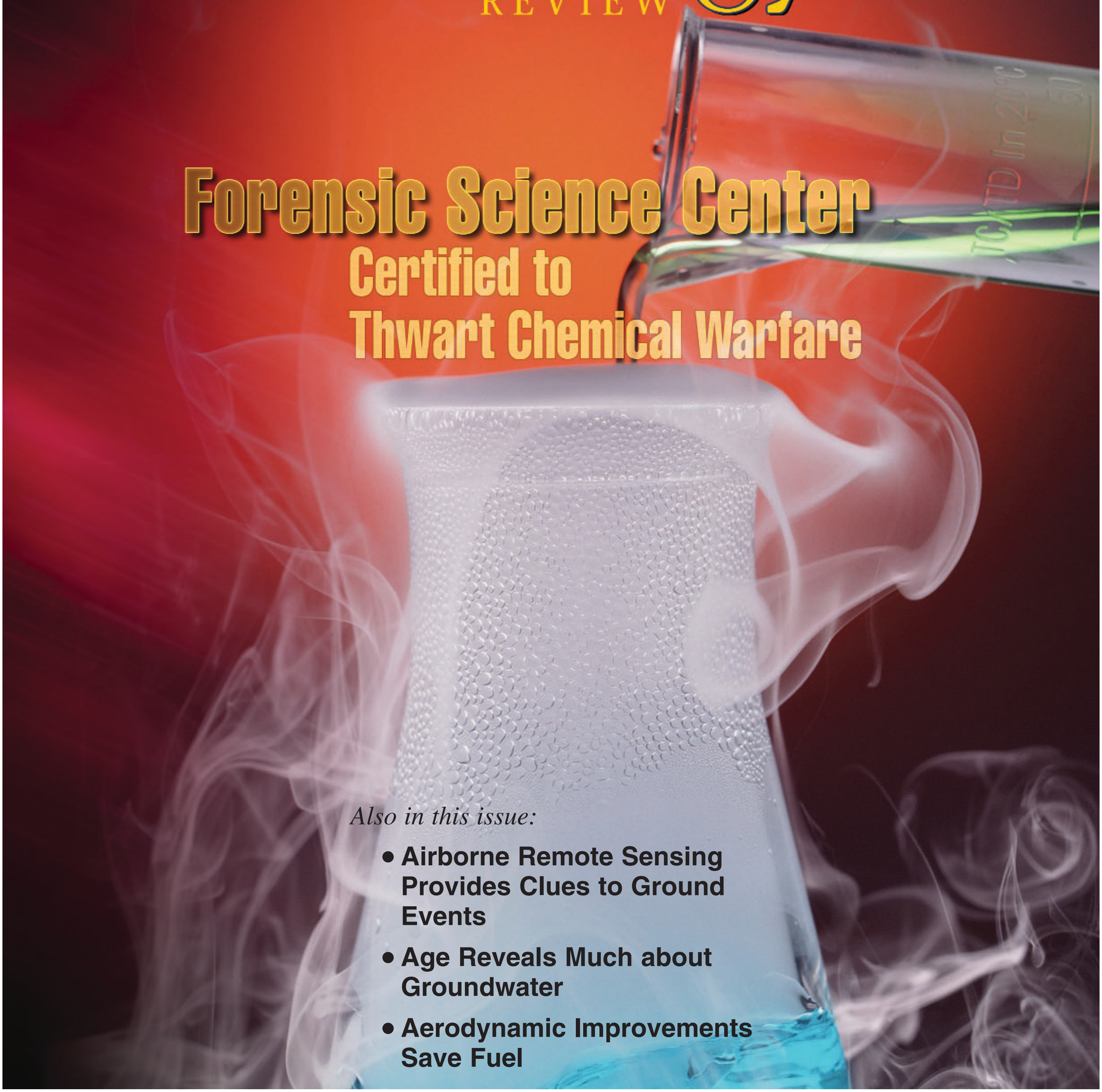
Science & Technology REVIEW

May 2003

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory



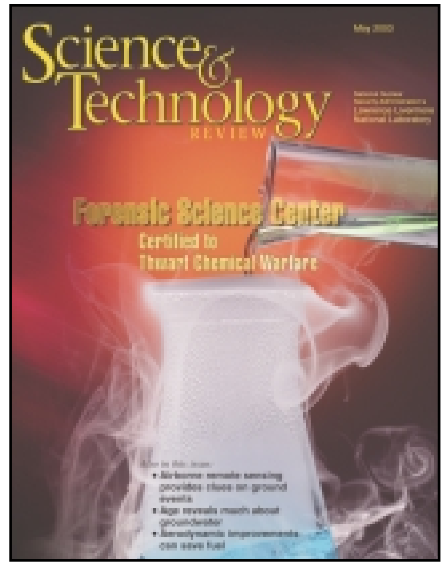
Forensic Science Center Certified to Thwart Chemical Warfare

Also in this issue:

- Airborne Remote Sensing Provides Clues to Ground Events
- Age Reveals Much about Groundwater
- Aerodynamic Improvements Save Fuel

About the Cover

Scientists in Livermore's Forensic Science Center passed three difficult proficiency tests given by the Organisation for the Prohibition of Chemical Weapons to prove their capabilities for detecting minute quantities of chemical warfare agents, their precursors, or decomposition products. For that accomplishment, the Forensic Science Center became one of two laboratories in the U.S. certified to support the international treaty banning chemical warfare weapons. The article beginning on p. 4 describes the proficiency test process and discusses the protocols for detecting chemical warfare compounds.



Cover design: Amy Henke

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. 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.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str/.

NNSA
National Nuclear Security Administration

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

Science & Technology Review

May 2003

Lawrence Livermore National Laboratory

S&TR Staff

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

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

Printed in the United States of America

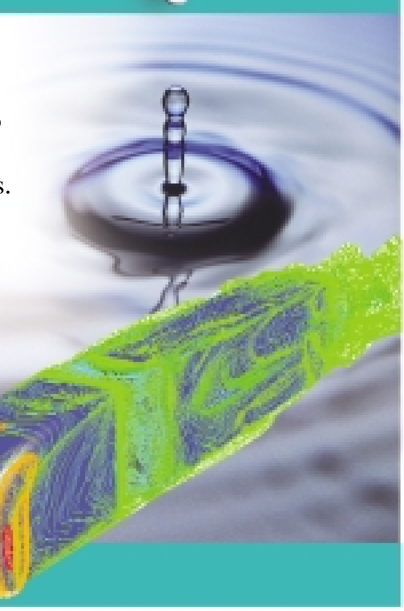
Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-52000-03-5
Distribution Category UC-99
May 2003

Contents

Features

Research Highlights



Departments

Human effects on the Great Barrier Reef

Stewart Fallon of the Laboratory's Center for Accelerator Mass Spectrometry collaborated with researchers from Australian National University and the Australian Institute of Marine Science to study the geochemistry of coral in the Great Barrier Reef. In the February 13, 2003, issue of *Nature*, they published findings concluding that in the 150 years since the first Europeans settled along the Australian coast, the settlers' land-use practices have led to a major degradation of the semiarid region and resulted in substantially increased amounts of sediment entering the Great Barrier Reef.

The researchers studied coral by measuring barium content within the coral skeleton, using a technique called laser ablation inductively coupled plasma spectrometry. Barium deposits can provide good records of how much sediment enters the reef. The barium comes loose from fine-grained particles in a low-salinity region of the estuary and is carried with a flood plume into the coral skeleton. Measurements of a 5.3-meter core from the Havannah coral reef showed a significant increase in barium beginning around 1870, about two decades after European settlers arrived in northern Queensland and began clearing land for raising sheep and cattle.

The *Nature* report warns that reducing sediment discharges must be a high priority if coral reefs are to survive the lethal combination of human-use effects and rapid climate change.

Contact: Stewart Fallon (925) 422-4396 (fallon4@llnl.gov).

More discoveries about neutron stars

An international group of researchers, which includes Laboratory astrophysicist Diego Torres, has shown through computer simulations that accreting neutron stars can be a source of high-energy neutrinos. The neutrinos—particles that rarely interact with other matter—are produced in amounts significant enough that they are expected to be detected by next-generation neutrino telescopes.

A neutron star is one possible end-point in the evolution of a massive star. In some binary star systems, two neutron stars are so close together that the strong gravity from one can steal gas from the other. The gas transfer onto a neutron star is accretion; it is a turbulent, shiny event.

Neutron stars have long been viewed as physics laboratories in space because they provide insights into the nature of matter and energy. Torres and his colleagues believe that astronomers will be able to use IceCube—an international high-energy neutrino observatory being built for installation in the deep ice below the South Pole—to detect neutron star neutrinos. This would mark the beginning of multiparticle astronomy, where photons in all wavelengths and neutrinos are detected at the same time.

Torres's collaborators include scientists from Northeastern University, Instituto Argentino de Radioastronomia, and the Max Planck Institut für Kernphysik. Their research is presented in the May 20, 2003, edition of *Astrophysical Journal*.

Contact: Diego Torres (925) 423-0750 (torres25@llnl.gov).

Containment of a fowl disease

A partnership of researchers from Livermore, the University of California at Davis, the California Animal Health and Food Safety Laboratory, and the U.S. Department of Agriculture has developed a rapid diagnostic assay to detect Exotic Newcastle Disease (END), a virus that has been attacking poultry in California and Nevada. The new assay, which is faster and more precise, is based on DNA fingerprinting methods that Livermore perfected for use in detecting bioterrorism. It can provide test results overnight, in contrast to the 6 to 12 days previously needed to identify infected birds.

The test is based on the polymerase chain reaction, a method of multiplying DNA. Livermore scientists use powerful computers to compare the multiplied DNA sequences of a pathogen with those of close genetic kin to discover the DNA regions, or signatures, that are unique to the pathogen. Scientists can then design an assay that includes fluorescent probes that signal the presence of a signature.

Developing an assay for END was challenging because its chromosome is made of RNA rather than DNA and because close cousins of the virus were hard to find. "These are very interesting pathogens," says Paula McCready, head of Livermore's DNA signature team. "They mutate quickly so it's difficult to find those regions that are unique to the virus."

Use of the new test spared 170,000 layer hens in Riverside County from euthanasia. The assay showed that the quarantined hens did not have END but were instead infected with a nonvirulent strain.

Contact: Paula McCready (925) 422-5721 (mccready2@llnl.gov).

Another Weapon in the Battle against Proliferation

WITH so much focus recently on homeland security and counterterrorism, it's easy to overlook the continuing importance of arms control treaties and the role played by Livermore's technologies and analytical capabilities in supporting them. Indeed, the strength of test ban treaties and arms reduction agreements rests, in large part, on the technical capabilities available for monitoring compliance.

Lawrence Livermore has a more than 40-year history of research and development in support of nuclear test ban treaties. The Laboratory played a major role during the original Comprehensive Test Ban Treaty (CTBT) discussions in the 1960s, the trilateral CTBT talks in the 1970s, the renegotiation of the Protocol to the Threshold Test Ban Treaty in the 1980s, and the more recent CTBT negotiations of the 1990s. Today, the Laboratory is a key participant in the national program to provide the U.S. government with the technical capabilities needed for worldwide nuclear explosion monitoring.

The Laboratory has also been involved in developing technologies to monitor nuclear arms reduction treaties and material disposition agreements. The sticking point in all of these negotiations is the need to measure attributes of classified objects while preventing the disclosure of sensitive weapons design information. To overcome this obstacle, Livermore has developed and demonstrated novel radiation detection instrumentation, data interpretation algorithms, information barriers, and monitoring procedures suitable for use by inspection personnel from the U.S., Russia, and the International Atomic Energy Agency.

Now, as described in the article beginning on p. 4, Livermore's Forensic Science Center has been certified to support the Chemical Weapons Convention (CWC). Unlike the nuclear treaties, which limit testing and the number and types of permitted weapons, the CWC bans an entire class of mass-destruction weapons. It outlaws the development, production, acquisition, stockpiling, and use of chemical weapons. Parties to the CWC must destroy any and all chemical weapons stockpiles and production facilities. Also banned is the transfer of chemical-weapon-related technologies to other countries or groups. The CWC is the first arms control treaty to widely affect the private sector. Because many of the chemicals of concern have legitimate civilian uses, industrial facilities, not just government sites, are subject to inspections.

The Organisation for the Prohibition of Chemical Weapons (OPCW), headquartered in The Hague, Netherlands, is responsible for implementing the CWC. More than a dozen OPCW-designated laboratories have been set up around the world, including two in the U.S.: one at the U.S. Army's Edgewood Chemical and Biological Forensic Analytical Center in Maryland and the other at Lawrence Livermore. OPCW requires that samples from sites under challenge by chemical weapons inspections be analyzed by two OPCW-certified laboratories, and U.S. legislation requires that all samples collected in the U.S. be analyzed within the country. Thus, two OPCW-certified laboratories in the U.S. are needed.

Endorsed by the departments of Energy, State, and Defense and the National Security Council, Livermore was selected to be the second U.S. OPCW-designated laboratory because of its unique capabilities in chemical analysis and forensic characterization of unknown samples. The work required for OPCW is technically challenging—analyzing samples for traces of any of thousands of possible compounds (chemical warfare agents, precursor chemicals, decomposition products), often in the presence of other compounds that complicate or confound the analysis; synthesizing the identified chemicals to verify the analysis; and reporting results—all in the space of 15 days. Clearly, this isn't your usual chem lab.

As current events in Iraq highlight, the threat posed by the acquisition and likely use of chemical weapons by rogue states or terrorists is all too real. Lawrence Livermore is working the entire spectrum of problems caused by weapons of mass destruction (WMD) proliferation and terrorism. Technical capabilities for detecting and characterizing activities indicative of WMD production are critical to national and global security. Certification by OPCW to support challenges during chemical weapons inspections is one more way the Laboratory is fighting against WMD proliferation and terrorism.

■ Wayne Shotts is associate director for Nonproliferation, Arms Control, and International Security and acting director for the Homeland Security Organization.

Chemical Weapons Can't Evade This Lab

Livermore's Forensic Science Center is certified to support the treaty that bans chemical weapons.

LAWRENCE Livermore has been among the leaders in supporting national and world efforts to detect chemical weapons and thwart their proliferation. In February, the international Organisation for the Prohibition of Chemical Weapons (OPCW) certified Livermore's Forensic Science Center (FSC) to support its chemical weapons inspections.

"Chemical weapons are a growing threat to the security of the U.S. and its allies," says Jeff Richardson, deputy program leader for the Proliferation Prevention and Arms Control Program in Livermore's Nonproliferation, Arms Control, and International Security Directorate. "Putting the capabilities of FSC to work in the effort to prevent the spread of chemical weapons is one more way the Laboratory can contribute to national and international security."

In light of its demonstrated capabilities to analyze and characterize unique samples, FSC was selected by the U.S. State Department in 2000 to become the second U.S. laboratory to support the OPCW, pending certification by the OPCW. (The other facility is the U.S. Army's Edgewood Chemical and Biological Forensic Analytical Center in Maryland.) Under the terms of the Chemical Weapons Convention (CWC), the international agreement banning chemical weapons that the OPCW oversees, all inspection samples must be analyzed at two OPCW-designated laboratories. In addition, the U.S. Senate has mandated that all samples obtained within the U.S. must be tested in the U.S. so that proprietary information belonging to American chemical manufacturers will be protected. (See the box on p. 8.)

