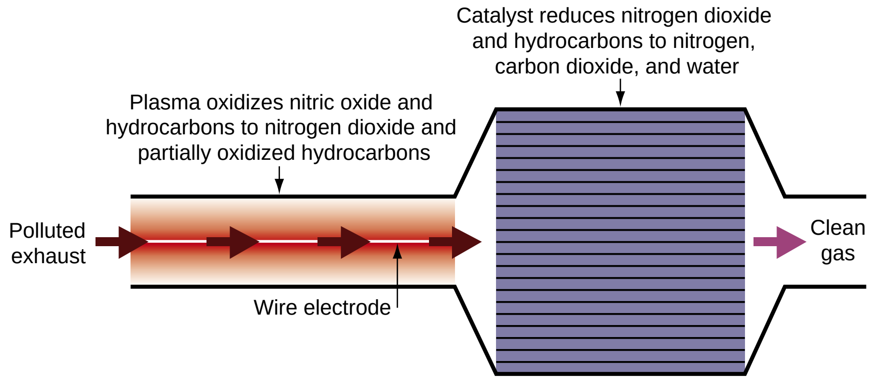


Temperature distributions before combustion in two possible Homogeneous Charge Compression Ignition (HCCI) combustion chamber designs, (a) and (b). Chamber design (a) produces significantly lower hydrocarbon emissions because it has a smaller "cold" crevice near the cylinder wall.

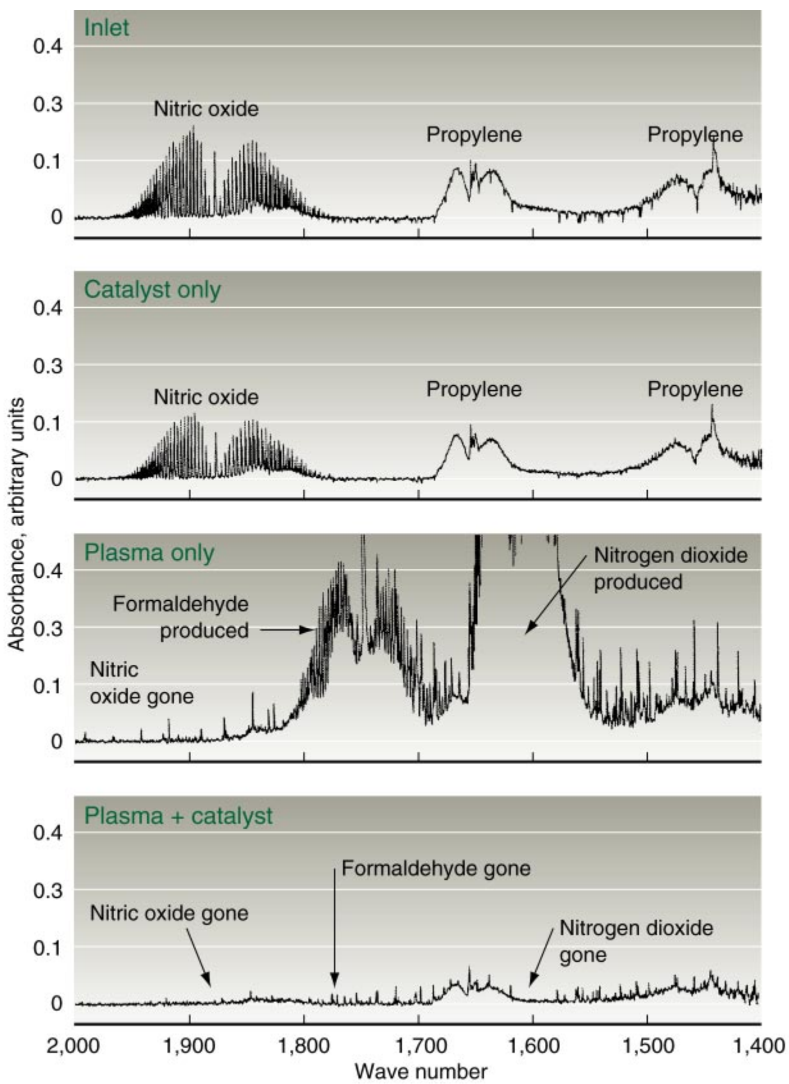
addition to oxygen, prompting the plasma not only to oxidize NO to NO_2 but also to oxidize NO_2 to nitric acid. Livermore's models are guiding the development of the PACR process, in which the plasma oxidizes NO to NO_2 without further producing acids.

Use of the plasma also avoids a problem that confounds most proposed diesel catalysis systems. The current state-of-the-art catalysis method uses platinum or another precious metal to convert NO_x to N_2 in diesel engines. But diesel fuels have a fairly high sulfur content. Catalysis with precious metals tends to oxidize sulfur dioxide (SO_2) to sulfur trioxide (SO_3), which then fouls the catalyst and produces particulates. Using low-sulfur fuels might avoid this problem, but the PACR process gets around it altogether without precious metals or low-sulfur fuel. By simulating the activity of the exhaust gases in the plasma, the team learned that the presence of unburned hydrocarbons makes the plasma "tolerant" of SO_2. The unburned hydrocarbons scavenge the reactive free radicals that would otherwise oxidize SO_2, thus allowing the plasma to be very selective.

Thus far, the team has developed a bench-scale prototype of the system. With it, they have successfully run tests on a portion of the exhaust from a diesel engine and on controlled laboratory gases that simulate exhaust mixtures.



A schematic of the plasma-assisted catalytic reduction system. A nonthermal plasma is produced by short pulses of high voltage on a metal wire inside a metal cylinder.



Spectrographic analysis of exhaust emissions demonstrates the benefit of plasma-assisted catalytic reduction. Plasma plus catalysis almost completely eliminates emissions from diesel engines.

The team has recently scaled up the system to handle the full exhaust flow from car and truck engines.

A New Look at Diesel Fuel

California's Air Resources Board and the U.S. Environmental Protection Agency are proposing regulations for substantially reducing emissions of NO_x and particulate matter. These regulations will pose a major challenge for diesel engines, which currently produce significant amounts of both types of emissions. Working with several engine companies, a Livermore team has been using the HCT code to simulate ignition and particulate production in advanced diesel engines running on oxygenated fuels.

In particular, they are looking at how fuel molecular structure influences emissions. Several alternative fuels—such as dimethyl ether and dimethoxy methane—have been suggested to reduce soot and NO_x in diesel engine operations. These fuels contain no carbon-to-carbon bonds and produce little or no soot, and, like other fuels containing oxygen atoms such as alcohols and ethers, they reduce NO_x emissions by lowering flame temperatures. Charlie Westbrook is leading the modeling effort to more fully understand how these fuels react and how to exploit their beneficial properties.

Environmental scientist Dave Layton and his team are contributing to this work in a novel fashion by preparing life-cycle analyses of the various fuels and additives under consideration. Looking beyond how the fuels will operate in an engine, they are examining the full effects of the fuels from their production through subsequent distribution, storage, and use.

Westbrook notes, "This kind of life-cycle analysis was not done for MTBE. Engineers knew it would suppress knock and reduce carbon dioxide, and at the time, that seemed to be enough. We now know that a more thorough investigation is needed before new fuels and additives are introduced."

Layton, Westbrook, and others at Livermore have proposed to the Department of Energy that a Consortium for Fuels Assessment be established at Livermore to perform life-cycle analyses of new fuels and additives. The goal is to learn as early as possible what the full ramifications of a new additive or fuel will be and to evaluate any necessary mitigation measures.

The Work Ahead

Given our peripatetic lifestyles, it is clear that automobiles powered by the internal combustion engine are with us to stay, at least until some better mode of transportation comes along. For most consumers, the car's flexibility and relatively low cost outweigh its deleterious effects on petroleum reserves and the environment.

But it is no accident that the U.S. Department of Energy and other organizations are focusing most of their research on diesel and HCCI engines. These fuel-efficient engines promise to make oil supplies last longer. Once autoignition in the HCCI engine is effectively controlled, it may well be the engine we use until the fuel cell becomes an economic option. Developing fuels that burn cleaner and affect the environment less will improve the overall picture even more.

Modeling engine processes is key to this research. Livermore researchers have already made major contributions and show no sign of stopping any time soon.