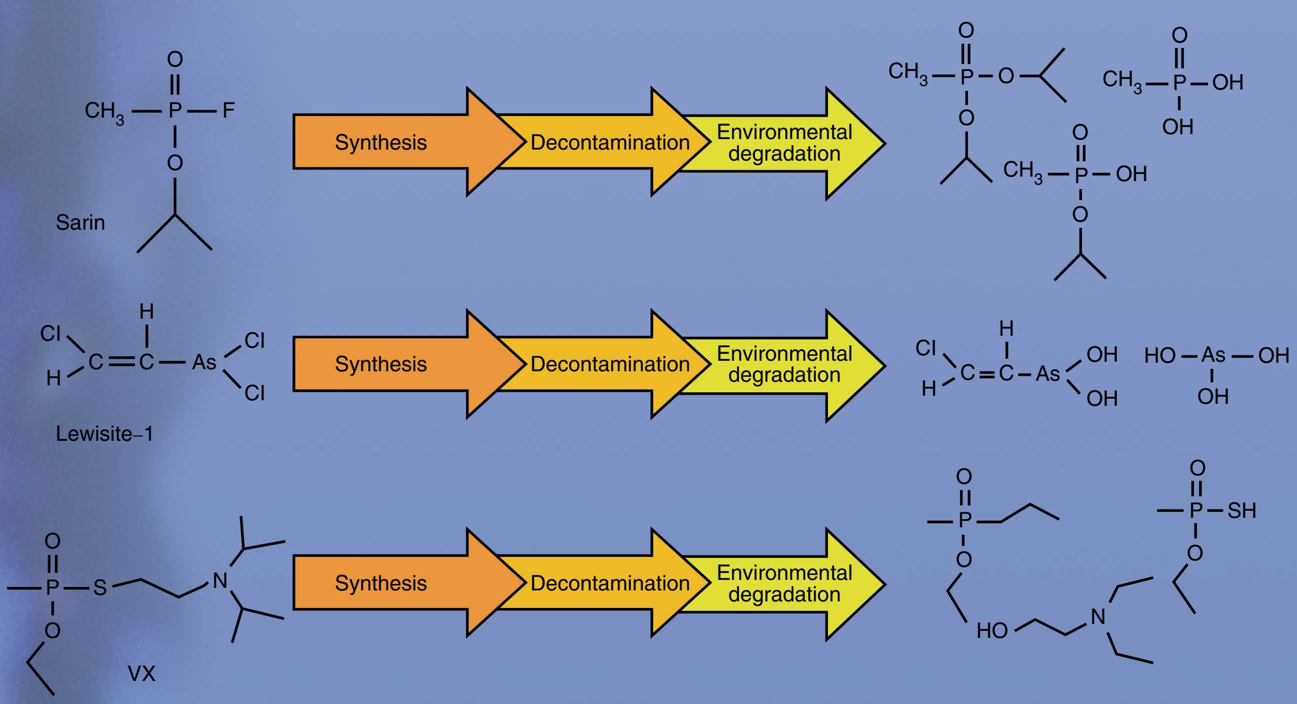
According to Livermore chemist and principal investigator Armando Alcaraz, FSC was originally selected by the State Department because of the Laboratory's advanced environmental controls and physical security and FSC's demonstrated capabilities in detecting and analyzing minute traces of unknown materials. Alcaraz also cites FSC's previous participation in international exercises to detect chemical agents and FSC chemists' work with colleagues at Edgewood. (See the box on p. 11.)

Livermore Joins Select Group

FSC joins about 15 other laboratories around the world that have been certified by the OPCW. The purpose of these laboratories is to test samples collected by OPCW inspectors from chemical plants and other sites to determine whether the samples contain scheduled chemicals (chemical weapons or their precursors) or their decomposition products. (The annex to the CWC has three schedules, or lists, of banned and monitored compounds: Schedule 1 compounds are the most toxic, and Schedule 3 compounds are less toxic or are dual-use chemicals.) To date, no samples have been officially collected from any sites. The only samples examined by the OPCW-certified laboratories have been those prepared for proficiency tests and exercises.

Livermore achieved its OPCW certification by passing three grueling proficiency tests. The tests involved the analysis and characterization of samples containing combinations of extremely dilute amounts of chemical warfare agents, precursor chemicals, and decomposition products as well as other chemicals included to complicate or obfuscate the analysis. The tests that led to accreditation took place in November 2001, April 2002, and October 2002. Different OPCW-designated laboratories formulated the test samples and graded FSC findings.

The proficiency tests used samples that simulated those the OPCW



Laboratories certified by the Organisation for the Prohibition of Chemical Weapons must be capable of detecting minute amounts of chemical warfare agents, precursor compounds, and their decomposition products.

Test samples occasionally contain emulsions of different layers, with each layer containing suspected chemical warfare agents, precursors, or decontamination products.

inspectors might send to Livermore for analysis. The test samples typically consisted of soil, a water-based solution, and an organic-based solution, each contained in sealed glass vials. One test sample looked like milk, but in reality was an emulsion of aqueous and organic phases, each containing suspected products.

Each vial contained one or more scheduled compounds that had to be identified. For each test, the Livermore team was given 15 days to analyze the samples and report its findings.

Background information was also provided on the simulated inspection scenario of the tests. For example, in one scenario, the note claimed that the samples were taken during an inspection of a foreign pesticide plant. Inspectors had supposedly obtained the samples from different locations around the plant, including soil from outside the plant because it might contain degradation products from illicit manufacturing of chemical weapons.

Analysis Plan Is Well-Rehearsed

Thanks to the three proficiency tests, the Livermore team of chemists now has a well-rehearsed plan for analyzing an OPCW sample. A large conference room is transformed into a "war room." Whiteboards on the walls are covered with flow diagrams and notes about possible compounds contained in the samples. "It's a pretty intense time, but we're very focused, and we have outstanding teamwork," says Hugh Gregg, coprincipal investigator.

During the 15 days of analysis, Rich Whipple prepares samples and Alcaraz and Gregg lead the analysis, aided by Robert Maxwell and Greg Klunder. Andy Vance, John Reynolds, and Phil Pagoria synthesize compounds used to confirm the presence of suspected compounds, and Tuijauna Mitchell-Hall provides quality control.

A large conference room is transformed into a "war room" for discussions and posting flow diagrams and notes about possible chemical warfare compounds contained in samples.

Alcaraz emphasizes that team members follow all applicable safety and security requirements for analyzing and synthesizing dilute chemical agents. In some cases, he says, the solvent is more hazardous than the target compounds because any chemical warfare compounds in the samples have been diluted to extremely low concentrations.

The team uses a variety of analytical techniques, including gas chromatography, mass spectrometry, atomic emission detection, gas chromatograph flame photometric detection, chemiluminescense, infrared spectrometry, liquid chromatography, inductively coupled plasma mass spectrometry, nuclear magnetic resonance, and capillary electrophoreses. With three nuclear magnetic resonance machines and more than 12 gas chromatograph–based analyzers at their disposal, the team has one of the world's best-equipped labs to analyze exceedingly small amounts of material.

"We use all the instruments because each gives us unique information," says Gregg. For example, FSC recently acquired a gas chromatograph capable of infrared detection because it yields structural information about a compound. The OPCW requires that at least two different analytical techniques be used for positive identification, and the Livermore team strives to obtain confirmation from three or four different techniques.

The workhorse instrument is the gas chromatograph–mass spectrometer (GC–MS), which can detect ultratrace quantities of organic compounds weighing a billionth of a gram or less. A few microliters of a sample are injected into the GC–MS, where the sample is vaporized and the sample components are separated and analyzed.

Looking for Suspicious Elements

One of the most important first steps in analyzing OPCW samples is doing quick screens with the GC–MS and element-specific detectors to look for a few key elements that indicate the possible presence of chemical warfare compounds. For example, lewisite contains arsenic, sarin contains phosphorous and fluorine, and VX contains phosphorous, nitrogen, and sulfur.

Alcaraz notes that just as important as finding actual chemical warfare agents is finding the chemicals that are associated with their manufacture. Many precursors are listed on Schedule 1 because they are unique to the manufacture of chemical weapons. The CWC list of scheduled chemicals includes tens of thousands of chemicals, most of which have never been synthesized or characterized but are thought to be as deadly as their well-known analogs. Identifying these "designer" agents is an extremely difficult but necessary part of the job.

Breakdown products of chemical agents also qualify as "smoking guns." The chemists must keep in mind the possible products that could be found, for example, in the wastes from a chemical or pesticide manufacturing plant. And the team must anticipate the products that might result from

(a) Chemist Armando Alcaraz logs in a proficiency test sample. (b) Chemist Bob Maxwell holds a sample in a tube that will be placed in a nuclear magnetic resonance instrument (in background). (c) Alcaraz injects a microliter of sample into a gas chromatograph–infrared spectrometer system. (d) Chemist Hugh Gregg uses solid-phase extraction cartridges to clean a sample of hydrocarbon compounds that might mask a chemical warfare agent.

decontamination procedures, as might happen if someone used bleach or another strong oxidizer to eliminate traces of illegal chemical agent manufacture. The team must also consider degradation products resulting from environmental factors such as sunlight and rain. Some chemical agents are stable while others, such as the nerve agent sarin, break down easily.

Whipple notes that the sample solutions may also contain agents, such as dirty diesel oil, that mask the target compounds present in vanishingly small quantities. In one case, when the diesel oil was carefully removed, the chemists found trace amounts of a chemical warfare agent precursor.

Watching for Red Herrings

Finally, the team must be ready to locate and identify any of thousands of possible compounds added to the samples as red herrings. These compounds are not found in any chemistry reference because they were created just for the test in an effort to fool the analysts. They are often similar or identical in molecular weight and elemental composition to well-known chemical warfare compounds.

"Many compounds will look like a Schedule 1 compound, but if we report it as such, we fail the test," says Vance. One such compound contained sulfur, phosphorous, and nitrogen, good indicators of a nerve agent, and the molecular weight was in the ballpark for a well-known nerve agent. With the aid of multiple syntheses and nuclear magnetic resonance analysis, the team figured out its structure, which was different from that of any nerve agent (and therefore not scheduled). The compound had been made by an OPCW laboratory to confuse chemists analyzing the sample.

Vance notes that OPCW has provided a database of thousands of compounds, complete with molecular weight, structure, and what the GC–MS spectrum should look like. In addition, the GC–MS will suggest the identity of a compound based on the 2,000 to 3,000 compounds in its

Chemical Weapons and the Treaty That Bans Them

The Convention on the Prohibition of the Development, Production, Stockpiling, and Use of Chemical Weapons and on Their Destruction (commonly known as the Chemical Weapons Convention, or CWC) defines chemical weapons as toxic chemicals and their precursors. Chemical and biological weapons have been referred to as the poor man's nuclear weapons. This is particularly true of chemical weapons, which are easily and affordably manufactured and can inflict mass casualties.

Chemical weapons are often grouped by their biological response. Nerve agents include sarin, soman, and VX; blister agents include mustard gas and lewisite; vomiting agents include diphenylcyanoarsine; and tearing agents include CS gas.

Many chemical warfare agents are similar to common industrial chemicals. In fact, troops during World War I used several unmodified industrial chemicals as weapons. For example, German troops opened canisters of chlorine and let winds disseminate the gas. Nerve agents, developed just before and during World War II, are related chemically to the organophosphorous insecticides and are among the most deadly: With some of them, one drop on the skin can cause respiratory failure and death.

The Geneva Protocol prohibiting the use of chemical weapons in warfare was signed in 1925. Several nations, including the U.S., signed with a reservation forswearing only the first use of the weapons. The U.S. ratified the protocol in 1975.

Chemical weapons were used by Italy in Ethiopia and by Japan in Manchuria and China prior to World War II, but no chemical weapons were deliberately employed by the Allies or the Axis powers during the war. Iraq used chemical weapons, including mustard gas, during the Iran–Iraq conflict of 1982 to 1987. Evidence indicates that it used chemical weapons within its own boundaries in 1988 when it killed about 5,000 Kurds in Halabja with a combination of mustard gas and the nerve gases sarin, tabun, and VX.

Until 1985, virtually all uses of chemical weapons had been as tactical weapons by nations. Then, in a terrorist attack, the Japanese cult Aum Shinrikyo released sarin gas in a Tokyo subway, killing 12 people and injuring more than 5,000. Currently, thousands of toxic chemicals could be used as chemical weapons. Many can be manufactured in existing chemical plants or individual laboratories.

Classes of chemical warfare agents.

1 Nerve	2 Blister	3 Vomiting	4 Tearing
• Sarin (GB)	• Mustard (HD)	• Diphenylcyanoarsine	• Chloracetophenone
• Soman	• Lewisite (L-1)	• Adamsite (DM)	• Chloropicrin (PS)
• VX, Vx	• Nitrogen mustard	• Diphenylchloroarsine	• CS

library. However, the instrument is not foolproof because more than one compound can have the same molecular weight and elemental composition.

As a result, once the team suspects the presence of a particular compound, it must obtain a reference sample, either from its storehouse of 500 to 1,000 stock chemicals or by synthesizing the compound. Either way, the reference is then screened by the same instruments to make sure it gives identical readings.

Vance points out that synthesizing the suspect chemicals poses no health or safety risk because chemists work in a special hood and use gloves. More importantly, they only synthesize extremely small amounts of material, never exceeding a concentration of 1 milligram per milliliter and a total of 10 milliliters of solution.

Because the GC–MS separates compounds, the synthesis chemists aren't concerned about purifying their product, which saves valuable time. They also aren't concerned about yield. "If we have only fractions of a microgram, the GC–MS will find it," Vance says. "The hard part is that doing things as fast as possible and not caring about yield is counter to my experience on other projects in which the focus was on maximizing yield and purity."

Aiding the synthesis effort are parallel synthesis techniques. A parallel synthesis instrument can perform up to 20 simultaneous reactions in temperature- and atmosphere-controlled reaction vessels. Vance can make multiple compounds that meet molecular weight and elemental composition requirements and then analyze all of them to find one that matches.

Alcaraz notes that as Day 15 approaches, "We feel the pressure. We're always thinking, 'Did we miss something?'" To answer that question, the team invites other Livermore chemists to a meeting about three to four days before the deadline to

---

The only toxin to exist naturally is ricin, made from the ubiquitous castor bean plant. British authorities found traces of ricin, for which there is no antidote, in a raid on a London apartment in January 2003. Instructions for making ricin have been found in the possession of several suspected terrorists and fighters in Chechnya.

CWC Extends Globally

The CWC is a global treaty that bans the development, production, stockpiling, and use of chemical weapons. Parties to the treaty are obligated to destroy their chemical weapons and production facilities within a specified period of time. They also must not assist other states in the production of chemical weapons. (The U.S. has been destroying its stockpile of chemical weapons at a cost of many billions of dollars.)

CWC negotiations began in 1980 as part of the United Nations Conference on Disarmament. The CWC went into effect on April 29, 1997, four days after the U.S. signed. Currently, more than 145 nations have signed the treaty, although nations such as Iraq and North Korea have not.

The CWC places controls on toxic chemicals and their precursors, which are listed on three schedules according to their toxicity, military and commercial utility, and risk. Schedule 1 lists military agents with no or low commercial use, such as nerve agents and mustards as well as their direct precursors. Schedule 2 lists high-risk precursors and toxic chemicals that are not produced in large quantities for commercial use. Schedule 3 lists dual-use chemicals, some of which have been used as weapons or precursors but which are produced in large quantities for purposes not prohibited by the CWC. The treaty allows states to produce an aggregate of 1 metric ton or less of Schedule 1 chemicals for research, medical, pharmaceutical, and protective purposes.

The CWC is the first arms control and nonproliferation treaty to widely affect the private sector. Although the U.S. does not manufacture chemical weapons, it does manufacture, use, import, and export a number of dual-use chemicals that could be used to produce chemical weapons. U.S. companies engaged in activities involving certain chemicals may be required to submit reports to the Department of Commerce and may be subject to inspections.

The CWC is implemented by the Organisation for the Prohibition of Chemical Weapons (OPCW), which is headquartered in The Hague, Netherlands. The OPCW has almost 500 employees, including a multinational corps of inspectors. Any treaty party that suspects another signatory of conducting activities prohibited by the CWC has the right to ask for a challenge inspection of the suspect site. The analysis of samples may be done at the suspect site, but samples can also be transferred to approved OPCW laboratories for additional analysis.

When the U.S. Senate ratified the CWC, it implemented a mandate, Condition 18, which states that no sample taken on U.S. soil shall leave the U.S. for analysis during an OPCW inspection. However, it is an OPCW requirement that two OPCW-accredited laboratories must analyze the samples and provide independent correlation. The two accredited U.S. laboratories are the U.S. Army's Edgewood Chemical and Biological Forensic Analytical Center and Livermore's Forensic Science Center.

review its analysis work and give comments and suggestions. The meeting, says Gregg, shows that “this is a real team effort, not just one person.”

Finally, the team sends its report, complete with instrument readouts and flow diagrams, to OPCW headquarters, where it is forwarded to a certified lab for grading. Gregg notes that OPCW has taken Livermore’s report format and made it the standard for all designated laboratories.

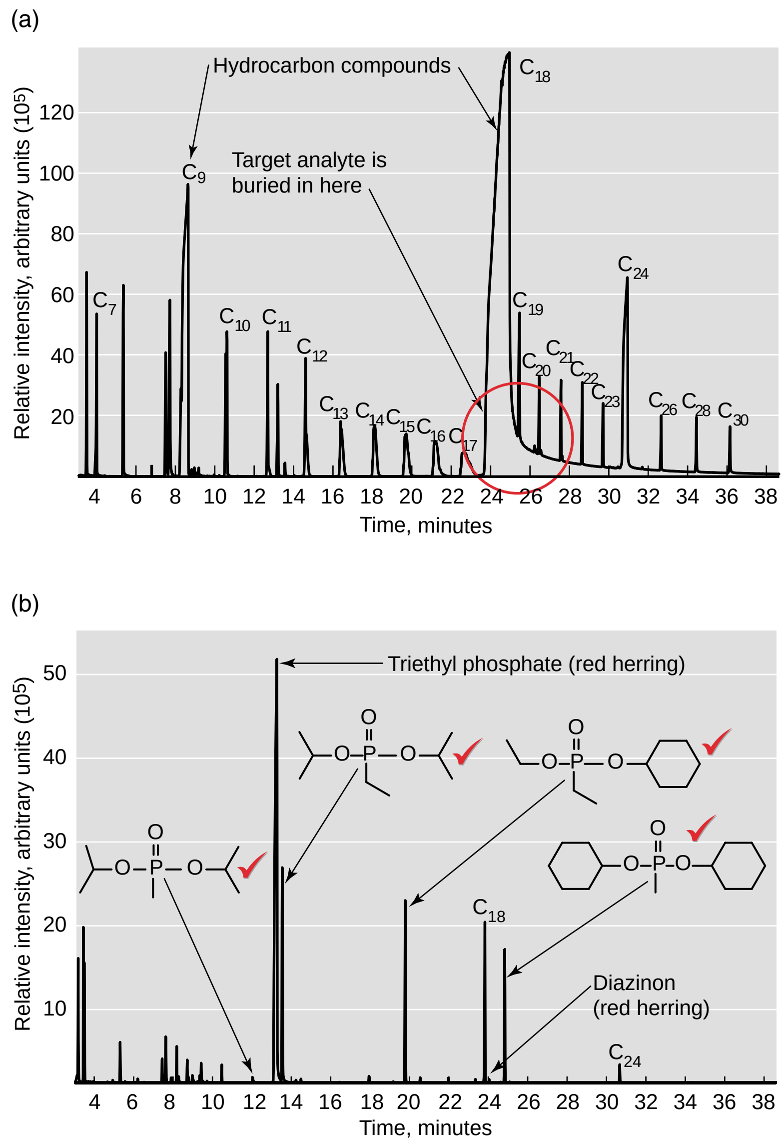
First Exercise Tests System

In early February, the team participated in OPCW’s first exercise designed to test all the procedures related to using the designated laboratories, including procedures for shipping and analyzing authentic samples. Not part of the proficiency tests, the exercise involved samples from a mock inspection site in Singapore that had been sent to OPCW headquarters in The Hague, Netherlands. OPCW added a quality control sample and a blank solution and placed them in a specially designed stainless steel case for transfer by commercial shippers to participating laboratories in Livermore, South Africa, and Britain.

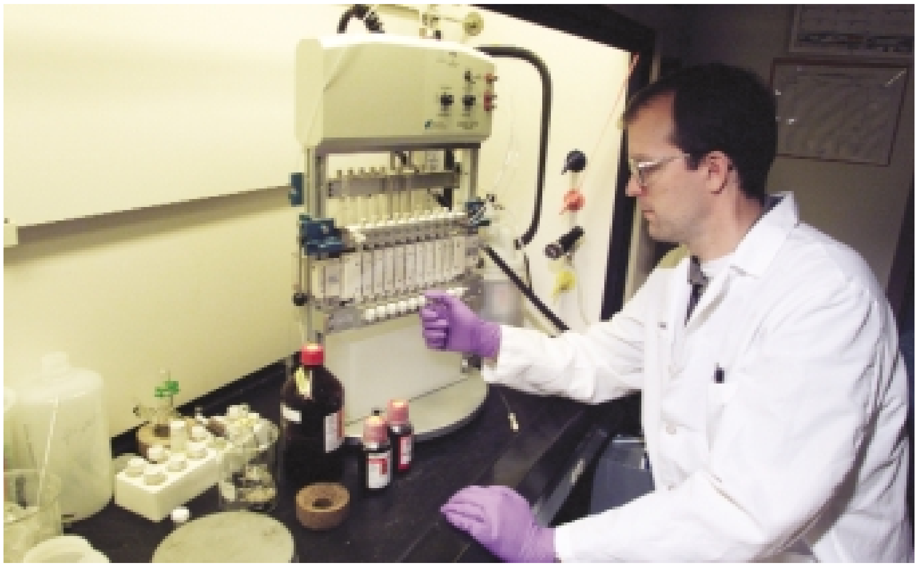
Before sending the samples to Livermore, OPCW notified the U.S. State Department, which notified Alcaraz and Gregg. Upon hearing from Alcaraz that FSC was ready, the OPCW sent the samples to Livermore. “We wanted to discover any customs and shipping problems that could come up with officially labeled samples from OPCW,” says Alcaraz. Because of paperwork and customs issues both in Europe and at the Los Angeles airport, the samples arrived a week later than expected.

An OPCW inspector from Zimbabwe was on hand at Livermore to verify the samples’ intact seals and weights. OPCW rules also allow a representative from the nation where the samples are taken to monitor the analysis. As with the proficiency tests, the Livermore team had 15 days to send in their analysis but finished the task in just one week. This sample handling exercise was beneficial to OPCW and the U.S. Potential and actual pitfalls in collecting, transporting, and analyzing authentic samples and reporting the results have been identified and are being addressed.

Alcaraz anticipates that FSC may receive samples for analysis several times a year from OPCW inspections.



(a) This chromatograph of a sample was produced by a gas chromatograph–mass spectrometer. Hydrocarbons could be masking trace amounts of chemical weapon agents. (b) Once the hydrocarbons are removed, the analysis reveals the presence of a compound that is a precursor to a chemical warfare agent.



Chemist Andy Vance uses parallel synthesis techniques to quickly prepare reference compounds and try to match them to what the team suspects are chemical warfare agents, precursors, or decontamination products.

Chemical Weapons Work Is Part of FSC Expertise

The laboratory certified by the Organisation for the Prohibition of Chemical Weapons (OPCW) operates as part of Livermore's Forensic Science Center (FSC). Founded in 1991, FSC offers a comprehensive range of analytical expertise to counter terrorism, aid domestic law enforcement and homeland security, and verify compliance with international treaties and agreements.

The center's human and technological resources have made it among the leading facilities for collecting and analyzing virtually any kind of evidence, some of it no greater than a few billionths of a gram. FSC has expertise in ultratrace chemical and isotopic analyses of nuclear, inorganic, organic (chemical warfare agents, illegal drugs, explosives), and biological materials (toxins, DNA).

FSC also develops new technologies for detecting and characterizing the source of weapons materials. A major effort is adapting forensic analysis technologies for field use. For example, FSC scientists have shrunk the standard gas chromatograph–mass spectrometer so it fits inside a wheeled suitcase. (See *S&TR*, April 2002, pp. 11–18.) When necessary, the center draws upon experts in Livermore's Chemistry and Materials Science and Nonproliferation, Arms Control, and International Security directorates.

Government and law enforcement agencies call upon FSC for analyses beyond the capabilities of their in-house laboratories and for interpreting samples demanding unusually high-quality forensic analyses. In 1998, the Federal Bureau of Investigation named FSC as the bureau's West Coast support laboratory. As part of the OPCW accreditation process, FSC in November 2001 obtained an International Organization for Standardization certification in the field of chemical testing by the American Association for Laboratory Accreditation.

Samples could contain just about any suspect material, including water, soil, gasket material, and even chips of concrete. As with the test samples, real samples will be diluted by inspectors before they are forwarded to an OPCW-designated laboratory.

In the meantime, the team is doing data validation work for the OPCW-developed libraries of scheduled chemicals. These libraries are used by inspectors with portable GC–MS instruments in the field and by designated laboratories performing analyses. Livermore chemists are evaluating the spectral data to make sure they are accurate. In addition, FSC, like all OPCW-designated laboratories, is expected to maintain high scores (at least two "A's" and a "B" on yearly proficiency tests) to keep its certification.

Alcaraz notes that FSC would like to make its chemical warfare agent analysis resources available to other government agencies. For example, he suggests the center could aid homeland security by providing technical support to first responders who suspect chemical agents. Agencies such as local health departments and the Environmental Protection Agency do not have expertise identifying chemical warfare agents, he says. Fortunately, Lawrence Livermore is certified to do the job.

—Arnie Heller

Key Words: chemical weapons, Chemical Weapons Convention (CWC), Forensic Science Center (FSC), Organisation for the Prohibition of Chemical Weapons (OPCW).

For further information contact Armando Alcaraz (925) 423-6889 (alcaraz1@llnl.gov).

Bird's-Eye View Clarifies Research on the Ground

Remote sensing of plant, soil, and water ecologies can yield important information about recent and historical events and conditions.

OUT in the backyard garden or in the wilderness, we've all seen how plants react to changes in environment. Too little water, too much sun, not enough nutrients, and normally green leaves wilt and turn yellow, evergreens shed their needles, grasses droop and die, new species of weeds and trees replace other plants that are struggling. In these and other ways, plants can provide valuable clues—some obvious, some subtle—about what's going on in their immediate world. Clues that, if interpreted correctly and combined with other information about an area's geology and ecology, can speak to scientists about the past and present and even give hints about the future.

Past events such as clandestine underground nuclear tests or surface digging that occurred many years ago could be revealed. Present events such as methane gas leaking from an underground pipeline, carbon dioxide leaking from geothermal formations, or chemical run-off in streams and estuaries could be pointed out. Future events such as impending landslides could be signaled. All these and more are reflected in the health and species mix of plants in the area.

Lawrence Livermore sensor physicist Bill Pickles first began noticing what plants can reveal after an underground test at the Nevada Test Site nearly a decade ago. (See the box on p. 14.) Since then, he has joined forces with researchers at the National Aeronautics and Space Administration (NASA), the University of California at Santa Cruz (UCSC), the University of Nevada at Reno, the University of Utah, and Pacific Gas and Electric's (PG&E's) Technical and Ecological Services (TES) Laboratory to explore and develop applications of geobotanical remote sensing. Their collaborations use multispectral imagery and airborne imaging spectroscopy, or hyperspectral imagery, to combine observed plant health and species mixes with soil and mineral distributions. They correlate these distributions to events both natural and human made. Such "translations" of the language of plants, soils, and water are contributing to Livermore's homeland security and energy resource development missions as well as providing insights into complex ecological systems such as coral reefs and wetlands.

Getting Details on the Big Picture

Geobotanical remote sensing uses both plants and geology to understand a region of interest; it gathers information with systems carried by either airplanes or satellites. Using remote sensors to map aspects of Earth's geology and biological ecosystems is not new. What is new about Livermore's Geobotanical Remote Sensing Program is that it combines commercial and national remote sensing systems of extremely high spatial and spectral resolution with an interdisciplinary methodology. As a result, it has brought together experts in many fields, including remote sensing technology, biology, botany, marine science, geology, ecology, and geothermal research. The team works together to produce an integrated interpretation of what is seen in the imagery and verified on the ground during field trips.

According to Pickles, today's commercial and NASA airborne sensor systems can record 50, 120, 256, and

even more bands in the visible and near-infrared wavelengths with spatial resolutions between 0.5 and 4 meters. Sensors with such a high number of spectral bands are referred to as hyperspectral. Commercial satellites have comparable pixel resolutions, but only image four bands over the same bandwidths. This low number of spectral bands is referred to as multispectral. High spatial resolution of a meter or so is essential for geobotanical analyses, he notes. With a hyperspectral scanner and 0.5- to 4-meter resolution, the spectra from rocks, soils, bushes, and trees aren't heavily averaged together in one pixel of the image but remain somewhat separate, or are only partially mixed. From hyperspectral data of this quality, researchers can obtain details such as determining the species of individual plants, identifying the locations of mineral outcrops, classifying clumps of plants, mapping unique soil types, detecting water conditions, differentiating road types, and exposing traces of disturbed earth.

Satellite multispectral imagery allows a broad overview of landscapes of interest. Once an area has been identified for further study, a plane carrying a spectroscopic system flies at a predetermined altitude, about 300 to 1,500 meters above ground elevation, gathering data for swaths usually 1 kilometer wide and tens of kilometers long in an overlapping pattern. Data are gathered in narrow, prescribed bands in the visible and infrared spectra. The spatial resolution of the data is usually detailed enough to pick out individual plants on the ground.

These data are processed by researchers using commercial image processing software such as ENVI or Imagine. "We're fortunate that many years of work by many remote sensing researchers has produced advanced suites of sophisticated image analysis software," says Pickles. "This software allows us to focus on analyzing the images and not on developing the computer codes. After all, the focus

Serendipity Leads to Sensing Technique

In the predawn light of September 23, 1993, Livermore physicist Bill Pickles drove his jeep onto Rainier Mesa on the northern part of the Nevada Test Site. He was looking for any changes that might be visual signatures of the 1-kiloton chemical explosion set off in a tunnel under the mesa 24 hours earlier. The shot, made during the international Nonproliferation Experiment, had representatives from many countries present.

The point of the experiment was to see whether underground nuclear explosions could be detected, located, and distinguished from other seismic events such as earthquakes, mine collapses, or large chemical explosions routinely used in mining, quarrying, and civil engineering projects. "It was a worldwide seismic party," remembers Pickles, who was trying to see if remote sensing could be used to pinpoint the location of a clandestine small underground explosion. He decided to piggyback on the event with advanced remote sensing available from the Department of Energy laboratory nearby at Nellis Air Force Base, Las Vegas. Pickles was hoping to find any signatures—such as cracks in the roads, fences knocked over—that might detect an explosion set off in violation of the Comprehensive Test Ban Treaty. At first glance, the visible results had been disappointing. There was no obvious damage to anything on the surface after the underground explosion.

Then 36 hours after the explosion, as dawn broke over the rim of Rainier Mesa, brilliant autumn colors from the surrounding pin oak trees flooded the inside of Pickles's jeep. "I drove into the area for my postshot inspection. I couldn't see anything different at all. It was very discouraging. So I kept driving and looking around. Something bothered me, tugged at the back of my mind as I drove, but I couldn't put my finger on it."

Two kilometers away from ground zero, it hit him as he gazed out the vehicle window. The pin oak trees surrounding him were green. "The fall colors that had so dazzled me near ground zero were gone! I drove back to ground zero and there, the fall colors were absolutely intense," says Pickles.

The scientific questioning began. Could the shock have precipitated the change to fall colors because it forced the plants into early senescence? Pickles approached National Aeronautics and Space Administration (NASA) botanist Greg Carter with the question. Carter said it was possible. The shock of the ground motion might have forced the plants to shut down their root systems, dehydrating and thus stressing the plants.

Carter had an ongoing NASA program to make spectral measurements of plants that all looked healthy to the naked eye but were in fact under some stress. He was in the process of determining which narrow wavelength bands in the reflected visible spectrum were an indicator of plant stress. "We got the list of his bands," says Pickles, "and found that two of my bands acquired using multispectral imaging just overlapped his bands." (The Livermore bands were 30 and 50 nanometers wide, while Carter's were only 2 nanometers wide.)

Pickles focused on the relevant bands to measure ratios of images before and after the shot. "The larger the ratio, the larger of our work is on understanding phenomena affecting vegetation and soil, not building applications."