—Katie Walter

Key Words: Combustion modeling, diesel fuels, HCT code, Homogeneous Charge Compression Ignition (HCCI), internal combustion engine, Plasma-Assisted Catalytic Reduction (PACR).

For further information contact Charles Westbrook (925) 422-4108 (westbrook1@llnl.gov).

Reference

1. Charles K. Westbrook, William J. Pitz, and William R. Leppard, "The Autoignition Chemistry of Paraffinic Fuels and Pro-Knock and Anti-Knock Additives: A Detailed Chemical Kinetic Study," paper no. 912314, Proceedings of the SAE International Fuels and Lubricants Meeting and Exposition, Toronto, Canada, October 7–10, 1991.

About the Scientist

CHARLES K. WESTBROOK received a B.S. in physics from Harvey Mudd College and a Ph.D. in applied science and engineering from the University of California at Davis. He joined Lawrence Livermore in 1968 in the Physics Directorate, where he served as division leader of the Computational Physics and Applied Physics Divisions. He recently became division leader of the Chemistry and Chemical Engineering Division in the Chemistry and Materials Science Directorate. His honors include the 1991 Horning Memorial Award from the Society of Automotive Engineers for the best paper of the year on engine–fuel relationships and the 1992 Thomas Midgley Award from the American Chemical Society for outstanding contributions in the field of chemistry related to the automotive industry. Westbrook has authored approximately 250 refereed publications on combustion, chemical kinetics, and physics.

Multilayers Illuminate the Sun's Secrets

TELESCOPES from Earth and from space have imaged the sun millions of times but have discerned its secrets very slowly, especially those concerning its ever-changing magnetic fields. Now, extremely detailed images from a NASA satellite called the Transition Region and Corona Explorer (TRACE) are revealing the role played by fluctuating magnetic fields in heating the sun's hot plasma and creating such fantastic features as solar flares, eruptions, and loops. Obtained with a telescope using multilayer-coated mirrors produced by Lawrence Livermore scientists, the images can be assembled into mosaics of the complete solar body or arranged sequentially into astonishing time-lapse movies.

TRACE is part of NASA's Small Explorer program of lightweight spacecraft designed to minimize the cost of scientific space exploration. In Earth orbit since April 2, 1998, the 1,030-kilogram satellite continuously studies the key solar regions: the photosphere (the 6,000-kelvin surface), chromosphere (the part of the sun's atmosphere where the temperature rises to about 10,000 kelvins), transition region (between the chromosphere and corona in which the temperature rises dramatically to 100,000 kelvins), and the corona (the multimillion-kelvin upper atmosphere).

TRACE observes the sun at unprecedented spatial resolution (1 arc second, or 740 kilometers across) and time resolution (from 2 to 30 seconds between images). Images at these resolutions effectively provide time-lapse movies that reveal how extremely fine magnetic loops appear, evolve, and reform.

Key to the high image resolution are the multilayer optical coatings produced by a Lawrence Livermore team led by materials scientist Troy Barbee, Jr. Multilayers are composed of alternating layers of two different materials as thin as a few atoms. (See "Atomic Engineering with Multilayers," *S&TR*, December 1997, pp. 12–19.)

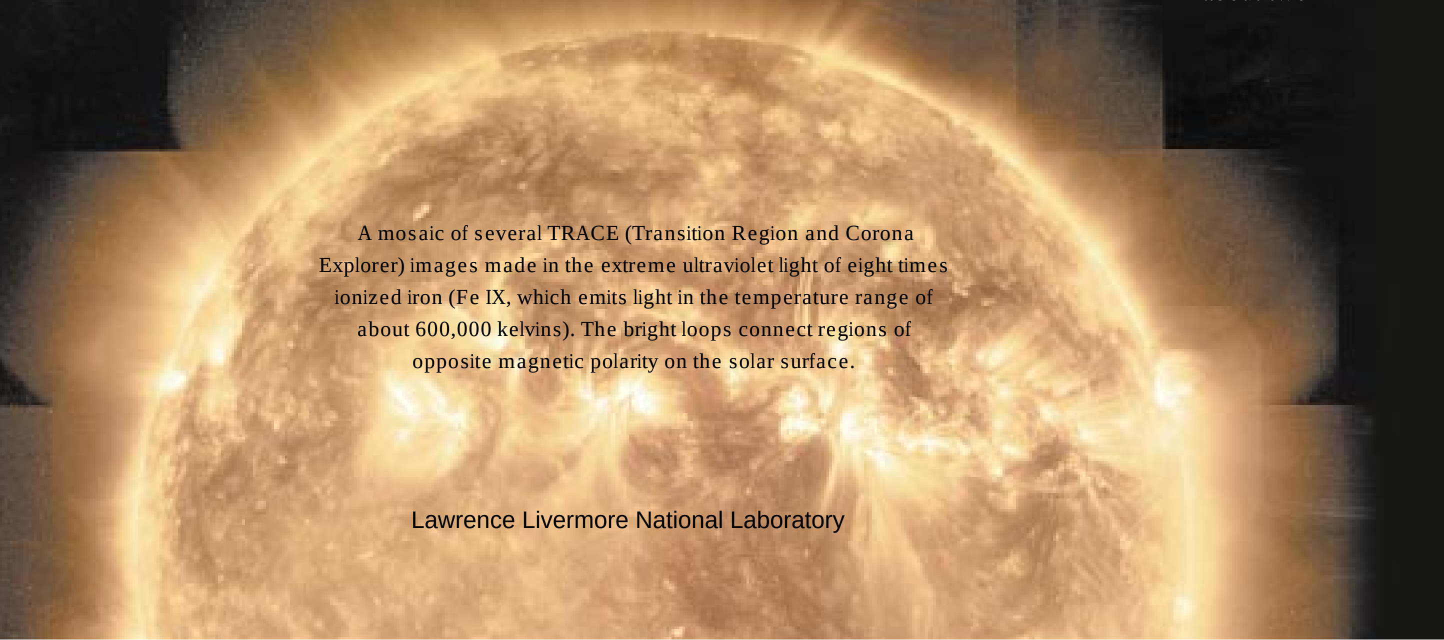
In recent years, multilayers have proved extremely valuable to astrophysicists for their ability to focus light in previously inaccessible narrow bands of the x-ray, soft x-ray, and extreme ultraviolet wavelengths. Their extraordinarily efficient optical performance reveals astronomical features that cannot be captured by instruments operating at longer wavelengths.