Researchers use the results of the computer software analysis and their ground observations to produce a wealth of detailed specialized maps. They superimpose and overlap these maps using geographic information systems (GISs), looking for patterns and relationships. For instance, a map of minerals produced by geothermal activity overlaid with a map showing distributions of plant species or plant health could pinpoint the location of a hidden geothermal source. The variety of maps include those of geology, botanical species and distributions,

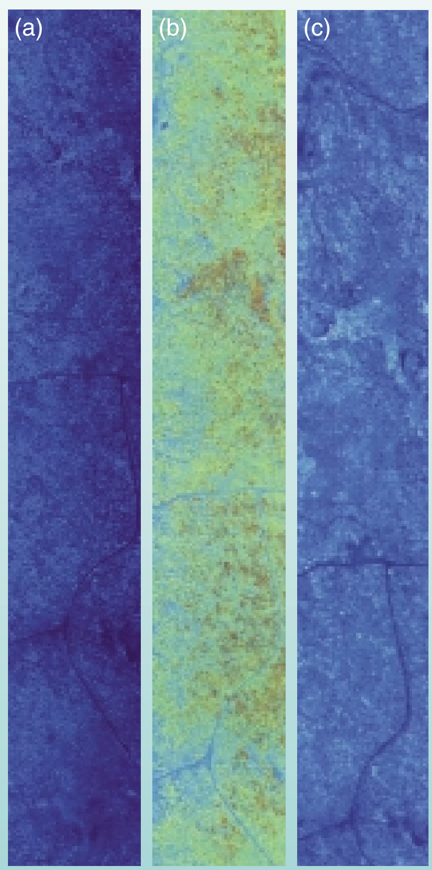
Members of the geobotanical remote sensing collaboration and the plane with a HyMap hyperspectral sensor on board. The sensor is mounted inside one of the doors and takes data through a hatch in the bottom of the aircraft.

the plant stress," says Pickles. "A ratio above 3.75 is definitely indicative of plant stress in Carter's research." He found a pattern of plants located near ground zero with ratios well above 3.75. This pattern does locate the area above the explosion to within several hundred meters.

It seemed entirely possible that the shock wave from the test's blast could have temporarily dehydrated the trees. Pickles and Carter tested this hypothesis by shocking trees at a large landscape contractor's tree-growing area in Calaveras Canyon near Sunol, a few miles from Livermore. To mimic the shock wave produced by the shot, which was known to produce a maximum vertical ground displacement of about 1 meter, a crew of workers hoisted trees growing in large containers to 1 meter above the ground and then dropped them. Using a small, narrowband filtered camera, Pickles and Carter recorded and measured previsual (before it is apparent to the human eye) stress in the trees' foliage as the plants went into shock. They measured several metabolic parameters for each tree.

The experiments showed the photosynthesis rates of the trees changed by the dropping. This finding was similar to what was seen at Rainier Mesa after the Nonproliferation Experiment. In both instances, the trees slowly recovered in about one week.

"Had the Nonproliferation Experiment occurred but two or three weeks later," says Pickles, "yellow autumn foliage would have been the norm for pin oaks up on the mesa. It was pure serendipity that the trees were thrown deep enough into senescence at a time when I could actually see the difference."



Ratio images of stressed vegetation at and around ground zero taken (a) 12 hours before, (b) 12 hours after, and (c) 1 week after the Nonproliferation Experiment shot. The last two images reveal that all the plants went into shock immediately after the shot, after which they recovered at different rates. Plant stress level is indicated by different colors. Blue represents normal or nonstressed, green and yellow are intermediate stressed, and red represents most-stressed plants.

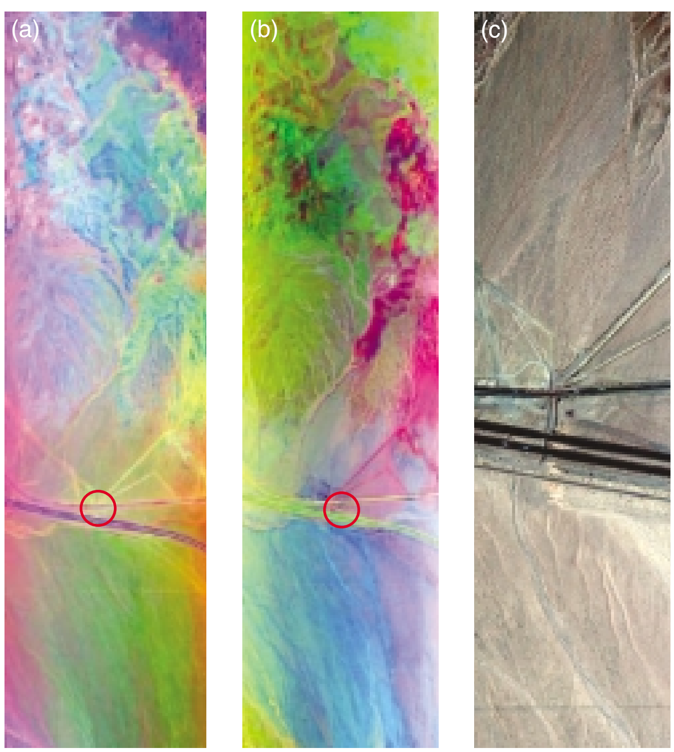
known as well as new and hidden faults, pockets of minerals that have been altered by high temperatures, the effects of carbon dioxide emissions on surface plants, and more.

Pickles works with Don Potts and Eli Silver, professors of biology and geology at UCSC who also head up a doctoral program in geobotanical

A Pacific Gas & Electric worker points to one of the discovered leaks in the exposed pipe.

remote sensing. The program focuses on gathering geological, biological, and ecological data over large areas of interest. Remote sensing techniques are used to create an overall picture of how plants respond to changes in the environment, such as those caused by heat, salinity, contamination, shock waves, and seasons.

Initially, the research program focused on analyzing imagery for plants under shock—to support studies for the Comprehensive Test Ban Treaty—but it has expanded to mapping soil types, soil contamination, plant species, plant health, minerals, water, and water content. The data are used for Livermore's missions in energy technology and homeland security. Geobotanical remote sensing techniques are also being applied to ecological studies in Elkhorn Slough in Monterey, California, and coral reefs in the new North West Hawaiian Islands Coral Reef National Sanctuary. (See the box on p. 18.)



Three views of a pipeline leak. (a) Minimum noise fraction (MNF) transformation in pseudo-color, showing leak area west of Ludlow, California. (b) Using different MNF transformed bands emphasizes features differently and is a common technique for sorting out what is seen in the imagery. (c) A true color, three-band image at 3-meter resolution.

Keeping Pipelines Safe

The Laboratory's Homeland Security Organization is responsible for providing comprehensive solutions for defending against terrorism. As a part of this mission, the Laboratory has been assessing the nation's energy infrastructure, including natural gas utilities. Geobotanical remote sensing is one method being developed to detect hazards to natural gas pipelines. "We are looking for ways to identify leaks, landslides, earthquakes, and third-party incursions—deliberate as well as accidental damage, such as the kind that could happen when fields are plowed too deep, subdivisions are built over pipelines, that sort of thing," says Pickles.

Pickles and Don Price of PG&E's TES Laboratory in San Ramon, California, are collaborating on this pipeline monitoring program. The collaboration, which includes UCSC graduate students, recently completed a pilot project in Cordelia, California, at a PG&E pipeline site in an area where a landslide bent the pipeline. (The bent part has now been bypassed with a new section of pipe.) The pilot project used high-resolution IKONOS satellite multispectral imagery to see if the landslide area could have been detected by remote sensing before it broke loose and damaged the pipe. Results of the project are being applied along other PG&E pipelines to reduce risk and enhance infrastructure reliability.

PG&E is providing instant information about new leak locations, site access, leak area appearance, repair details, and historical site information. When Pickles and Price are informed of a new leak location, they arrange for low-altitude overflights by NASA Jet Propulsion Laboratory, NASA Ames Research Center, or commercial hyperspectral imaging providers such as SpecTIR Corporation or HyVista Corporation. "Geobotanical changes are much more sensitive indicators than, for instance, airborne detection of methane in a plume that accumulates over a leak," says Pickles.

So far, two areas have been successfully imaged. One area is on the main pair of PG&E pipelines that run through the California desert. The leaks there were between the towns of Ludlow and Amboy. The other is in the Sunol Canyon in the San Francisco Bay Area. For the Amboy–Ludlow site, the team had NASA Ames acquire spectroscopic data in 50 spectral bands, including in thermal infrared and infrared portions of the spectrum, in bandwidths of a few nanometers, and at a spatial resolution of 3 meters. They then used the resulting imagery to map species types, plant health within species types, soil types, and soil conditions.

PG&E's failure analysis showed that the Ludlow and Amboy leaks occurred in the original welds of the pipeline when it was buried nearly 40 years ago. "The area and vegetation has been subject to 40 years of methane leakage," says Pickles. "You can tell when you go into the Amboy area on foot that there's something going on. The plants in the vicinity of these leaks look strange."

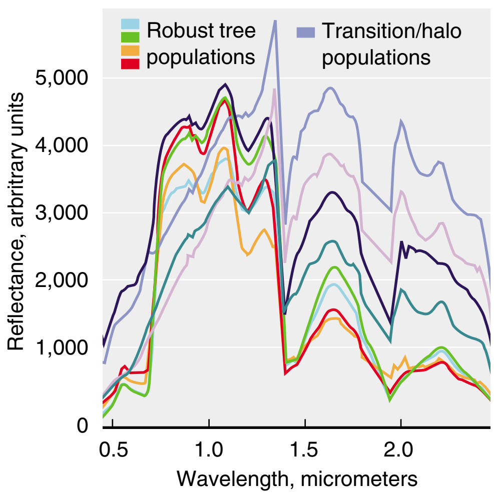
In the Sunol leak, the failure was much more recent and of shorter duration. Although only leaking for a few months, the grass above the leak was clearly in stress and looked brown compared with the surrounding vegetation. Pickles and Price are currently analyzing hyperspectral imagery acquired by SpecTIR within three days of the leak being noticed to see if the brown spot is visible in the images.

Pickles says that the technique shows promise for continuous, real-time monitoring of the pipelines. "The detail we pick up can't be obtained by satellite imagery yet. Basically, our approach provides an alert that something is up, something that requires a closer look. Where to look is important to utilities like PG&E because in California alone there are some 12,000 miles of transmission gas pipelines to monitor."

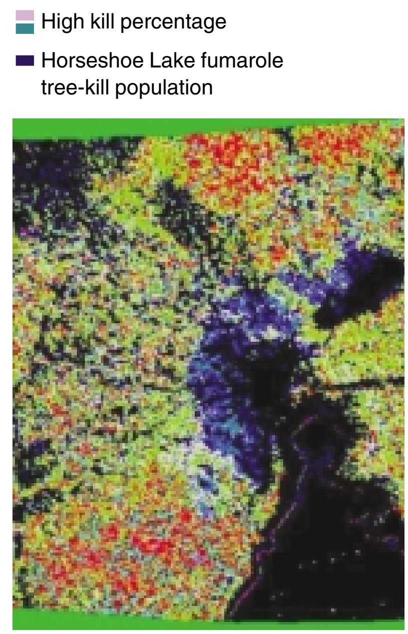
Uncovering Geothermal Sources

Geobotanical remote sensing is also being used to support the DOE mission to discover new hidden geothermal resources that could be used as energy sources. This application got its start in 1996, when Livermore's geothermal program funded a team that included Pickles, Silver, Potts, and UCSC graduate student Brigette Martini to see if geobotanical remote sensing could identify plants stressed by geothermal activity. "If you hike into a geothermally active area and look

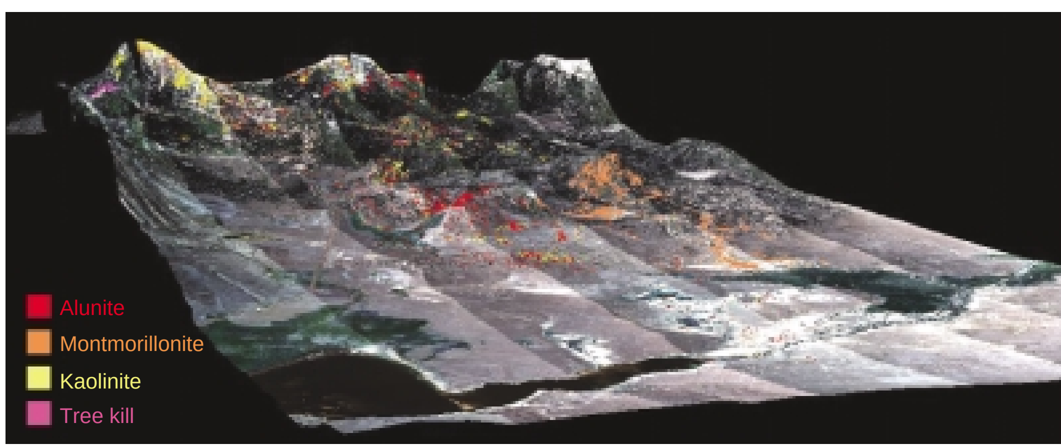
(a)



(b)



(a) Spectral signatures of quantitative stages of tree health. These signatures were used to produce (b), a map of tree health in and around the tree-kill area, using the same spectral colors.



Long Valley Caldera mapped with HyVista 3-meter hyperspectral imagery, showing tree-kill areas and the high-temperature mineralization that marks historical geothermal effluents.

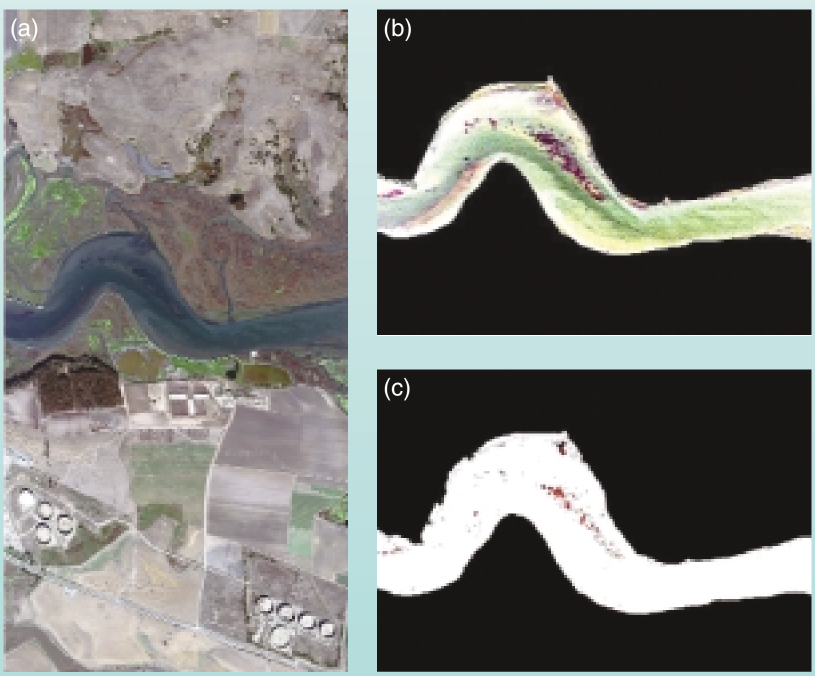
Studying Sensitive Ecological Systems

The techniques developed by Livermore and University of California at Santa Cruz (UCSC) researchers also have potential applications in monitoring and setting baseline conditions for ecologically sensitive areas, such as wetlands and reef systems. UCSC graduate students under professor Don Potts are pursuing these possibilities in two projects that are mapping Elkhorn Slough (a coastal wetland near Monterey, California) and shallow coral reefs off the coast of Hawaii's Oahu Island.

Coastal zones contain some of the most biologically diverse and productive ecosystems on Earth. Over half of the world's current population inhabits these coastal regions, as will much of its expected increase. Along with the human encroachment comes increased environmental impacts and biological stress in coastal and shallow marine ecological systems, stresses that deplete natural resources. Collecting comprehensive data about the extent of resources and impacts and having the ability to document temporal changes in these areas are essential requirements for successful management and planning.

UCSC researchers are using geobotanical remote sensing techniques to identify and map environmental stress in vegetation found around the terrestrial–aquatic interface of Elkhorn Slough. The home to many species of fish and invertebrates, Elkhorn Slough is also on the migratory path of West Coast birds, and its wetlands provide important nursery and breeding grounds for many animals. UCSC researchers and graduate students are using geobotanical remote sensing techniques to search for patterns of stress in vegetation. Although hyperspectral methods have been used in terrestrial systems for years, there have been fewer applications in coastal and shallow marine systems. UCSC researchers are creating a spectral library for this ecosystem and systematically evaluating different stress indices for use with its estuarine plants as well as evaluating chemical inputs to the system such as those from pesticides and nutrients. The end result will be maps of vegetation distributions and stress that will provide a tool for sustainable ecosystem planning.