Wanted: Higher Resolution

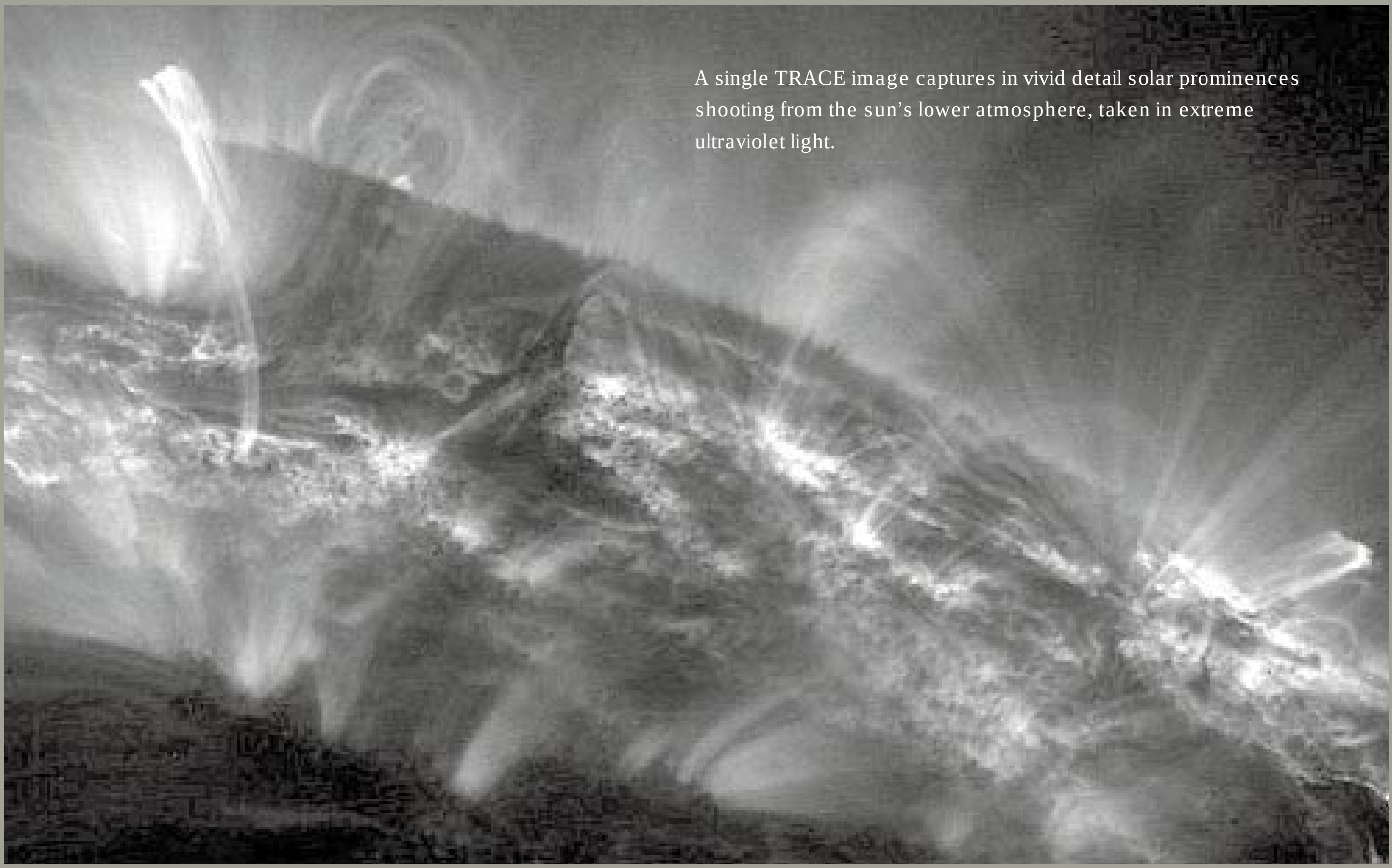
When planning for the mission began, says Barbee, the TRACE team asked for multilayers that could provide much higher resolution and reflectivity than had ever been achieved. The team also requested more robust materials; previous space-born multilayers have degraded in time as a result of the harsh environment.

In response, Barbee's team developed multilayers made of alternating layers of molybdenum carbide and silicon. The multilayers were applied to a substrate of titanium silicate glass, supplied by the group at the Smithsonian Astrophysical Observatory responsible for TRACE optics.

Barbee reasoned that the carbon in the molybdenum carbide reacts with silicon to form silicon carbide, an extremely stable material, at the interfaces between the layers. To test the multilayers' stability, Barbee annealed some test materials for eight hours at 673 kelvins—equivalent to being in space for about two



A mosaic of several TRACE (Transition Region and Corona Explorer) images made in the extreme ultraviolet light of eight times ionized iron (Fe IX, which emits light in the temperature range of about 600,000 kelvins). The bright loops connect regions of opposite magnetic polarity on the solar surface.



A single TRACE image captures in vivid detail solar prominences shooting from the sun's lower atmosphere, taken in extreme ultraviolet light.

years at 90˚C. No changes were observed in the performance of the annealed structures, demonstrating that they are dramatically more stable than other potential multilayer material combinations. In space, the TRACE multilayers have proved so stable that they are used to calibrate multilayers on other satellites.

The Livermore materials are exceptionally smooth and flat; their 47-percent reflectivity is a factor of 2 better than any multilayer previously used in space. Such high reflectivity results in much shorter exposure times for the satellite's charge-coupled device (CCD) camera.

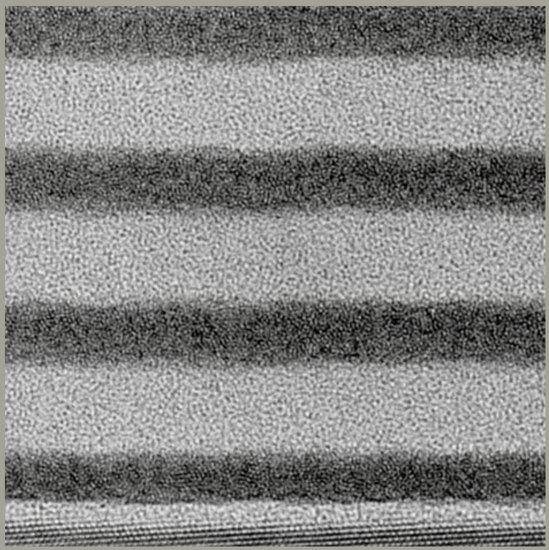
The 30-centimeter primary TRACE telescope has a different multilayer coating on each quadrant of its surface, making it in effect four different telescopes. The telescope shutter selects one quadrant at a time. Coatings for three quadrants were each designed for a specific band of extreme ultraviolet light corresponding to one of these excited ions of iron: Fe IX, Fe XII, or Fe XV. These three excited states are formed at temperatures of 600 thousand, 1.5 million, and 2 million kelvins, respectively.

The fourth quadrant of the telescope reflects visible and ultraviolet light; a filter wheel near the focal plane selects this light from the regions of 6,000 to 30,000 kelvins. One piece of the surprising information yielded by TRACE's high-resolution images is that temperatures in the outer solar atmosphere vary from less than 30,000 to more than 2,000,000 kelvins over distances of only a few thousand kilometers.

Putting Observations Together

By combining observations taken at different wavelengths only a few seconds apart, scientists can follow the evolution of the sun's magnetic fields from the photosphere into the highest reaches of the corona. The quality of the images is further refined by internal stabilization of the telescope optics against spacecraft jitter.

To date, more than two million TRACE images have been captured and relayed to Earth for analysis. Viewed individually, combined into giant mosaics, or rapidly sequenced as time-lapse movies, the images have sparked a revolution in understanding solar atmosphere dynamics, especially those events occurring in the transition region and corona. "We're seeing for the first time how magnetic fields determine solar phenomena," says TRACE principal investigator Alan Title, solar astrophysicist at the Lockheed–Martin Solar and Astrophysics Laboratory and physics professor at Stanford University.



TRACE multilayers are made of extremely thin, alternating layers of molybdenum carbide and silicon, as seen in this electron micrograph at about 4 million times magnification.

Title says that aside from observations from a couple of five-minute rocket flights into the Earth's atmosphere, the sun's corona had not been seen with such resolution. "Suddenly, TRACE extended our observing window from five minutes to several years."

TRACE observations, he says, reveal a richly detailed portrait of the corona, where magnetic fields play a dominant role. Especially obvious are bright loops of different lengths of plasma that connect regions of opposite magnetic polarity.

"The images show that virtually all of the sun's loops have a structure at scales near or below the CCD camera's resolution of 1 arc second," says Title. "No one had appreciated that the solar atmosphere was as finely detailed and as rapidly evolving as we're seeing with the TRACE movies. We really hadn't expected so much information."

Title cites the light-gathering capabilities of the multilayer mirrors, which permit taking rapid sequences of images. "If you're only taking a picture every 15 minutes, magnetic waves with periods of a few minutes don't get recorded."

Important Data with Multiple Uses

The data are important to NASA and other agencies because magnetically induced solar events, such as flares and coronal mass ejections, can have huge consequences millions of miles away. Although they last only a couple of minutes, large flares emit enormous amounts of high-energy radiation and fast particles that can endanger astronauts, disrupt satellites in orbit, and even cause power outages in electrical grids on Earth.

The problem of flare emission and coronal mass ejection is sufficiently important that a National Sun Weather Program has been established. A better understanding of the physical processes in the outer solar atmosphere is also important to astronomers for understanding the processes of other stars and to magnetic fusion scientists for designing methods to confine hot plasmas and produce magnetic fusion energy.

The wealth of information contained in images from TRACE and other solar satellites was the focus of an international conference held at Monterey, California, in August 1999 that was attended by scientists from the U.S., Japan, China, Europe, Russia, and Canada. Barbee, who attended the conference, says the proceedings showed that TRACE observations are forcing a reconsideration of traditional theories underlying the physics of the sun and its atmosphere.

In particular, he says, TRACE movies are providing new insights into how the corona becomes heated to extremely high temperatures by magnetic fields. Astrophysicists have long been perplexed by the fact that the sun's outer atmosphere is so much hotter than its surface; computer models have not accounted for this heating satisfactorily.

Images and movies are not reserved for scientific investigators. TRACE is the first U.S. research mission with a completely open policy; all data are available to other scientists, students, and the general public soon after they become available to investigators. Sample movies of TRACE images can even be seen on the Internet at http://vestige.lmsal.com/TRACE/.

Barbee points out a final and seemingly unrelated payoff to the successful application of multilayers in solar astrophysics: computer chip manufacturing. Multilayer mirror coatings are a key technology for extreme ultraviolet lithography (EUVL), now under development by Lawrence Livermore and its industrial research partners. The technology promises manyfold increases in computer performance by shrinking the size of lines and features within chips. "The first images of the sun with multilayers in 1987 really put EUVL in motion," says Barbee. "We demonstrated we could get these resolutions, so the researchers pushed ahead in the lithography area."

From the vast atmosphere of the sun to the tiniest computer chips, multilayers are helping scientists push ahead on many fronts.

—Arnie Heller

Key Words: chromosphere, corona, extreme ultraviolet lithography (EUVL), multilayers, photosphere, sun, Transition Region and Corona Explorer (TRACE).

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Of Mice and Men

RODENTS and people may not appear to be closely related, but consider this the next time you look in a mirror: the genes of human beings and mice are 85 percent identical. This similarity is one of the reasons Lawrence Livermore scientists are studying mice. At Livermore's Human Genome Center, biomedical scientist Lisa Stubbs is leading a team that is studying the mouse genome to better understand the functions of human genes. Comparative genomics—analyzing and comparing the genetic material of different species—is viewed by bioscientists as an important method for studying evolution, the functions of genes (what they do and why), and inherited diseases.

Hunting Down Damaged Chromosomes

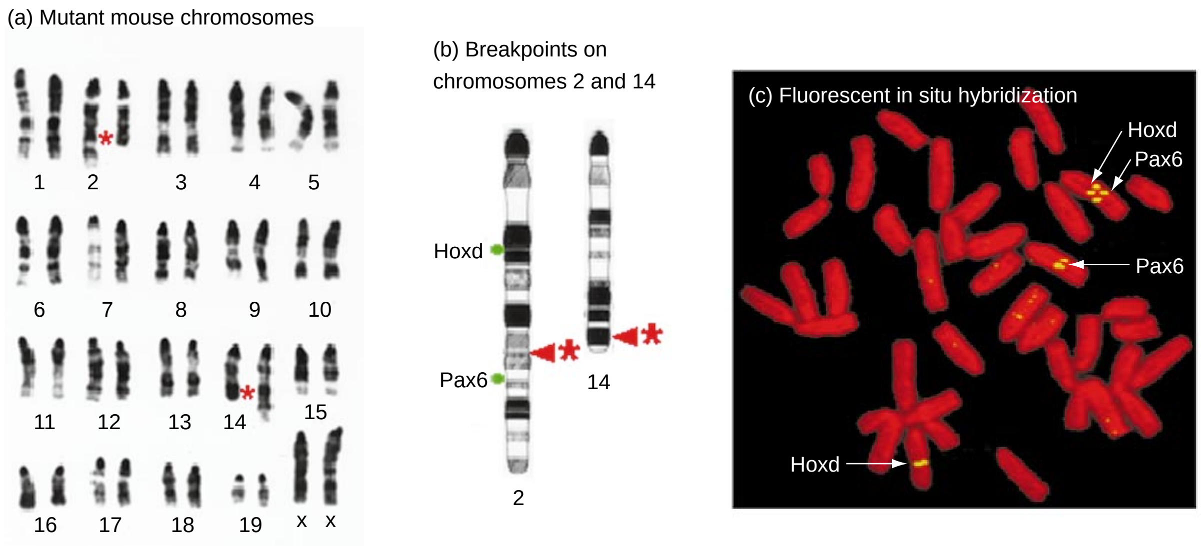
The mice used by Stubbs and her team were initially bred at the experimental mouse genetics facility at the Oak Ridge National Laboratory, one of the largest of such facilities in the world. It was originally established to conduct genetic risk assessment and toxicology studies. The mice brought to Livermore comprised some 130 unstudied mouse family lines, descendants of mice that were exposed years ago to radiation or chemicals for the purpose of studying the genetic effects of these agents. The offspring of the original mice were normal, although they were carriers of a mutation. But some of the descendants of those offspring, inheriting two copies of a mutated gene, showed anomalies (phenotypes) that are visible signs of the genetic mutations. Stubbs brought the carrier mice to Livermore in 1997 to identify inherited traits associated with the mouse lines and to find the genes disturbed by each mutation. "We look for phenotypes such as deafness, movement disorders, limb deformities, obesity, and susceptibilities to cancer," says Stubbs. If the trait is passed down to successive generations of a single mouse line, the team knows it is genetic.

Laura Chittenden, Lawrence Livermore biomedical scientist, with furry friend. This rotund mouse has a chromosomal defect in an unknown gene that leads to obesity.

To find out which gene is responsible, a researcher takes a small snip of skin from a mouse tail and grows the skin cells in a petri dish. Chromosomes from those cells are then spread on a microscope slide. In the laboratory, the researchers look for one particular kind of mutation called a translocation, which involves obvious changes in chromosome structure. Because the chromosomes are visibly disrupted, researchers can easily map the position of the mutated gene using only a simple light microscope. For example, the figure at right shows two mouse chromosomes—2 and 14—where such a translocation has occurred. "We knew immediately that the gene responsible for the trait would be found on one of those two chromosomes," Stubbs explains.

The researchers then use a procedure called fluorescent in situ hybridization (FISH), a technique for painting chromosomes with a fluorescent dye, to pinpoint the gene's location. They label a gene from a normal chromosome 2 with the fluorescent dye and add it to a slide containing the mutant mouse chromosomes. The labeled gene probe recognizes DNA sequences spread over the slide that are identical to its own and binds to the chromosome at that site. "In this way," Stubbs says, "we can map any gene relative to the translocation and 'trap' the mutated gene in a small, well-defined region."

The researchers repeat the process for other genes on chromosome 2 until they have narrowed down the "breakpoints," that is, the end pieces of the two broken and rejoined chromosome segments. Once they zero in on the chromosome section involved, they search the



Translocations are a type of mutation that change chromosome structure and can be detected by looking at stained chromosomes under a light microscope. In (a), a translocation involving mouse chromosomes 2 and 14—caused by breaking and rejoining of those two chromosomes—is shown. The mouse carrying these translocations has one normal (at left) and one mutant (at right) copy of each chromosome. (b) The locations of the chromosome breaks, marked by arrows, are determined by comparing the light- and dark-staining bands of normal vs mutant chromosomes. The break marks the location of the gene that no longer functions correctly. (c) To map the mutant gene more precisely, researchers paint genes from a normal chromosome (in this case, the genes Hoxd and Pax6 on chromosome 2) with fluorescent dyes and mix them with chromosomes spread over a microscopic slide. Here, both painted gene "probes" bind to a normal chromosome 2 that contains an identical sequence of them. But two other chromosomes show only one binding gene probe each, because the translocation has occurred in the region between the two genes and has separated them. The translocation maps the mutated gene to the region between Hoxd and Pax6 on chromosome 2.

Of Human Genes and the Department of Energy

Humans have 23 pairs of chromosomes that are made up of DNA (deoxyribonucleic acid), chemical characters arrayed in a particular order in a chain. The chromosomes contain the three billion characters that make up the human genome.

Sequencing is the work of determining the exact order of four individual chemical building blocks that form DNA. These four chemical bases—commonly abbreviated as A, G, C, and T—bind together to create base pairs of DNA molecules. After researchers sequence a piece of DNA, they search for the special strings of sequences that form genes.

The Department of Energy's Joint Genome Institute (JGI) combines the work of Lawrence Livermore, Lawrence Berkeley, and Los Alamos national laboratories. JGI operates around the clock as researchers work to determine the sequence of the information-carrying units that comprise the DNA of three human chromosomes—5, 16, and 19—as part of the international effort to decipher the human genetic code. The purpose is to understand the genetic basis of life. This understanding, in turn, will enable us to understand and attack the root causes of hereditary disorders and susceptibility to diseases such as cancer, heart disease, stroke, diabetes, schizophrenia, Alzheimer's disease, and many others. Because comparison to genomes of other, distant species such as the mouse aids in the discovery and analysis of genes embedded in the human sequence, the JGI will also contribute significantly to sequencing of the mouse genome. That sequencing is part of an international effort slated to proceed in earnest as the human sequence nears completion.