Coral reef ecosystems are also extremely sensitive to changes in their environment—whether those changes are natural or induced by humans. UCSC is using hyperspectral remote sensing to study the coral reef system in Kaneohe Bay, on the northeast coast of Oahu. The reef is subject to constant change, including natural change such as large freshwater flows and the deposition of land-derived sediments and human-driven changes from agriculture, grazing, and the ever-increasing urbanization of the coast. Researchers are using hyperspectral remote sensing data to characterize the organisms that make up the reef, including corals, algae, and invertebrates. The spectral data are being compared with oceanographic and water quality data to look for biological indicators of environmental stress in the spectral response. In particular, UCSC researchers are examining whether spectral signatures can characterize the physiological response of corals to salinity, temperature, dissolved oxygen, and concentration of nutrients, and they are looking for spectral indicators of coral health.



Although hyperspectral methods have been used in terrestrial systems for years, there have been few applications in coastal and shallow marine systems. UCSC graduate students Daria Siciliano and Stacy Jupiter are using geobotanical remote sensing techniques to map eelgrass beds in Elkhorn Slough, looking at vegetation distribution and for signs of stress. These maps and others like them will provide tools for sustainable ecosystem planning. (a) Red-green-blue (RGB) image of the area. (b) Stretched RGB image with the land masked out. (c) The (b) image showing only the eelgrass.

around at the vegetation growing there," says Pickles, "you'll see that some of the plants are not doing well. Some species might be struggling. Others—which you'd expect to find in the region—are completely absent, yet other species are flourishing. We wondered if we could go into an area where the geothermal activity isn't so obvious and check plants for geothermal stress, thereby tracking down geothermal resources."

The team decided to focus on southern California's Mammoth Mountain located on the western rim of the much larger Long Valley Caldera—an area well known for its geothermal volatility, with many hot springs and fumaroles. One of three active calderas within the contiguous U.S., Long Valley has witnessed periodic volcanic degassing and increased seismic activity over the past 20 years.

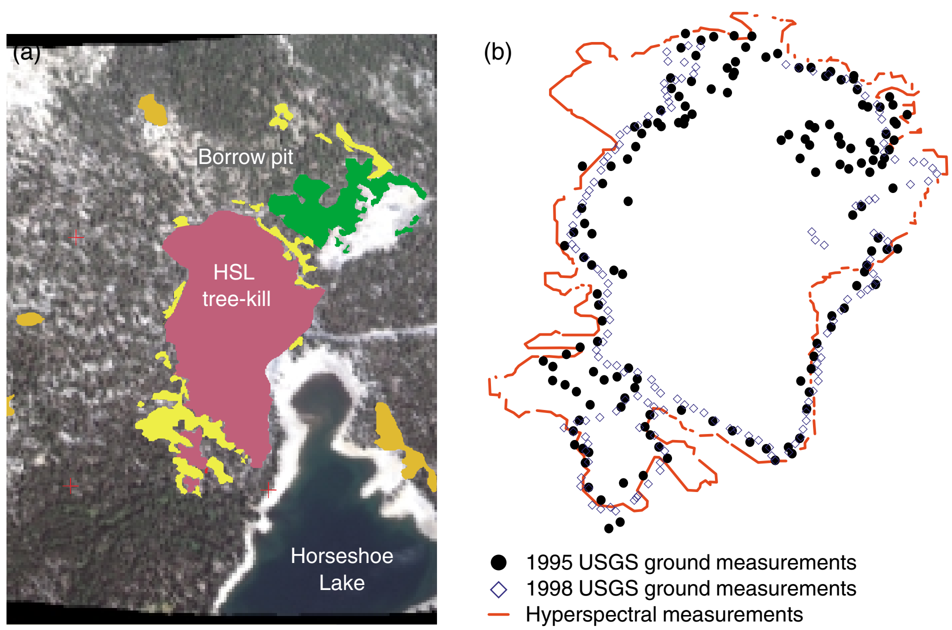
The Horseshoe Lake region located on the southeast flank of Mammoth Mountain was the team's specific focus. In May 1990, a year after a six-month swarm of earthquakes, dead trees were seen in increasingly large numbers at this site. In 1994, soil gas measurements made by the U.S. Geological Survey (USGS) proved that the trees had been asphyxiated by an enormous quantity of carbon dioxide in the ground. In some cases, up to 90 percent of the gas measured in the soil was carbon dioxide, compared with less than 1-percent concentrations in soils outside the tree-kill areas. Carbon dioxide is outgassed by geothermal systems, and the trees died because of geothermal stress. The tree-kill area was a good place to see if hyperspectral images would corroborate the USGS measurements and be a good detector of geothermal resources.

Martini received her Ph.D. in December 2002 from UCSC. Under advisers Silver and Potts, her thesis was on the Long Valley Caldera and Mammoth Mountain system. As part of the thesis, Martini used low-altitude, high-resolution hyperspectral imagery to map altered minerals, hidden faults, and the tree-kill areas of Mammoth Mountain. She extracted spectral signatures of healthy robust trees, dead trees, and physiologically stressed trees from the imagery and used it in several mapping schemes. She was able to characterize geothermal activity along the Long Valley fault lines by detecting the release of carbon dioxide and identifying areas where carbon dioxide was coming out of the ground in measureable amounts.

When she compared her mapping of carbon dioxide leakage areas with those measured on the ground by John Rogie of USGS at Menlo Park, the agreement was, notes Pickles, remarkable. Her results show that hyperspectral data can provide accurate geologic and biological information about a geothermal system quickly and without a host of ground-based monitoring programs. Says Pickles, "Martini showed that when we move away from the center of the tree-kill area, plant health improves as we get further away. She discovered that it was possible to spot carbon dioxide leaks that were not previously mapped." (For more information about Martini's work, see www.es.ucsc.edu/ ~hyperwww/.)

The part of the collaboration dealing with the geothermal exploration project has expanded to include the University of Nevada at Reno and the University of Utah. It is now using geobotanical remote sensing techniques to look for possible new geothermal sites in many places in the western United States.

The expanded collaboration is funded by a DOE program that has the goal of dramatically increasing the use of geothermal energy in the western U.S. To accomplish that goal requires identifying and locating new geothermal fields that could potentially



Plant-stress mapping results at Horseshoe Lake (HSL) using 3-meter hyperspectral imagery.
(a) The Horseshoe Lake tree-kill mapping results. The lightest shades represent transitional zones, while the darker shades show the present boundaries of dead populations.
(b) Hyperspectral-based size estimates of the tree kills compared with contours of average carbon dioxide emissions measured on the ground by the U.S. Geological Survey (USGS) over several years.

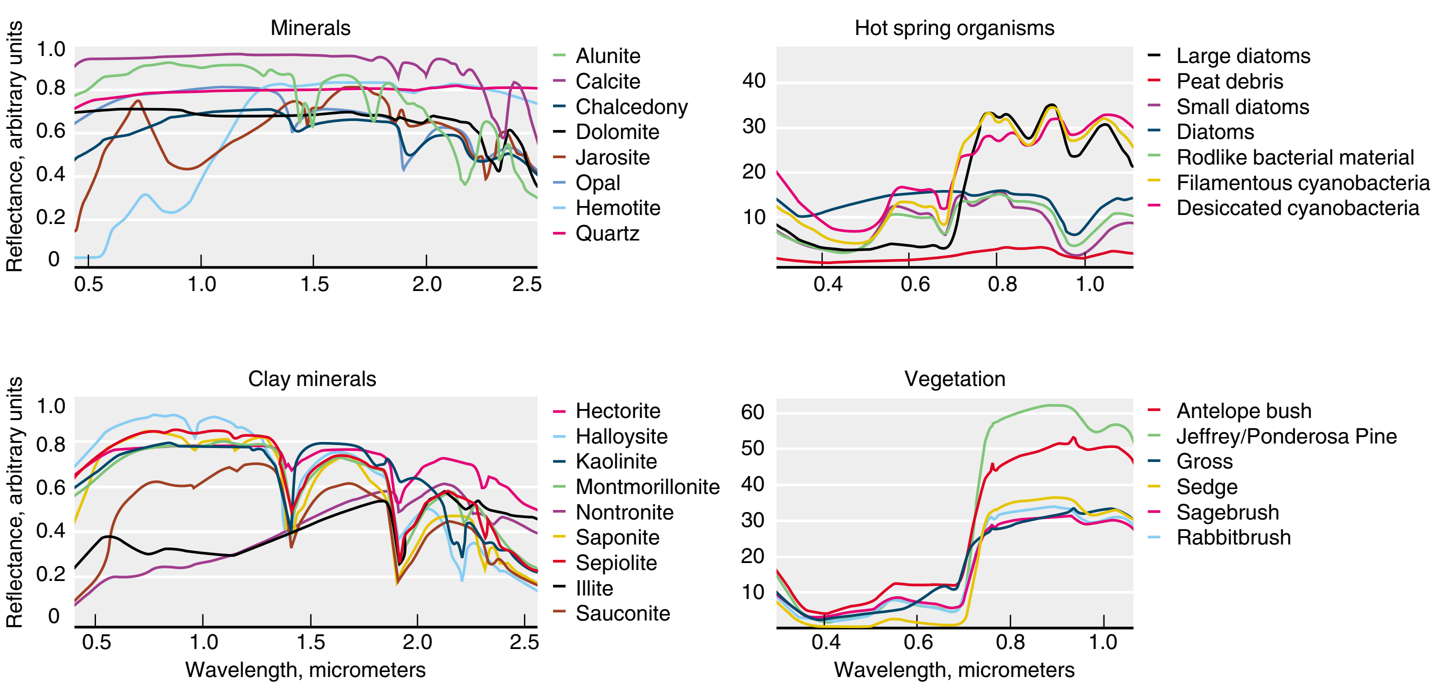
be used to produce electric power. In the past, geothermal fields have mostly been discovered by their characteristic surface effluents—springs and fumaroles, for instance.

Most of these fields in the western U.S. are now well catalogued. But questions remain as to whether there are a large number of currently undetected hidden thermal systems, systems that have little outflow to the surface, and whether there are large resources that are untapped in the known fields. Geobotanical remote sensing images in the visible and near-infrared spectra have proved successful in mapping subtle geobotanical surface clues that could lead to such discoveries. Currently, geothermal exploration projects are being conducted with newly acquired hyperspectral imagery of the Dixie Meadows and Fish Lake Valley fields in Nevada.

Watching Sequestered Carbon

As fossil fuel burning and tropical deforestation cause more carbon dioxide to make its way into the atmosphere, the U.S. and other nations are researching strategies to capture excess carbon dioxide and inject it into appropriate underground formations. Once there, it would either remain sequestered from the atmosphere for thousands of years or be available for near-term industrial use. Livermore has been involved in carbon sequestration research in a number of ways, such as developing criteria for identifying subsurface geologic formations that could be used for carbon dioxide storage. (See *S&TR*, December 2000, pp. 20–22.) Livermore's geobotanical remote sensing technique has also emerged as a primary, region-wide, early warning system for detecting carbon dioxide leaking from underground formations where it has been sequestered. Pickles explains, "This was a natural outgrowth of our work on looking for geothermal resources since we also would be monitoring the vegetation on the surface above. But instead of looking for any plant response to a geothermal resource, we'd be looking for carbon dioxide leaking from a reservoir to the surface."

The Laboratory's geobotanical remote sensing program is contributing to the Storage, Monitoring, and Verification task force for the Carbon Capture Project (CCP), an international effort funded by international energy companies and a number of governments. The goal of the project is to reduce carbon emissions and contribute toward a sustainable, environmentally acceptable, and competitively priced energy supply for the world. Among other efforts, the project is developing technologies to reduce the cost of capturing carbon dioxide from combustion sources and safely store it underground, where it can then be retrieved as needed. As Pickles notes, carbon dioxide has a value. It can be pumped into a geologic formation to promote increased oil flow and enhance oil recovery. Carbon dioxide is also an important industrial component used in making dry ice and in various chemical



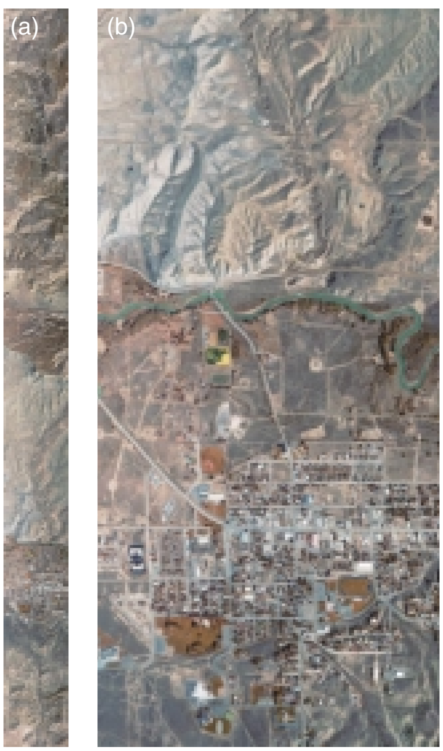
Hyperspectral images provide distinctive spectral shapes that allow identification of mineral types, clay soil types, plant species, plant health within species types, and hot and cold spring microorganisms. These spectra are from Mammoth Mountain–Long Valley hyperspectral imagery but are representative of most areas.

processes. (For more about the CCP, go to www.co2captureproject.org/.)

Livermore and UCSC researchers are testing their remote sensing techniques at the Rangely, Colorado, Enhanced Oil Recovery field. They hope to detect and discriminate hidden faults, establish geobotanical baselines, and look for effects of leaking carbon dioxide on plants and microorganisms in soil and water from low-altitude airborne hyperspectral imagery. Armed with on-the-ground carbon dioxide emission maps for plant species at Mammoth Mountain and high-resolution remote imagery of the same area, Martini established a semiquantitative relationship between plant health and amounts of average carbon dioxide emission. The team then acquired high-spatial-resolution imagery of the Rangely oil field in August 2002 and conducted an on-the-ground study of Rangely in collaboration with Ron Klusman, a professor from the Colorado School of Mines. Pickles and UCSC graduate student Wendy Cover are now analyzing the imagery and beginning to map signatures of carbon dioxide leakage, plant species, and soil types. Preliminary results show some interesting plant and soil signatures.

Pickles, Cover, Potts and Charles Christopher of British Petroleum-America, the CCP manager for this research, will return to the Rangeley field in June to check their interpretation of the imagery analysis, make more carbon dioxide measurements on the ground, and make detailed spectral measurements of special features. The next steps are to produce detailed geobotanical maps and maps of hidden faults, start some continuous carbon dioxide monitoring at potential leak points, and begin connecting surface features to subsurface modeling and existing oil field data.

The goal, says Pickles, is to develop a technique where a leak from an underground carbon dioxide reservoir could be detected quickly and dealt with. "Suppose an earthquake happens, and an underground carbon dioxide reservoir forms a crack. Carbon dioxide would then begin to appear at the surface." Pickles says. "Ideally, we would quickly see something strange going on in the vegetation above the fractured area. We would have already mapped out hidden faults and know about the earthquake. We would provide the early warning, so that a team could go out into the field, monitor the area, and remediate as necessary. Successful carbon sequestration involves many aspects; we provide the vigilance that will keep it safe."



(a) One line of hyperspectral imagery of the town of Rangely, Colorado. This image is shown (b) closer and (c) even closer. Note in (c) that the resolution is good enough to see cars on Main Street. The imagery is useful for learning how to prepare geobotanical maps of carbon dioxide leakage under towns.

Focusing at Ground Level

The geobotanical remote sensing program has come a long way and developed in many different directions from its initial beginnings. From providing early warning on pipeline infrastructure to geothermal energy to carbon sequestering and charting delicate ecological systems, the program has thrived on synergy. As remote sensing techniques improve, bringing better spatial and wavelength resolution, field work requirements have been minimized. In the end, it's the unique point of view of the researchers that brings the real power to this program.