DNA sequence of that region to identify the genes that have been disrupted by the chromosome break.

"By the time we go to the DNA sequence and begin searching out individual genes," Stubbs says, "we know exactly which spot on the chromosome we must deal with." She continues, "When an organism is exposed to radiation or chemicals, we don't know ahead of time which genes will be affected. It's random, like potluck. All genes 'do something,' but some genes are less important than others—their activities affect our development or our health in very subtle ways. If such genes are mutated, we see no visible effects. Others genes, such as those that predispose someone to cancer or obesity, are essential, and their mutations have very obvious impact. All of our mice have mutations. But by focusing specifically on those

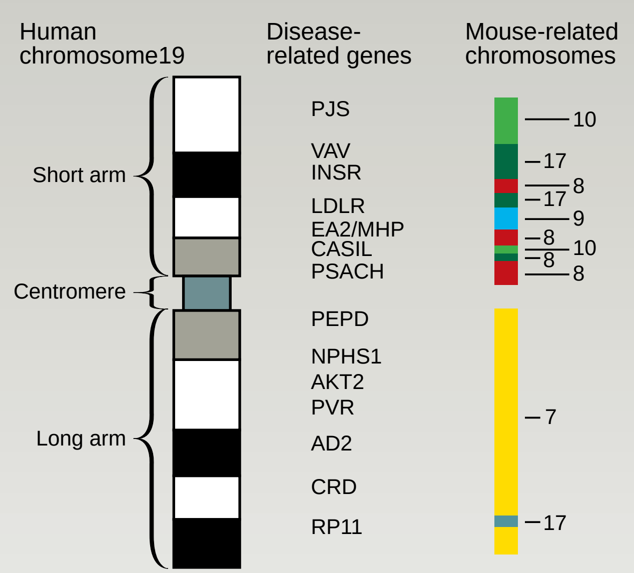
Similar but Different

Imagine taking human chromosomes, shattering them into pieces of varying lengths, and putting them back together in a different order. "That's what mouse chromosomes look like," says Lisa Stubbs, a Lawrence Livermore bioresearcher. For instance, as the figure shows, almost all of the long arm of human chromosome 19 is related to mouse chromosome 7. That is, the two chromosomal regions contain human and mouse versions of the same genes, organized roughly in the same order. In contrast, the short arm of human chromosome 19 comprises nine segments, each containing 20 to 100 genes and corresponding to different mouse chromosomes. Despite this scrambling of the genetic material, gene content and order within each mouse and human segment mirrors the other quite closely. Humans have this genetic material contained in 23 pairs of chromosomes, whereas mice have 20 pairs. But this difference reflects organization of genes and not their relative numbers.

Humans and mice also have about the same number of genes—now estimated to be approximately 140,000—and with some exceptions, each human gene has a clear and quite similar counterpart in the mouse. Those rare exceptions may prove to be quite important to the differences between humans and mice and must be understood more fully. For example, mice have some members of the cytochrome gene family that encode proteins needed to metabolize toxins, which humans do not possess. This genetic difference is reflected in the fact that mice and humans deal with certain toxins differently. Likewise, humans carry a gene encoding a protein called Apo(a) that plays an important role in developing atherosclerosis. Normal mice do not have the gene and never exhibit the symptoms of this deadly cardiovascular disease.

However, these species-specific genes altogether account for roughly 1 percent or less of the two gene sets and do not determine all the differences between humans and mice. The major differences between the species arise from the wide variation in the coding sequences of the counterpart genes. When the average 15 percent difference in mouse and human protein coding sequences is multiplied by 140,000 genes, the overall genetic difference is quite significant.

Not all genes are indispensable, and many of the differences found when mouse and human genes are compared have little effect on our biology. Many living organisms, including humans, carry single-gene changes and chromosomal defects such as translocations (swapped bits) and deletions (missing bits). These changes can mean nothing, or everything. "Consider," says Stubbs, "that because of the large coding capacity and complexity of the genome, a mere 15 percent difference in genes gives you a completely different organism—a human instead of a mouse. But turning the tables around, it is also quite remarkable that humans and mice are as genetically similar as we actually are."



That the human and mouse genomes are both similar and different is shown here. The long arm of human chromosome 19 has a close counterpart in mouse chromosome 7—the human and mouse versions of the same genes (see middle column) are found in them in roughly the same order. However, genes in human chromosome 19's short arm correspond to mouse versions that are located in many different mouse chromosomes, as indicated by colored bars to the right, labeled by chromosome number.

with visible abnormalities, we are aiming at those genes that play the most important roles in maintaining health."

Tracking a Cancer Gene

One case the team researched involves a particular kind of stomach cancer known as adenocarcinoma. In some cases, this cancer begins with the *Helicobacter pylori* bacteria commonly found in human stomachs. Although many people carry these bacteria, only some develop chronic gastritis—a painful inflammation of the stomach lining. If the bacterial infection is left untreated, many of the infected will develop a low-grade stomach lymphoma, which can progress with time. A small but significant percentage of lymphoma patients will eventually develop adenocarcinoma if the bacterial infection persists long enough. "We know," says Stubbs, "that whether or not one develops gastritis and cancer is determined at least in part by genetic predisposition. However, no one knows which genes encode these predisposing factors."

The stomach cancer issue arose when Stubbs identified a family of mice susceptible to gastritis, lymphoma, and adenocarcinoma. "This mouse mutant family develops a disease that looks precisely like what has been documented in susceptible, *Helicobacter*-infected people," says Stubbs. "These mice therefore provide a unique model for tracing the elusive genetic susceptibility factors."

The first thing the researchers did was to raise this mouse family in an environment without *Helicobacter* or other known pathogenic bacteria. "Although mice that have been exposed to bacteria quickly develop lymphoma," she says, "these pathogen-free animals did not. However, they did exhibit precancerous changes in cells of the stomach lining. We are observing some of those animals over time to see if the precancerous changes will progress to adenocarcinoma. Our hypothesis is that the genetic defect carried by these mice makes them susceptible to infection. But because they develop precancerous lesions without bacteria, the mutation must also mimic the effects of bacterial infection in some unknown but important way."

Using the FISH technique, they tracked down a mutation in a gene that produces a component of the mucus normally coating the intestinal lining. The mutant mice turn this gene on in the wrong location—the stomach—and have the properties of their stomach linings altered in significant ways. "It may be," says Stubbs, "that people who have a defect in the corresponding human gene may also have a higher susceptibility to this kind of stomach cancer. We hope to verify this possibility in future research."

For the Future: Playing Off the Strengths

On the one hand, much less sequencing has been completed for the mouse than for the human genome. On the other hand, a wealth of knowledge exists regarding the inheritance of genetic traits in mice.

Every family has some undesirable hereditary trait—whether near-sightedness, obesity, asthma, allergies, high cholesterol, or other ailments. In such cases, says Stubbs, it's almost impossible to see the pertinent genetic signal over the general noise of random—and often unimportant—changes that distinguish our highly varied genomes. Humans are a heterogeneous population with a huge amount of genetic variation—some important, some not. Which change is the one that accounts for the asthma, the obesity? "Mutant mice will help us find out," says Stubbs. "We can study groups of mice that are genetically identical, like identical twins, except that one mouse carries a mutation in a single, unknown gene. Because the background is stable, we can follow the activities of that single gene with good certainty. We study the pathology of the mutant mouse, track down the gene involved, and then identify its human counterpart to study whether that gene plays a role in human diseases with similar pathology [see box on p. 16 for comparison of mouse and human genes]. Knowing which gene is responsible for a health disorder is the first step toward designing treatments to alleviate the condition."

The mouse is a powerful genetic model that is being used worldwide for gene-function studies. As new information about human genes is developed at the Department of Energy's Joint Genome Institute and through the international sequencing effort, there will be more and more new genes to study and understand. And as more and more health-related genes—such as those for obesity, deafness, and developmental disorders—are discovered first in the mouse, the power of studying a human gene through its mouse counterpart is increasingly obvious. Stubbs sums it up this way: "It's very exciting to be working at the center of the next wave of genome research."

—Ann Parker

Key Words: adenocarcinoma, chromosome, comparative genetics, DNA, fluorescent in situ hybridization (FISH), gene, Human Genome Center, Joint Genome Institute, translocation.

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For more genetic research information, see these Web sites:
http://wwwbio.llnl.gov/genome/genome.html.
http://www.jgi.doe.gov/JGI_about.html.
http://www.ornl.gov/TechResources/Human_Genome/publicat/primer/intro.html.

Experiment Mimics Nature's Way with Plasmas

FOR the past decade, most research in magnetic fusion energy has centered on the doughnut-shaped tokamak approach to generating fusion reactions. Tokamak work continues in the United States and abroad, but Department of Energy fusion energy scientists are also revisiting the spheromak, an alternative concept for attaining magnetic fusion.

Much of the renewed interest in spheromaks is focused on a research effort at Lawrence Livermore called the Sustained Spheromak Physics Experiment (SSPX). The SSPX was dedicated on January 14, 1999, in a ceremony attended by representatives from DOE and collaborating scientists from the Sandia and Los Alamos national laboratories. SSPX is a series of experiments designed to better determine the spheromak's potential to efficiently contain hot plasmas of fusion fuel, in this case, the hydrogen isotope deuterium.

According to SSPX leader David Hill, the tokamak concept is considered the leading contender to generate sustained fusion reactions by heating plasmas to more than 100 million degrees Celsius (much hotter than the core of the sun) and confining them with magnetic fields. However, the tokamak's magnetic fields are generated by large, external magnetic coils surrounding the doughnut-shaped reactor. These large coils would increase the cost and complexity of generating electricity.

Spheromaks, however, confine hot plasma in a simple and compact magnetic field system that uses only a small set of external stabilizing coils. The necessary strong magnetic fields are generated inside the plasma by what's known as a magnetic dynamo. In this regime, the plasma—fast-moving, superhot ions and electrons—produces its own confining magnetic fields. The magnetic fields pass through the flowing plasma and generate more plasma current, which in turn reinforces the magnetic fields.

The powerful internal currents and magnetic fields become aligned so that they are nearly parallel to each other. Together, they form what Hill describes as something akin to a very hot smoke ring made of electrical currents.

Simple Design, Complex Behavior

"The beauty of a spheromak is that the main magnetic fields are generated by the plasma itself. It's a physical state the plasma wants to make naturally," Hill says. Indeed, the spheromak state is produced by the same mechanisms responsible for the behavior of galactic jets, solar prominences, and Earth's molten magnetic core.

Many scientists believe the spheromak's simple design and lower operating costs make it a potentially better candidate than the tokamak for a power-producing fusion reactor. "Tokamaks are big and expensive," says Hill. "If one coil goes down, it's a big repair job."

Technician Richard Kemptner adjusts the high-voltage lines that initiate the plasma in the 1-meter-diameter vacuum vessel.

Although the physical spheromak design is simple, its dynamo activity produces plasma behavior that is extremely complex and more difficult to predict and control than that found in tokamaks. Livermore researchers are guided in understanding this plasma behavior by accumulated theoretical expertise and by CORSICA, an advanced Livermore simulation code developed over the past decade. (See *S&TR*, May 1998, pp. 20–22.)

The SSPX is the latest of the experiments in magnetic fusion energy research that date back to Lawrence Livermore's founding in 1952. Over the years, Lawrence Livermore scientists performed some of the pioneering spheromak work, along with Los Alamos National Laboratory and other DOE and university research centers.

Enthusiasm for spheromaks waned in the early 1980s, however, when experiments at Los Alamos and other facilities achieved lower temperatures than experiments using tokamak designs. As a result, the nation's magnetic fusion research community focused on advancing the tokamak design, while spheromak research continued in Japan and Great Britain.

Reanalysis Revived the Concept

Interest in reviving the spheromak concept was triggered by a review of data from key Los Alamos experiments conducted more than 10 years ago. A thorough reanalysis led by Ken Fowler and Bick Hooper, former associate director and the assistant associate director, respectively, for Magnetic Fusion Energy at Livermore suggested that the plasma's energy confinement was up to 10 times better than originally calculated.

The analysis also showed that plasma confinement improved as the temperature increased. The thinking, says Hill, is that as temperatures increase in the spheromak, electrical resistance in the plasma decreases, so fusion reactions can occur more easily.

In light of the reanalysis, the scientific community and DOE managers considered it worthwhile to pick up where the Los Alamos experiments left off some 10 years earlier. Hill notes that the experiment is one of several alternative concepts being supported by DOE's Office of Fusion Energy Sciences, concurrent with its funding of tokamak research. (The Lawrence Livermore spheromak research is also supported by the Laboratory Directed Research and Development program.)

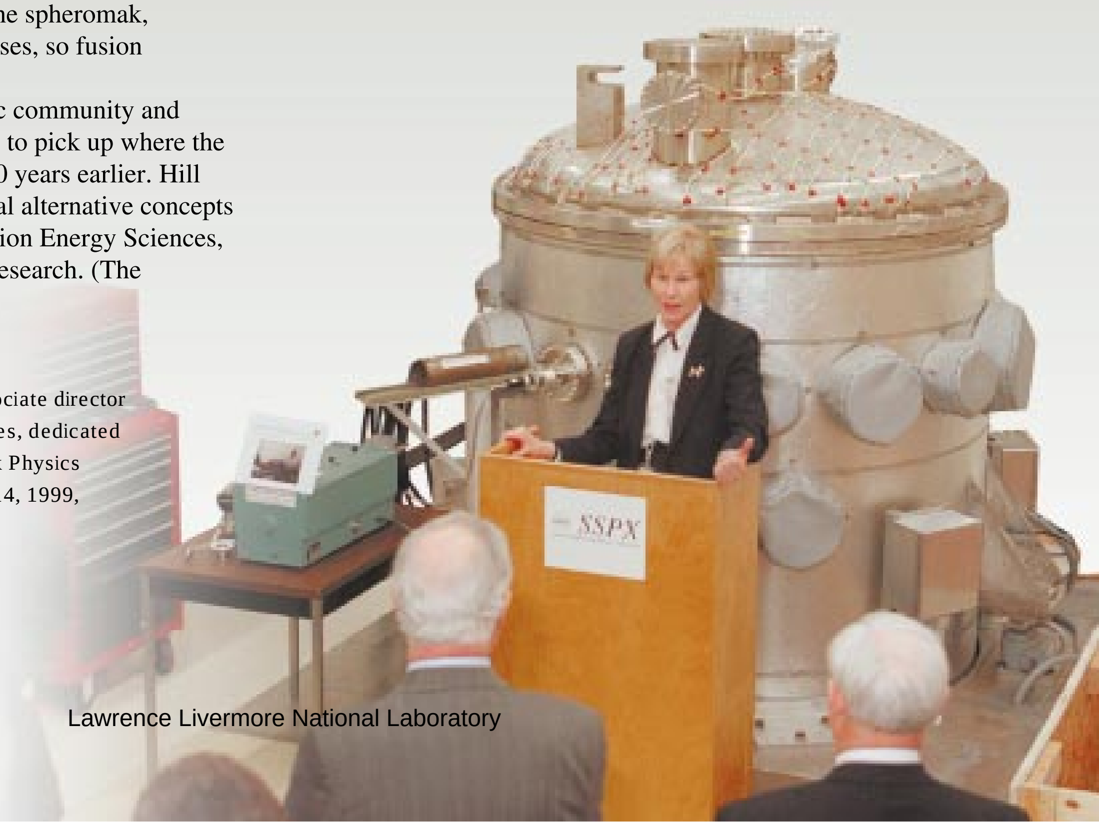
The overall goal of SSPX is to better understand spheromak physics by studying how magnetic fluctuations affect confinement. The experiments are designed to reach plasma temperatures of about 4 million degrees Celsius, similar to what the Los Alamos experiments obtained. Although this temperature is some 25 times cooler than that necessary to achieve fusion, it is sufficiently hot that energy is lost by processes similar to those that would occur in a fusion reactor. The experimental team will also attempt to keep the dynamo maintained in a hot plasma for 2 milliseconds instead of the 0.5 milliseconds achieved at Los Alamos.

The team is in the early phases of the project and is performing activities such as learning how to form the deuterium plasmas, achieving vacuum conditions, removing plasma impurities, and debugging diagnostic instruments.