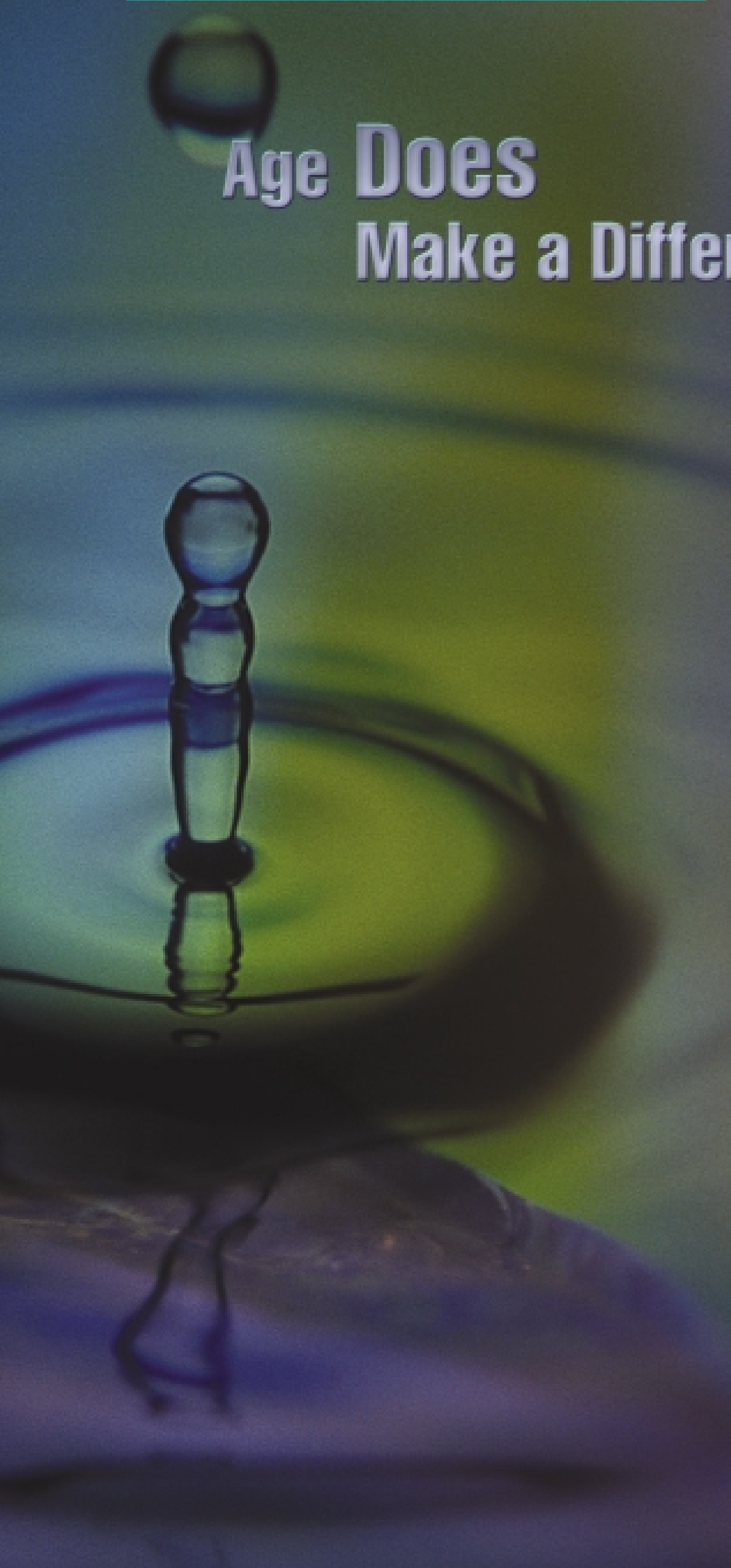
"At first, people were skeptical. Being able to sort out events from plant health was just a little hard for some folks to swallow," says Pickles. "But time has proven that high-resolution geobotanical imaging really works. It provides a complete picture and history. If you can learn how to read the signs, nature will tell you everything you need to know."

—Ann Parker

Key Words: carbon sequestration, Elkhorn Slough, energy infrastructure, geobotanical remote sensing, geothermal energy, homeland security, Mammoth Mountain, Nonproliferation Experiment.

For further information contact Bill Pickles (925) 422-7812 (pickles1@llnl.gov).

Age Does Make a Difference



When you drink a glass of water, the first question that might come to mind is not “how old is this water?” but “what’s in this water?” A study at Lawrence Livermore is demonstrating that, in many cases, answering the first question can help answer the second.

California residents have been asking a lot of questions about their drinking water, in particular about their groundwater—the source for 50 percent of the state’s drinking water. The closing of several public drinking wells because of contamination has concerned citizens so much that in 1999, the state mandated the Groundwater Ambient Monitoring and Assessment (GAMA) Program to investigate to what degree groundwater is susceptible to contamination.

The GAMA Program calls for testing every one of the approximately 16,000 public drinking wells scattered throughout the state. It is a daunting task, to be sure, but Livermore is a natural choice for tackling the challenge. “Livermore has a history of working with the state on groundwater issues and providing solutions,” according to environmental scientist Dave Rice. In 1999, for example, the Laboratory was part of an investigation that looked at leaking underground fuel tanks (LUFTs) and their effects on the state’s groundwater. (See *S&TR*, April 1999, pp. 21–23.) The Laboratory developed GeoTracker, a geographic information system that provides online access to data such as LUFT sites and all public well sites in California. Maintained by the state, GeoTracker is providing a repository for data generated by the GAMA Program.

According to physicist Bryant Hudson, Livermore scientists have partnered with the California State Water Resources Control Board and the U.S. Geological Survey to test 1,200 wells so far. Two years into the project, the scientists have analyzed wells in the Los Angeles–Orange County basin, the Santa Clara Valley, the Livermore–Niles area, and the counties of Sacramento, Butte, Fresno, and San Joaquin. During this testing, they have also been educating the public and students in schools about groundwater.

Young and Vulnerable

With a suite of analytical tools at their disposal, Laboratory scientists are developing a comprehensive picture of the state's groundwater resources. They are determining where contamination has occurred, what the groundwater flow pattern is, and from where the groundwater originates. The work begins with age-dating water from municipal drinking water wells. For groundwater geologists, the age of water is a good indicator of its probability of contamination.

Geochemist Jean Moran says using age to assess the vulnerability of groundwater to contamination is based on a simple concept: younger water has been in the aquifer for a shorter time, so it has more recent contact with ground surfaces where contaminants are present. Older water that has been in the subsurface for hundreds or thousands of years will have stayed relatively isolated and protected from any pollutants on the surface.

To determine how long the water has been out of contact with the atmosphere, Livermore scientists use the tritium–helium-3 method, a capability available only in a handful of laboratories worldwide. Tritium, a radioactive hydrogen isotope, occurs naturally at very low levels in Earth's upper atmosphere, but it was produced in much greater amounts during atmospheric nuclear testing in the 1950s and 1960s. Thus, it is an excellent tool for age-dating water that has entered an aquifer in the past 50 years. Tritium has a half-life of 12.3 years; it decays into helium-3, a stable noble gas.

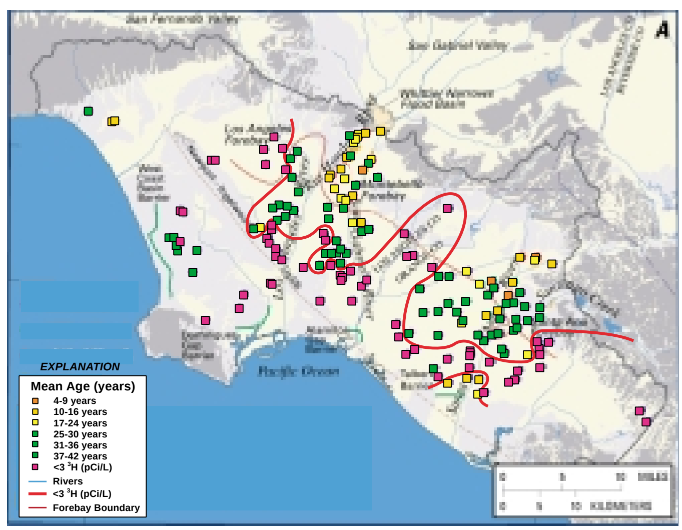
That helium-3 remains in solution once water containing tritium enters an aquifer. As tritium continues its decay over time, the amount of helium-3 in the water grows and the amount of tritium declines; the sum of both stays constant. By measuring both the remaining tritium and the decay product helium-3, scientists can determine the time at which the water entered the aquifer.

To measure tritium, the scientists remove all of the helium from a large water sample so they can see the decay of tritium into helium-3 over a two-week period. "The beauty of all of this is in the sensitivity of the measurements," Moran notes. Noble gas mass spectrometry allows measurements sensitive to just a few thousand helium-3 atoms. With such precision, the scientists can determine the age of a water sample to within about one year. These age determinations allow them to directly infer the direction and rate that the groundwater in the aquifer is flowing.

Tracking the Contamination

To test the principle that younger water is more likely to be contaminated, Livermore scientists perform several types of

An important part of the Groundwater Ambient Monitoring and Assessment Program is public education. Here, at the 2002 Edward Teller Science and Technology Education Symposium, Bryant Hudson uses a groundwater model to show students how water moves in a simulated aquifer.



A map of tritium–helium-3 ages measured in drinking water wells from Los Angeles and Orange counties. A general pattern of increasing age away from the artificial recharge areas (where water entering the aquifer reaches saturation) is observed. The red line shows the boundary between younger groundwater and groundwater more than 50 years old. The measured age shows the direction and rate the groundwater in the aquifer is flowing.

analyses to get a larger picture about groundwater resources in the state. One analysis detects actual contamination at ultratrace levels, using gas chromatography in combination with mass spectrometry to track volatile organic compounds (VOCs) such as the gasoline compound methyl tertiary-butyl ether (MTBE) and the dry cleaning solvent perchloroethylene (PCE). Such VOCs are ubiquitous and can be detected at very low concentrations nearly anywhere on Earth's surface. The analyses require that the mass spectrometer used to detect VOCs in groundwater be stringently clean; the responsibility for keeping it that way falls to Livermore scientist Roald Leif, who makes it possible to detect VOCs to parts-per-trillion sensitivity. The detection results indicate where groundwater has been contaminated and also verify the age-dating results.

In another analysis to round out their information about the state's groundwater, the scientists measure two stable oxygen isotopes (oxygen-16 and oxygen-18) to determine the origin and flow patterns of contaminated water. The ratio of oxygen-16 to oxygen-18 in the water varies, depending on where the water precipitated, the elevation at which it was found, and its distance from the ocean. For example, water from the Sierra Nevada has a different ratio of these oxygen isotopes than that found in precipitation in the San Francisco Bay Area. Using a mass spectrometer, the team can measure the isotope ratio and determine the source of the water.

Older May Be Better

Some of the data analysis shows that older water can remain relatively contaminant-free, despite its location. For example, the Silicon Valley, with its large number of contaminated waste disposal sites and more Superfund sites than anywhere else in the nation, has remarkably uncontaminated drinking water wells. Because most of the Silicon Valley water has been resident in underground aquifers for longer than the contaminants have been present, the water has been relatively protected, and very few VOCs have been detected. A similar example is in the Los Angeles and Orange County basins. Despite their urban location, 59 of 176 wells tested were devoid of tritium, and those same wells were free of VOCs. The pathway of water into the aquifer is blocked by thick layers of clay, and that has kept most of the water underneath the basin protected from surface contaminants over the past 50 years.

The vulnerability of younger water to contamination can be seen in the Livermore Valley. The east side of the water basin (under the city of Livermore) has widespread PCE occurrence and younger groundwater ages than the west side. Water located on the west side of the basin, under the city of Pleasanton, approximately 10 kilometers away, is protected by a confining layer that prevents the direct transport of water from the surface to the aquifer.

Being Prepared

Next year, the group hopes to take the age data accumulated so far and study nitrate contamination, which is the most frequent cause for shutting down a drinking water well in California. In the meantime, Livermore's data showing that newer isn't better will help the state make informed decisions to protect wells and plan future development. Moran says California intends to increase its use of groundwater for drinking purposes, and these data could keep the state from making costly mistakes.

"If you know the age of the groundwater in a basin, it can tell you how fast water is moving, where it is being replenished in the ground, how much storage you have, how fast water turns over—a complete picture," Moran says. "Water is a huge issue in California, so the more data you have, the better."

—Laurie Powers

Acknowledgment: This work is managed by the Environmental Protection Department in collaboration with the Chemistry and Materials Science and the Energy and Environment directorates.

Key Words: age-dating, groundwater contamination, stable oxygen isotopes, tritium–helium-3 analysis.

For further information contact Jean Moran (925) 423-1478 (moran10@llnl.gov).

Reducing Aerodynamic Drag

FOR every mile down the freeway, the average-size American car has to push 5.5 metric tons of air out of its way. That is, quite literally, a drag. Overcoming this aerodynamic drag takes a lot of energy. In fact, at 70 miles (110 kilometers) per hour, the typical highway speed, as much as 65 percent of the fuel the car uses goes to overcoming air resistance.

The numbers are similar for big-rig tractor–trailers, despite their far greater weight, and even higher for high-speed trains. Traveling as fast as 185 miles per hour, high-speed trains may use up to 80 percent of their fuel to overcome drag.

Truck aerodynamics researchers with scale model truck inside the wind tunnel at Ames Research Center, National Aeronautics and Space Administration. Clockwise from top left are James Ross of NASA Ames and Rose McCallen, Kambiz Salari, and Jason Ortega of Livermore.

For more than five years, Livermore has led a Department of Energy project to examine possible ways to make heavy trucks more aerodynamic, reducing air resistance and thus increasing fuel efficiency. Obviously, air resistance cannot be eliminated entirely. But engineers estimate that truck drag coefficients could be reduced by as much as 25 percent over the next 20 years. In the future, such a reduction would save billions of liters of diesel fuel annually, or 12 percent of the fuel used.

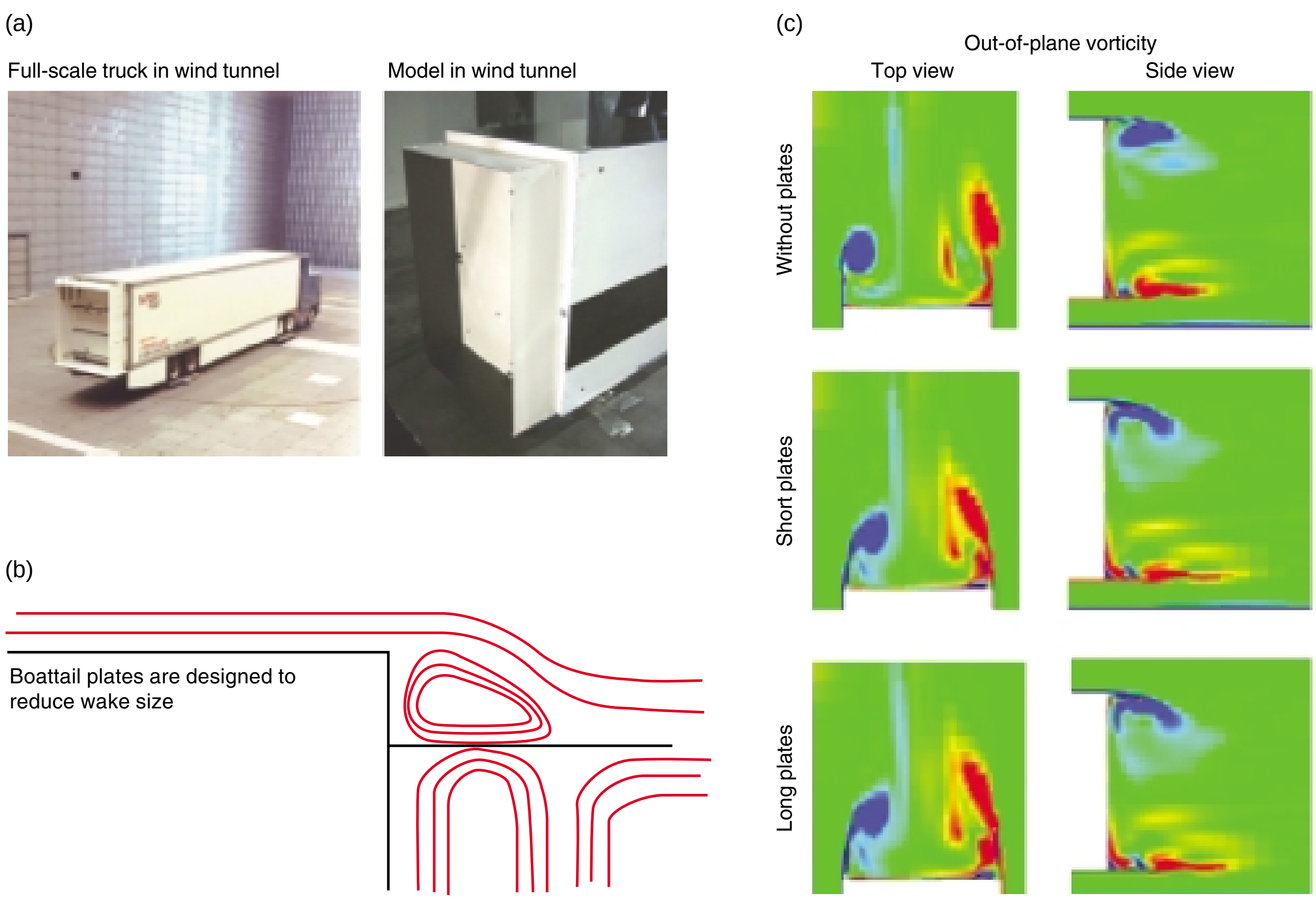
"Our nation's dependence on oil is a national security issue," says project leader Rose McCallen. "Minimizing vehicle aerodynamic drag can significantly reduce this country's dependence on foreign oil."