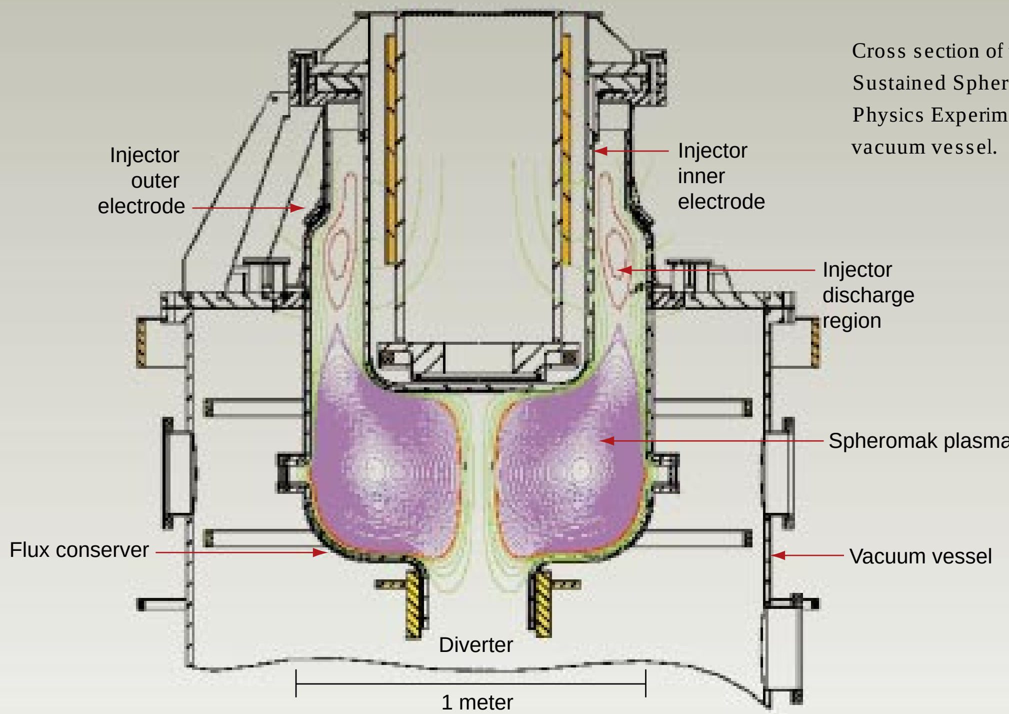
Measuring Hot, Moving Currents

The experiments involve injecting deuterium plasma into a reactor's 1-meter-diameter by 0.5-meter-high vacuum vessel. A 10-kilovolt, 0.5-megajoule startup capacitor bank supplies a voltage across two electrodes to form the deuterium plasma. A separate 5-kilovolt, 1.5-megajoule power system sustains the plasma for 2 milliseconds. During this brief moment, the plasma balloons down into the vessel, forming a hot, moving circular current of ions that creates magnetic fields, which in turn induce more current within the plasma.

Improving the understanding of spheromak physics requires accurate measurements of plasma density, temperature, turbulence, and magnetic field fluctuations. Because probes inserted into the plasma would disrupt the



Anne Davies, DOE's associate director for Fusion Energy Sciences, dedicated the Sustained Spheromak Physics Experiment in a January 14, 1999, ceremony.



Cross section of the Sustained Spheromak Physics Experiment (SSPX) vacuum vessel.

experiments, the researchers must rely on remote measurements taken through a slot located around the spheromak's center.

One measurement instrument, called a reflectometer, was designed by scientists at Lawrence Livermore and the University of California at Davis. It yields profiles of the magnetic field strength by injecting waves of varying polarized light into the plasma. The reflected waves carry information about the changing plasma density and the magnetic fields. Another measurement instrument injects a glass pellet across the plasma; a laser views the pellet and determines the magnetic field from the reflected light.

Hill notes that although situated at Livermore, the SSPX work benefits from contributions from colleagues at Los Alamos, Sandia, General Atomics, California Institute of Technology, University of California at Berkeley and at Davis, University of Wisconsin, University of Washington, and Swarthmore College. He adds that SSPX also benefits from the wealth of information about plasmas that has been gained from the past decade of tokamak studies.

In light of the extensive collaborations with researchers from other institutions, the experiment control room is equipped with video cameras that permit collaborators to view experiments remotely from their computers. The video cameras are part of a system developed by Livermore researchers to link magnetic fusion experimental sites nationwide.

If the results from SSPX are sufficiently promising, the research team will develop a larger, follow-up experiment. This experiment would aim at achieving much hotter, longer lasting plasmas.

Clearly, many experts are speculating that the method nature chooses to confine plasmas in space may well be the process scientists should mimic in designing a fusion reactor to generate electricity on Earth.

—Arnie Heller

Key Words: CORSICA, deuterium, dynamo, magnetic fusion energy, plasma, spheromak, Sustained Spheromak Physics Experiment (SSPX), tokamak.

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Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Richard W. Pekala Steven T. Mayer James L. Kaschmitter Robert L. Morrison	**Method for Making Thin Carbon Foam Electrodes** U.S. Patent 5,932,185 August 3, 1999	A method for fabricating thin, flat carbon electrodes by infiltrating highly porous carbon papers, membranes, felts, metal fibers and powders, or fabrics with an appropriate carbon foam precursor material. The infiltrated carbon paper, for example, is then cured to form a gel-saturated carbon paper that is subsequently dried and pyrolyzed to form a thin sheet of porous carbon. The material readily stays flat and flexible during curing and pyrolyzing to form thin sheets. Precursor materials include polyacrylonitrile, polymethylacrylonitrile, resorcinol–formaldehyde, catechol–formaldehyde, phenol–formaldehyde, etc., or mixtures thereof. These thin films are ideal for use as high-power energy electrodes in batteries, capacitors, and fuel cells and are potentially useful for capacitive deionization, filtration, and catalysis.
Anthony F. Bernhardt Vincent Malba	**Attachment Method for Stacked Integrated Circuit (IC) Chips** U.S. Patent 5,933,712 August 3, 1999	A method for connecting stacked integrated circuit (IC) chips, such as DRAM memory chips. Pads on the individual chips are rerouted to the side of the chip. When the chips are stacked on top of each other, the side-located pads can be used to form interconnections to other chips or to a circuit board. The side pads are connected to metal lines on a flexible plastic tape (flex) using anisotropically conductive adhesive (ACA). The metal lines on the flex are likewise connected to other pads on chips and/or to pads on a circuit board. In the case of a stack of DRAM chips, pads to corresponding address lines on the various chips may be connected to the same metal line on the flex to form an address bus. This method has the advantage of reducing the number of connections to circuit boards required by busing. The flex can accommodate dimensional variation in the alignment of chips in the stack. The bonding of the ACA is accomplished at low temperature and is otherwise simpler and less expensive than solder bonding; chips can be bonded to the ACA all at once if the sides of the chips are substantially coplanar, as in the case for stacks of identical chips such as DRAM.
Thomas C. Kuklo	**Concentric Ring Flywheel without Expansion Separators** U.S. Patent 5,941,132 August 24, 1999	A concentric ring flywheel configured to eliminate the need for differential expansion separators between its adjacent rings. In this configuration, a circumferential step is formed on an outer surface of an inner concentric ring and a matching circumferential step is formed on the inner surface of an adjacent outer concentric ring. During operation, the circumferential steps allow the rings to differentially expand without forming gaps that then need expansion separators to take them up.
David J. Erskine	**Multichannel Heterodyning for Wideband Interferometry, Correlation, and Signal Processing** U.S. Patent 5,943,132 August 24, 1999	A method for processing a high-bandwidth signal by coherently subdividing it into many narrow-bandwidth channels for individual processing, in parallel, at lower frequencies. Phase and amplitude information about the original frequencies is preserved. This multichannel heterodyning can be used to interfere, correlate, autocorrelate, delay, filter, record, and synthesize waveforms as well as combinations of these processes. This invention allows the use of inexpensive, low-bandwidth and low-frequency signal processing components to manipulate signals of much higher bandwidth and frequency. Furthermore, signal comparisons can be performed using reference frequencies that may slowly drift. Not requiring stabilization of this drift reduces device costs.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Robert J. Deri Eugene D. Brooks III Ronald E. Haigh Anthony J. DeGroot	**Massively Parallel Processor Networks with Optical Express Channels** U.S. Patent 5,943,150 August 24, 1999	An optical method for separating and routing local and express channel data. Nodes in a network are interconnected with fiber-optic cables that carry both express channel traffic and local channel traffic. Express channel traffic is placed on, or filtered from, the fiber-optic cable at a light frequency (color) different from that of the local channel traffic. On its light carrier, the express channel traffic skips over local nodes one by one by reflecting off mirrors selectively placed at each local node. The local-channel-traffic light carriers, on the other hand, pass through the mirrors. A single fiber-optic cable can thus be threaded throughout a three-dimensional matrix of nodes with the *x*, *y*, and *z* directions of propagation color-encoded for local or express channel traffic. This frequency division multiple access eliminates the bucket-brigade latencies that would result if express traffic had to hop between every local node to reach its ultimate destination.
Abraham P. Lee Peter A. Krulevitch M. Allen Northrup	**Micromachined Electrical Cauterizer** U.S. Patent 5,944,717 August 31, 1999	A micromachined electrical cauterizer, in which microstructures are combined with microelectrodes for highly localized electrocauterization. The microcauterizer is fabricated by bulk-etching silicon to form knife edges, then aligning parallel microelectrodes adjacent to the knife edges. While most of the microelectrode lines are electrically insulated from the atmosphere by depositing and patterning silicon dioxide on the electric feedthrough portions, a window is opened in the silicon dioxide to expose the microelectrodes. This helps reduce power loss and assists in focusing the power locally for more efficient and safer procedures.

Awards

Jack Campbell, lead scientist for optical materials research and development for the National Ignition Facility (NIF), recently received the **1999 Otto Schott Research Award** at the European Society of Glass Conference in Prague, Czech Republic. The award is named after the famous 19th-century German glass chemist and is given for “exemplary new research work in the field of glass and glass ceramics.”

Campbell and his research group have focused on working with industry to develop technology for making large, high-quality laser glass for Lawrence Livermore’s inertial confinement fusion lasers—Nova, Beamlet, and NIF.

Campbell joined the Laboratory in 1975 after receiving his Ph.D. in physical chemistry from the University of Illinois at Champaign–Urbana and his bachelor’s degree from Rochester Institute of Technology.

Jack Kolb has been elected **president** of the **Livermore chapter of Sigma Xi**, the national scientific research society. With about 85 members, most of them employees or retirees from Lawrence Livermore and Sandia National Laboratories/California, the chapter’s activities over the past year have most notably included cosponsorship of Livermore’s Science on Saturday lecture series and presenting awards at the Tri-Valley Science and Engineering Fair. Kolb said, “We seek to continue those activities, particularly youth education and science outreach activities, and are interested in expanding efforts to further the cause in pursuit of science whenever we can.”

Serving with Kolb on the chapter’s board are **Ron Weinberg** of the Classification Office, elected vice president; **Harold Ackler** of the Electrical Engineering Department, elected treasurer; and **Jack Harrar** of the Environmental Protection Department, reelected secretary.

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Abstract

The Internal Combustion Engine at Work—Modeling Considers All Factors

Livermore scientists have been modeling the inner workings of the internal combustion engine for almost 25 years. They developed HCT (hydrodynamics, chemistry, and transport), a chemical kinetics code, specifically for modeling the combustion process. Combustion modeling is invaluable for several projects today. For the Homogeneous Charge Compression Ignition engine, a cross between the spark-ignition and diesel engines, modeling is helping to determine the best way to control ignition timing, which is now the limiting factor for the engine. Modeling was important in developing the Plasma-Assisted Catalytic Reduction process for treating emissions from diesel engines; it determined what the plasma can and cannot do. Yet another project is using the HCT code to simulate ignition and unburned hydrocarbon production in advanced diesel engines running on oxygenated fuels.

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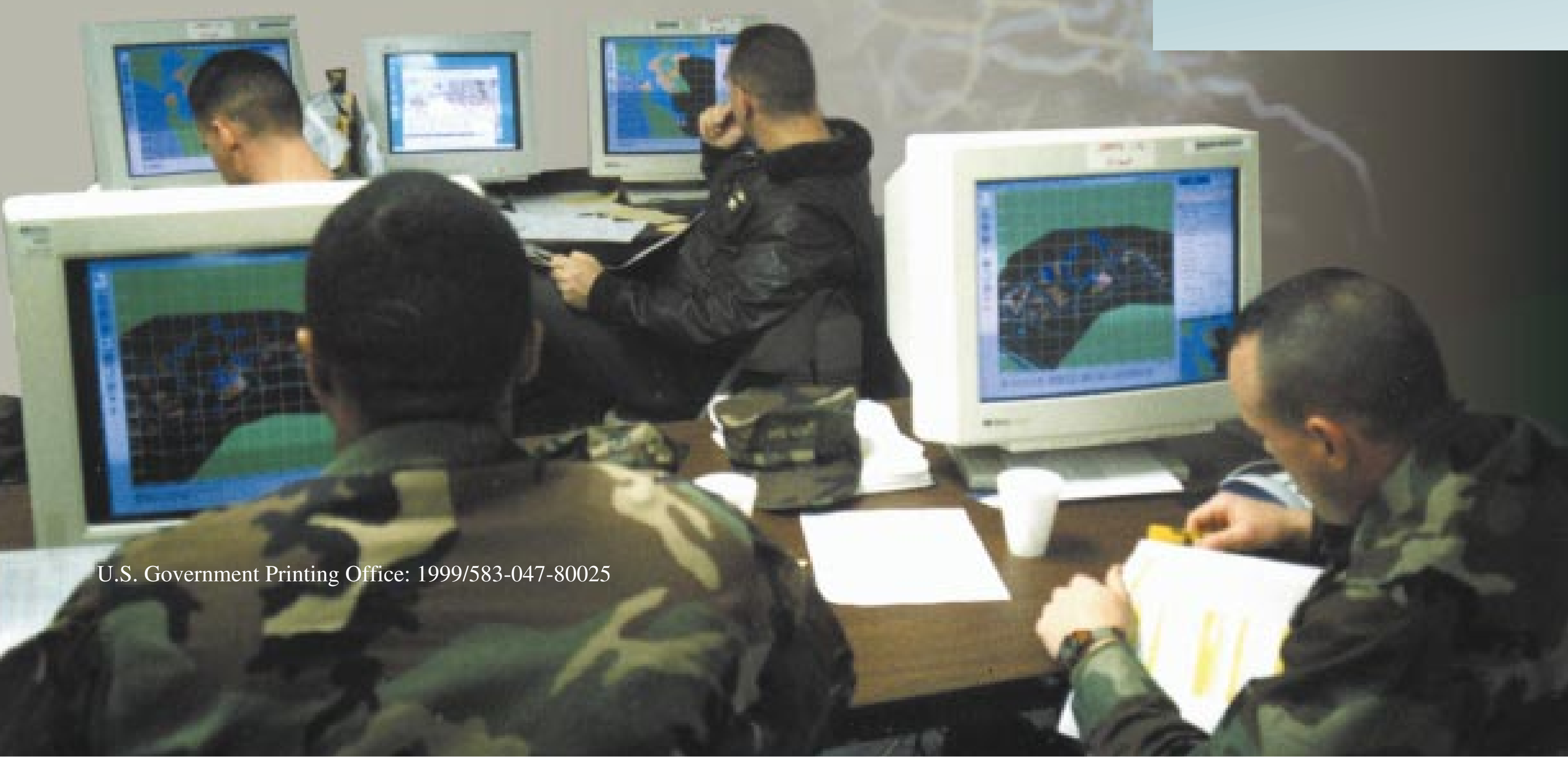
Coming Next Month

Livermore's Conflict Simulation Capabilities Pass a Major Test

The powerful combat simulation program JCATS (Joint Conflict and Tactical Simulation) was put to a major test in a San Francisco Bay Area exercise.

Also in January/ February 2000

- *Understanding the complex hydrodynamics of the death of stars.*
- *Agile manufacturing technologies that meet the U.S. Army's variable and changing munitions needs.*
- *HyperSoar, an aircraft concept that could revolutionize air travel.*



U.S. Government Printing Office: 1999/583-047-80025