Current predictions are that at present rates of consumption, world energy demand will begin to exceed energy available from all sources by the year 2050. Reducing consumption is just one approach to meeting this challenge head on.

After the first oil crisis in the early 1970s, trucking companies adopted a shield that curves up over the top of the trailer to reduce drag. But two major components of drag on a heavy truck remain: the gap between the tractor and the trailer and low pressure in the trailer's wake. Friction losses—the air shear resistance on the trailer–tractor sides—contribute 10 to 20 percent to the total vehicle drag.

"Trucks are much more complicated than cars and planes, which are integrated and streamlined," notes McCallen. "Not only do trucks come in two parts, with a gap in between, but the trailer has to be a big unstreamlined box to maximize cargo space."

As if the aerodynamic situation weren't complicated enough, tractors and trailers are built by different companies. "It would be wonderful to be able to manufacture a single unit," she adds, "but it just isn't going to happen."



Large-eddy simulations of the back end of a trailer with boattail plates. (a) The full-scale truck and the scale model, (b) diagram of the flow field of boattail plates, and (c) simulations of a truncated vehicle (showing just the back end of the trailer) with and without boattail plates. Red and blue indicate counterrotating vortices. The flow is from left to right in the side view.

An Aerodynamic Partnership

Responding to the complex physics problem of truck aerodynamics is a consortium of Livermore, Sandia, and Argonne national laboratories, University of Southern California (USC), California Institute of Technology (Caltech), National Aeronautics and Space Administration Ames Research Center (NASA Ames), and Georgia Tech Research Institute (GTRI), under the leadership of McCallen in Livermore's Energy Technology and Security Program. The DOE Energy Efficiency and Renewable Energy, Office of FreedomCAR & Vehicle Technologies (CAR stands for Cooperative Automotive Research), is supporting the consortium's effort. Four tractor manufacturers have joined the partnership as well: AB Volvo, which owns Mack Trucks, Inc.; International Truck and Engine Corporation; Freightliner Limited; and Paccar Inc., which manufactures both Kenworth and Peterbilt trucks.

The aerodynamic design of heavy trucks is currently based on performance estimates derived from wind tunnel, track, and road experiments. Now, with the availability of powerful supercomputers, scientists can begin to simulate complex tractor–trailer air flows. The trick is to make the simulations reliable and thus predictive. The simulations must also run efficiently, with quick turnaround times. Only then will they be useful for designers of heavy tractors and trailers.

The simulations must be able to accurately portray the complex interaction between a vehicle's many different surfaces and the air striking or moving past it. The air flow around the front end of the tractor is complicated by the bumper, head lamps, hood, mirrors, and any other trim that the driver has chosen to add. The contribution to drag from the gap flow between the tractor and the trailer and behind the trailer has already been noted. Air also flows along the underbody of the truck and in the wheel wells. Computational fluid dynamics, McCallen's area of expertise, is the tool of choice on this project.

As computer simulations of various parts of a truck's air flow are being performed by Caltech and the Lawrence Livermore, Sandia, and Argonne national laboratories, companion wind tunnel experiments using models of tractor–trailers are under way at NASA Ames, USC, and GTRI. Livermore, USC, and GTRI are also developing devices that can be attached to tractors or trailers that reduce aerodynamic drag.

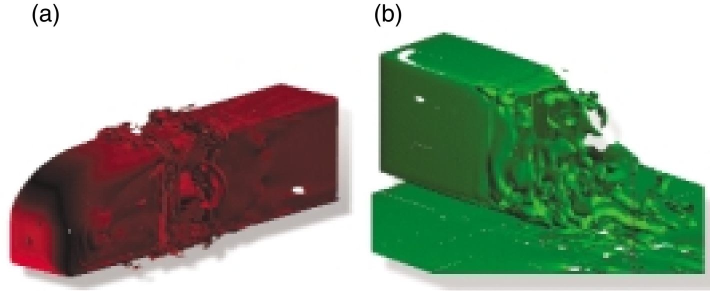
Air Flow in Action

Complex turbulent flows—whether in the explosion of a nuclear weapon or in the wake of a heavy tractor–trailer—are particularly challenging problems in fluid dynamics. Livermore has been working to simulate turbulence for decades, first for weapons design and more recently for stewardship of the nation's nuclear stockpile. For this project, Livermore's focus is again on turbulence, this time in the trailer's wake. Engineer Kambiz Salari is leading the Livermore effort.

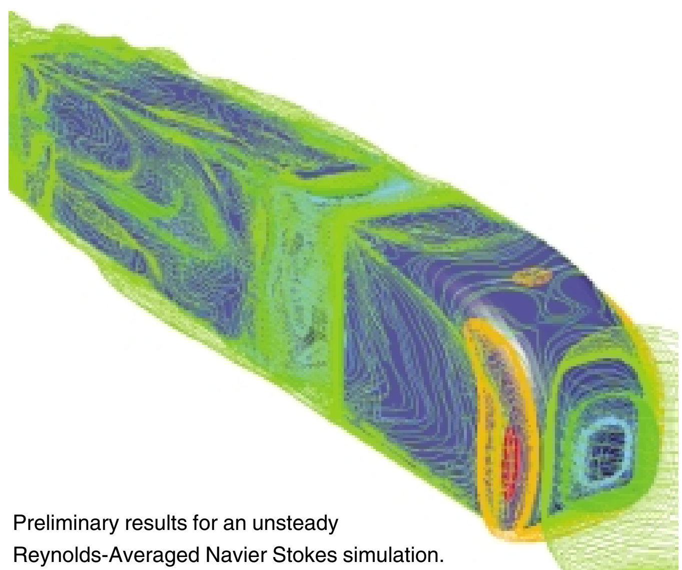
Salari's team first developed a simplified three-dimensional (3D) form representing the typical tractor–trailer combinations, a geometry that is now being used by other researchers around the world. With this form, Salari and his team are using large-eddy simulations (LES) to model what happens at the back end of the trailer.

Some of their simulations have included boattail plates attached to the back of the trailer to reduce the wake. The

(a) (b)



Models using large-eddy simulation software show air flow in (a) the tractor–trailer gap and (b) the trailer's wake.



Preliminary results for an unsteady Reynolds-Averaged Navier Stokes simulation. The truck model used is the cab-over design. Air flow in the gap between the tractor and the trailer and in the trailer's wake are visible. This simulation methodology more accurately models wake and hence total drag than steady Reynolds-Averaged Navier Stokes methods.

figure on p. 26 shows "snapshots" of the flow field with short and long boattail plates and without these plates. (The plates were designed by a private firm not involved in the partnership.) The simulations with the plates indicate a reduction in the trailer wake, which is consistent with wind tunnel experiments at NASA Ames.

The consortium recently obtained the first 3D particle image velocimetry (PIV) results in a large production wind tunnel. Three-dimensional PIV techniques being developed at NASA Ames use laser beams to measure the velocity and direction of air flow in a series of planes. Two-dimensional PIV is far more common, and experiments usually take place in small research wind tunnels. But NASA Ames is home to a 2-meter by 3-meter wind tunnel, where the first 3D PIV images were obtained using a one-eighth scale model. More recently, experiments were run in a 3.5-meter pressurized wind tunnel at NASA Ames.

The pressurized tunnel is capable of simulating the air flow at realistic highway speeds. Because the wind tunnel is housed in a pressure vessel, the PIV experiments in the vessel are controlled remotely to avoid blowdown (pressure release) of the vessel when the laser or cameras are repositioned; obviously, no one can be in the tunnel during an experiment.

Engineer Jason Ortega, a member of Salari's team, has been developing new devices that show promise for reducing aerodynamic drag. Detailed tests incorporating these devices started this spring at one of the wind tunnels at NASA Ames.

Sandia has been using steady Reynolds-Averaged Navier Stokes (RANS) models to simulate air flow around a heavy tractor–trailer. But researchers are finding that steady RANS models, which are routinely used to simulate fluid dynamics and are computationally efficient, do not accurately predict tractor–trailer wake or low-pressure region. So Livermore is developing hybrid techniques that combine LES and unsteady RANS turbulence models, resulting in more accurate, predictive simulations. Drag estimates must be correct before solutions can be found.

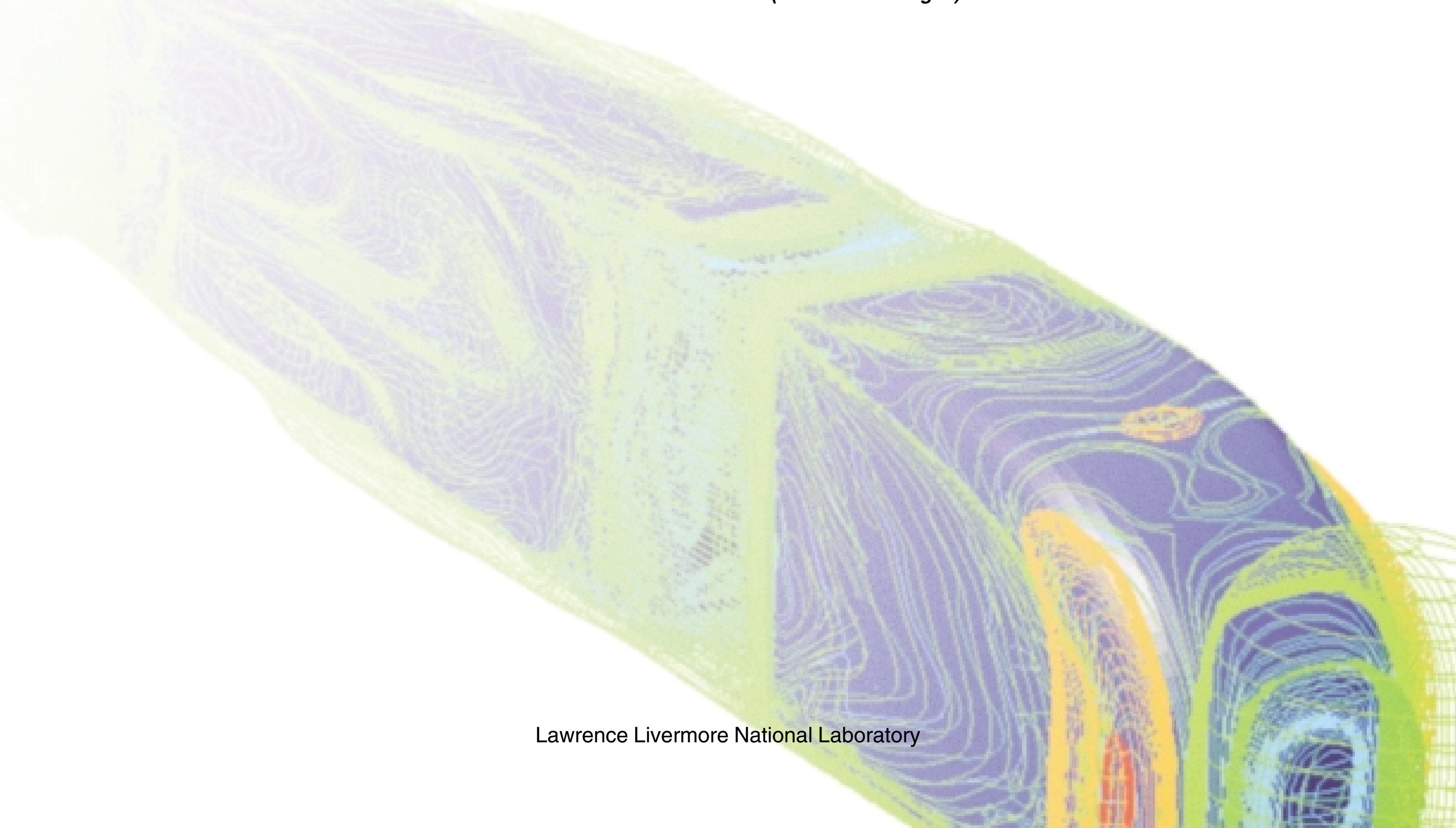
A World of Interest

Outside interest in the partnership's work was evident in the large turnout for a December 2002 conference in Monterey, California, on "The Aerodynamics of Heavy Vehicles: Trucks, Buses, and Trains." DOE and the United Engineering Foundation sponsored this conference that brought together researchers in aerodynamics from national laboratories, universities, and corporations around the world. Interest was so high that a similar conference is planned for 2004. Saving energy is important—reducing drag on heavy vehicles is one way to do it.

—Katie Walter

Key Words: aerodynamics, computational fluid dynamics, heavy trucks, large-eddy simulations (LES), Reynolds-Averaged Navier Stokes (RANS) models.

For further information contact Rose McCallen (925) 423-0958 (mccallen1@llnl.gov).



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

Method for Producing Damage Resistant Optics
Lloyd A. Hackel, Alan K. Burnham, Bernardino M. Penetrante, Raymond M. Brusasco, Paul J. Wegner, Lawrence W. Hrubesh, Mark R. Kozlowski, Michael D. Feit
U.S. Patent 6,518,539 B2
February 11, 2003
A system that mitigates the growth of surface damage in an optic. In an embodiment of the invention, damage sites in the optic are initiated, located, and then treated to stop the growth of the damage sites. The step of initiating damage sites in the optic includes a scan of the optic with a laser to initiate defects. The exact position of the initiated sites is identified. A mitigation process is performed that locally or globally removes the cause of subsequent growth of the damaged sites.

High Air Volume to Low Liquid Volume Aerosol Collector
Donald A. Masquelier, Fred P. Milanovich, Klaus Willeke
U.S. Patent 6,520,034 B1
February 18, 2003
A high-air-volume to low-liquid-volume aerosol collector. A high-volume flow of aerosol particles is drawn into an annular, centripetal slot in a collector that directs the aerosol flow into a small pool of liquid contained in a lower center section of the collector. The annular jet of air impinges upon the liquid, embedding initially airborne particles in the liquid. The liquid in the pool continuously circulates in the lower section of the collector by moving to the center line, then upward, and then, with assistance from a rotating deflector plate, passes back into the pool at the outer area adjacent to the impinging air jet. The air jet moves upward through the liquid pool, through a hollow center of the collector, and is then discharged via a side outlet. Any liquid droplets escaping with the effluent air are captured by a rotating mist eliminator and moved back toward the liquid pool. The collector includes a sensor assembly for determining, controlling, and maintaining the level of the liquid pool. It includes a lower, centrally located valve assembly connected to a liquid reservoir and to an analyzer for analyzing the particles that are impinged into the liquid pool.

Method for Fabricating Beryllium-Based Multilayer Structures
Kenneth M. Skulina, Richard M. Bionta, Daniel M. Makowiecki, Craig S. Alford
U.S. Patent 6,521,101 B1
February 18, 2003
A process for fabricating beryllium-based multilayer mirrors useful in the wavelength region greater than the beryllium K-edge (11.1 nanometers). The process includes alternating sputter deposition of beryllium and a metal—typically from the fifth row of the periodic table—such as niobium, molybdenum, ruthenium, and rhodium. The process includes not only the method of sputtering the materials but also the industrial hygiene controls for safe handling of beryllium. The mirrors made in accordance with the process may be used in soft x-ray and extreme ultraviolet project lithography, which requires mirrors of high reflectivity (greater than 60 percent) for x rays in the range of 6.0 to 14.0 nanometers.

Microfabricated Electrochemiluminescence Cell for Chemical Reaction Detection
M. Allen Northrup, Yun-Tai Hsueh, Rosemary L. Smith
U.S. Patent 6,521,181 B1
February 18, 2003
A detector cell for a silicon-based or nonsilicon-based sleeve-type chemical reaction chamber that combines heaters, such as doped polysilicon for heating and bulk silicon for convection cooling. The detector cell is an electrochemiluminesence cell constructed of layers of silicon with a cover layer of glass. It has electrodes spaced between various layers forming the cell. The cell has a cavity into which fluid inlets direct reaction fluids. The reaction chamber and detector cell may be used in any chemical reaction system for synthesis or processing of organic, inorganic, or biochemical reactions, such as the polymerase chain reaction, or other DNA reactions, such as the ligase chain reaction. These are examples of synthetic, thermal-cycling-based reactions. The electroluminescence cell may also be used in synthesis instruments, particularly those for DNA amplification and synthesis.

Ion Beam Collimating Grid to Reduce Added Defects
Walter B. Lindquist, Patrick A. Kearney
U.S. Patent 6,521,897 B1
February 18, 2003
A collimating grid located after the exit grid of an ion source that collimates the ion beamlets, disallows beam spread, and limits beam divergence during transients and steady-state operation. The additional exit or collimating grid prevents beam divergence during turn-on and turn-off and prevents ions from hitting the periphery of the target where there is redeposited material. Or it prevents ions from missing the target and hitting the wall of the vessel where there is deposited material, thereby preventing defects from being deposited on a substrate to be coated. Thus, the addition of a collimating grid to an ion source ensures that the ion beam will hit and be confined to a specific target area.

Optical Detection Dental Disease Using Polarized Light
Matthew J. Everett, Billy W. Colston, Jr., Ujwal S. Sathyam, Luiz B. Da Silva, Daniel Fried
U.S. Patent 6,522,407 B2
February 18, 2003
A polarization-sensitive optical imaging system is used to detect changes in polarization in dental tissues to help diagnose diseases such as caries. The degree of depolarization is determined by illuminating the dental tissue with polarized light and measuring the polarization state of the backscattered light. The polarization state of this reflected light is analyzed with optical polarimetric imaging techniques. A handheld fiber-optic dental probe is used in vivo to direct the incident beam to the dental tissue and collect the reflected light. For depth-resolved characterization of the dental tissue, the polarization diagnostics may be incorporated into optical coherence domain reflectometry and optical coherence tomography systems, which enable identification of subsurface depolarization sites associated with demineralization of enamel or bone.

Microfabricated Sleeve Devices for Chemical Reactions
M. Allen Northrup
U.S. Patent 6,524,532 B1
February 25, 2003
A silicon-based sleeve-type chemical reaction chamber that combines heaters, such as doped polysilicon, and bulk silicon for convection cooling. The reaction chamber combines a critical ratio of silicon- and nonsilicon-based material to provide the desired thermal properties. For example, the chamber may combine a critical ratio of silicon and silicon nitride to the volume of material to be heated (for example, a liquid) in order to provide uniform heating at low power requirements. The reaction chamber will also allow the introduction of a secondary tube (for example, plastic) into the sleeve containing the reaction mixture, thereby alleviating any potential material incompatibility issues. The reaction chamber may be used in any chemical reaction system for synthesis or processing of organic, inorganic, or biochemical reactions, such as the polymerase chain reaction, and other DNA reactions, such as the ligase chain reaction. These are examples of synthetic, thermal-cycling-based reactions. The reaction chamber may also be used in synthesis instruments, particularly those for DNA amplification and synthesis.

Cryogenic High-Resolution X-Ray Detector with High Count Rate Capability
Matthias Frank, Carl A. Mears, Simon E. Labov, Larry J. Hiller, Andrew T. Barfknecht
U.S. Patent 6,528,814 B1
March 4, 2003
A cryogenic high-resolution x-ray detector with high count rate capability. The new detector is based on superconducting tunnel junctions and operates without thermal stabilization at or below 500 millikelvins. The x-ray detector exhibits good resolution (approximately 5 to 20 electronvolts full width at half-maximum) for soft x rays in the kiloelectronvolt region and is capable of count rates of more than 20,000 counts per second. Simple field-effect-transistor–based charge amplifiers, current amplifiers, or conventional spectroscopy–shaping amplifiers can provide the electronic readout of this x-ray detector.

Electro-Mechanical Heat Switch for Cryogenic Applications
Marcel L. van den Berg, Jan D. Batteux, Simon E. Labov
U.S. Patent 6,532,759 B1
March 18, 2003
A heat switch includes two symmetric jaws. Each jaw is composed of a link connected at a translatable joint to a flexible arm. Each arm rotates about a fixed pivot and has an articulated end that includes a thermal contact pad connected to a heat sink. The links are joined together at a translatable main joint. To close the heat switch, a closing solenoid is actuated and forces the main joint to an over-center position. This movement rotates the arms about their respective pivots, forces each of them into a stressed configuration, and forces the thermal contact pads toward each other and into compressive contact with a cold finger. The closing solenoid is then deactivated. The heat switch remains closed because of a restoring force generated by the stressed configuration of each arm, until actuation of an opening solenoid returns the main joint to its starting open-switch position.

Correlated Histogram Representation of Monte Carlo Derived Medical Accelerator Photon-Output Phase Space
Alexis E. Schach Von Wittenau
U.S. Patent 6,535,837 B1
March 18, 2003
A method is provided to represent the calculated phase space of photons emanating from medical accelerators used in photon teletherapy. The method reproduces the energy distributions and trajectories of the photons originating in the bremsstrahlung target and the photons scattered by components within the accelerator head. The method reproduces the energy and directional information from sources up to several centimeters in radial extent, so it is expected to generalize well to accelerators made by different manufacturers. The method is computationally fast and efficient, with overall sampling efficiency of 80 percent or higher for most field sizes. The computational cost is independent of the number of beams used in the treatment plan.

HEPA Filter Encapsulation
Dianne D. Gates-Anderson, Scott D. Kidd, John S. Bowers, Ronald W. Attegery
U.S. Patent 6,537,350 B2
March 25, 2003
A low-viscosity resin is delivered into a spent HEPA filter or other waste. The resin is introduced into the filter or other waste using a vacuum to assist in the mass transfer of the resin through the filter media or other waste.

Bubble Diagnostics
Steven R. Visuri, Beth M. Mannimini, Luiz B. Da Silva, Peter M. Celliers
U.S. Patent 6,538,739, B1
March 25, 2003
A means of diagnosing the presence of a gas bubble and incorporating the information into a feedback system for optoacoustic thrombolysis. In optoacoustic thrombolysis, pulsed laser radiation at ultrasonic frequencies is delivered intraluminally down an optical fiber and directed toward a thrombus or otherwise occluded vessel. Dissolution of the occlusion is therefore mediated through ultrasonic action of propagating pressure or shock waves. A vapor bubble in the fluid surrounding the occlusion may form as a result of laser irradiation. This vapor bubble may be used to directly disrupt the occlusion or as a means of producing a pressure wave. It is desirable to detect the formation and follow the lifetime of the vapor bubble. Knowledge of the bubble formation and lifetime yields critical information as to the maximum size of the bubble, density of the absorbed radiation, and properties of the absorbing material. This information can then be used in a feedback system to alter the irradiation conditions.

Process for Direct Integration of a Thin-Film Silicon P-N Junction Diode with a Magnetic Tunnel Junction

Daniel Toet, Thomas W. Sigmon
U.S. Patent 6,541.316 B2
April 1, 2003
A process for direct integration of a thin-film silicon p-n junction diode with a magnetic tunnel junction for use in advanced magnetic random access memory cells of high-performance, nonvolatile memory arrays. The process is based on pulsed laser processing for the fabrication of vertical polycrystalline silicon electronic device structures, in particular p-n junction diodes, on films of metals deposited on low-temperature substrates such as ceramics, dielectrics, glass, or polymers. The process preserves underlayers and structures onto which the devices are typically deposited, such as silicon integrated circuits. The process involves the low-temperature deposition of at least one layer of silicon, either in an amorphous or a polycrystalline phase on a metal layer. Dopants may be introduced in the silicon film during or after deposition. The film is then irradiated with short-pulse laser energy, which is efficiently absorbed in the silicon, resulting in the crystallization of the film and simultaneously in the activation of the dopants by ultrafast melting and solidification. The silicon film can be patterned either before or after crystallization.

System and Method for Characterizing, Synthesizing and/or Canceling Out Acoustic Signals from Inanimate Sound Sources

John F. Holzrichter, Greg C. Burnett, Lawrence C. Ng
U.S. Patent 6,542, 857 B1
April 1, 2003
A system and method for characterizing, synthesizing, and/or canceling out acoustic signals from inanimate sound sources. Propagating-wave electromagnetic sensors monitor excitation sources in sound-producing systems, such as machines, musical instruments, and various other structures. Acoustical output from these sound-producing systems is also monitored. From such information, a transfer function characterizing the sound-producing system is generated. From the transfer function, acoustical output from the sound-producing system may be synthesized or canceled. These methods enable accurate calculation of matched transfer functions relating specific excitations to specific acoustical outputs. Knowledge of such signals and functions can be used to effect various sound replication, sound source identification, and sound cancellation applications.

Awards

Steve Grey, head of the Laboratory's American Indian program, has been chosen **Indian affairs director** for the **Department of Energy**. Grey grew up on the Navajo reservation and has managed a DOE field office at the Navajo Community College in Shiprock, New Mexico. He is also chairman of the Navajo Nation Telecommunications Regulatory Commision.

Bill Durham of the Geophysics and Global Security Division of the Energy and Environment Directorate has been elected a **fellow** of the **American Geophysical Union (AGU)**. Among Durham's contributions to geophysics is his work on the rheology of ice, synthesis of methane hydrates in the laboratory, and laboratory measurements of the physical properties of rocks and minerals.

AGU awards fellowships to scientists who have attained acknowledged eminence in one or more branches of geophysics. It elects no more than one-tenth of a percent of its membership as fellows.

Bob Schanilec of the Lawrence Livermore Television Network has earned a **Crystal Award of Excellence** from the **Communicator Awards 2002 Video Competition** for his editing and videography on "Fifty Years of Innovation in Nuclear Weapon Design," which was commissioned by the Defense and Nuclear Technologies Directorate. Shanilec also won an **Award of Distinction** for the Laboratory's 50th anniversary video, "Making History—Making a Difference."

Another **Award of Distinction** was won by **Donald Harrison**, also of the Lawrence Livermore Television Network. He was recognized in the "External Communications/Meeting Opener" category for "Beyond Boundaries," a video about the Laboratory's supercomputing program, which was produced for the 2001 Supercomputing Conference in Denver.

The Communicator Awards is an international competition that recognizes outstanding work in communications. Entries in the competition are judged by industry professionals who look for work that serves as a benchmark for the industry.

Additionally, Schanilec received an **Aegis Award** for his production work on "Making History—Making a Difference." The Aegis Awards are the video industry's premier competition for peer recognition of outstanding video production and nonnetwork television commercials.

Laboratory scientists **Claire Max** and **Ellen Raber** have been inducted into the **Alameda County Women's Hall of Fame**. Inductees are chosen by the Alameda County Board of Supervisors, the Alameda County Health Care Foundation, and the Commission on the Status of Women.

Max is an astrophysicist in the Institute of Geophysics and Planetary Physics and associate director of the National Science Foundation's Center for Adaptive Optics based at the University of California at Santa Cruz. She specializes in using adaptive optics to minimize the blurring effects of turbulence in Earth's atmosphere, thereby improving the view of celestial objects through ground-based telescopes.

Raber is head of the Environmental Protection Department. In her 22 years at the Laboratory, she has used her background in geochemistry to resolve a variety of environmental issues related to geothermal energy, underground coal gasification, the strategic petroleum reserve, and nuclear waste management. Her most recent accomplishment has been in the development of L-gel, a decontaminating agent that is effective against chemical and biological warfare agents and breaks down to environmentally acceptable byproducts.

The recipients of the **2002 Edward Teller Fellowships** are **Fred Milanovich** and **Cynthia K. Nitta**. The fellowship is awarded to employees who have made outstanding contributions to the Laboratory.

Milanovich is being recognized for his outstanding scientific contributions and technical leadership, particularly for his recent role as an intellectual leader supporting the nation's programs to counter the threats posed by biological weapons and for developing innovative detection capabilities.

Nitta's contributions are to the Laboratory's weapons program. She was nominated for the fellowship by Associate Director Bruce Goodwin, who proposed that she be given the opportunity to pursue a program of research and studies to explore the implications of recent nuclear policy changes stemming from the Nuclear Posture Review.

Chemical Weapons Can't Evade This Lab

The international Organisation for the Prohibition of Chemical Weapons (OPCW) has certified Livermore's Forensic Science Center (FSC) to support its chemical weapons inspections. The FSC was selected by the U.S. State Department in 2000 to become the second U.S. laboratory to provide this support. OPCW-certified laboratories test samples collected by OPCW inspectors from chemical plants and other sites. Under the terms of the Chemical Weapons Convention, which is the international agreement banning chemical weapons, all inspection samples must be analyzed at two OPCW-designated laboratories. In addition, the U.S. Senate has mandated that all samples obtained within the U.S. be tested within the U.S. to protect proprietary information belonging to American chemical manufacturers.

Livermore achieved certification by passing three grueling proficiency tests that involved the analysis and characterization of samples containing combinations of extremely dilute amounts of chemical warfare agents, precursor chemicals, and decomposition products as well as other chemicals included to complicate or obfuscate the analysis.

Contact:
Armando Alcaraz (925) 423-6889 (alcaraz1@llnl.gov).

Bird's-Eye View Clarifies Research on the Ground

Nearly a decade ago, physicist Bill Pickles noticed an interesting phenomenon during an underground nonproliferation experiment at the Nevada Test Site. The shock of the underground explosion shocked the plants into early senescence. Those stressed plants showed up clearly in spectroscopic imagery taken with a remote sensor system mounted to an airplane that imaged the area the day before and the day after the experiment. In the ensuing 10 years, geobotanical remote sensing—using airborne spectroscopic imagery to analyze plant health and correlate it to events both natural and human made—has found a wide variety of applications. Such sensing is now part of efforts to develop methods of detecting damage to natural gas pipelines and to uncover hidden geothermal resources that could be used in the future as energy sources. Geobotanical remote sensing is also being considered to provide a region-wide, early warning system for detecting carbon dioxide leaking from underground formations where it has been sequestered for future use. Researchers from the University of California at Santa Cruz, in collaboration with Pickles, are also using geobotanical remote sensing to monitor and set baseline conditions for ecologically sensitive areas such as wetlands and coral reef systems.

Contact:
Bill Pickles (925) 422-7812 (pickles1@llnl.gov).

U.S. Government Printing Office: 2003/583-060-70041

Coming Next Month

Riding the Waves of Supercomputing Technology

Livermore's Computation Directorate is riding the crest of three technology waves to ensure high-performance, cost-effective computing for Livermore scientists today and in the future.

Also in June

- ***As part of the Human Genome effort, Livermore scientists have focused on mapping and sequencing the genes of chromosome 19.***
- ***For the first time, scientists have determined the mass of a star in isolation from other celestial bodies.***
- ***A Livermore team is testing a fuel tank for passenger vehicles that can simultaneously store three types of hydrogen fuel.***

University of California
Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

Nonprofit Org.
U. S. Postage
PAID
Albuquerque, NM
Permit No. 853

Printed on recycled paper.