April 2004

Science & Technology Review

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Mapping Pathogens for Biodefense

Also in this issue:

- **Yucca Mountain's Engineered Barrier System**
- **Controlling Combustion for a Cleaner, More Efficient Engine**

About the Cover

A Livermore team is developing DNA and protein signatures for pathogens and deploying validated assays in the field as part of the national effort to defend against bioterrorism. As the article beginning on p. 4 describes, signatures have been developed for virtually every biothreat pathogen for which adequate genomic sequences are available. Advances in computing science have significantly reduced the time of a key step in the signature development process, resulting in faster and more reliable biodetection capabilities.

Cover design: Kitty Madison

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.

National Nuclear Security Administration

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

Science & Technology Review

April 2004

Lawrence Livermore National Laboratory

Contents

Features

Research Highlights

Departments

S&TR Staff

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

S&TR is available on the 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-TR-52000-04-4
Distribution Category UC-99
April 2004

Discovery of new superheavy elements 113 and 115

The two newest superheavy elements, 113 and 115, were recently discovered through a collaborative effort between researchers from the Joint Institute for Nuclear Research (JINR) in Russia and scientists from Livermore's Glenn T. Seaborg Institute and the Chemistry and Materials Science Directorate.

In experiments conducted between July 14 and August 10, 2003, at the JINR U400 cyclotron with the Dubna gas-filled separator, the team of scientists observed atomic decay patterns, or chains, that confirm the existence of elements 113 and 115. In these decay chains, element 113 is produced via the alpha decay of element 115. Energy Secretary Spencer Abraham says, "These elemental discoveries underscore both the value of federally supported basic research and the benefit of unfettered international scientific collaboration."

The experiments produced four atoms each of element 113 and element 115 through the fusion reaction of calcium-48 nuclei impinging on an americium-243 target. The team observed three similar decay chains consisting of five consecutive alpha decays, which combined took less than 30 seconds and terminated in a spontaneous fission of an element-105 (dubnium) isotope with a very long half-life (16 hours). Results from the team's research are featured in the February 2, 2004, issue of *Physical Review C*.

Joshua Patin, Livermore's primary data analyst on the team, says the three similar decay patterns were a "positive identifier that something good had been seen, because the long decay chains just don't happen that often." Scientists at Livermore and JINR independently verified the data.

Contact: Joshua Patin (925) 422-6341 (patin1@llnl.gov).

Details of water-to-air interface revealed

Using the Laboratory's terascale computers, Livermore scientists have revealed details of the reactive states and faster relaxation of molecules at the interface of water and air. Christopher Mundy and I-Feng Kuo created the first ab initio simulations of a stable liquid–air interface. Ab initio simulations present an unbiased representation of water in different environments and are ideal for explaining surface conditions.

The data analysis shows a faster relaxation of water molecules at the interface and reveals that the surface contains far more reactive states than the bulk water. "These simulations serve as an important step toward the use of terascale resources to produce simulations of water in complex environments," says Mundy.

In addition, the models successfully captured surface phenomena of water recently observed experimentally by Professor Richard Saykally's group at the University of California at Berkeley. A paper describing this work appeared in the January 30, 2004, issue of *Science*.

Contact: Christopher Mundy (925) 422-9571 (mundy2@llnl.gov).

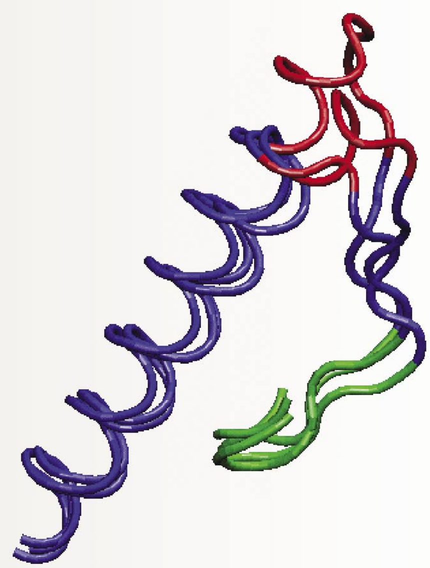
Scientists unveil melting point of iron at Earth's core

Livermore physicists Jeffrey Nguyen and Neil Holmes have discovered that iron at conditions comparable to Earth's core melts at a pressure of 225 gigapascals and a temperature of about 5,100 kelvins. Determining the melting point of iron is essential to determining the temperatures at core boundaries and the crystal structure of Earth's solid inner core. To date, the properties of iron at high pressure have been investigated experimentally through both laser-heated, diamond-anvil cell experiments and shock-compression techniques as well as through theoretical calculations.

However, those techniques have not produced a consensus on the melt line or the high-pressure, high-temperature phase of iron in the inner core. Using the Laboratory's two-stage gas gun, the researchers demonstrated that a shocked sample of iron crosses the melt line at a pressure between that of the core–mantle boundary and the pressure of the inner–outer core boundary.

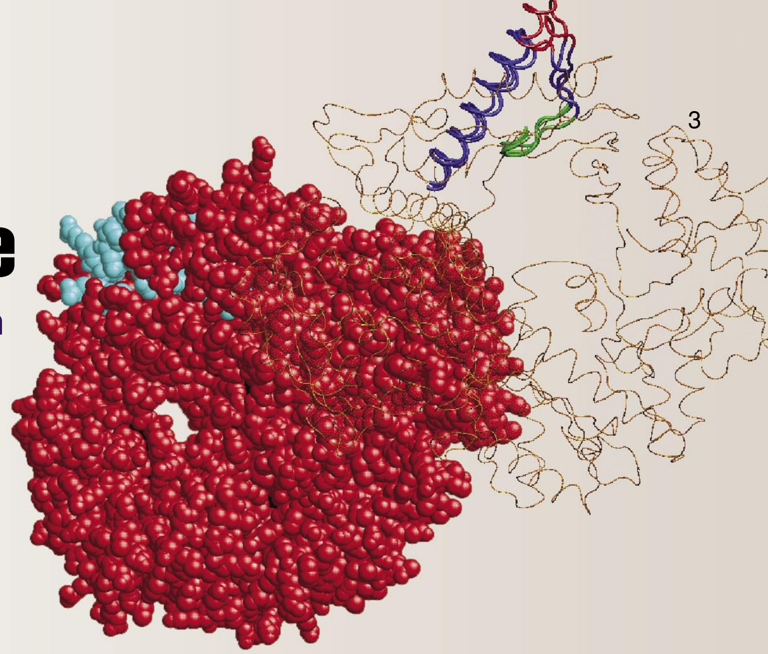
"By determining the melting point of iron, we can estimate the temperature at the core boundaries," Nguyen said. "These data provide us with more information to study the temperature of Earth's core." Nguyen and Holmes's results appeared in the January 22, 2004, issue of *Nature*.

Contact: Jeffrey Nguyen (925) 423-6838 (nguyen29@llnl.gov).



Computing Science

One Arrow in the Quiver for Homeland Security



WHEN the legislation establishing the Department of Homeland Security was being drafted, eyebrows were raised across the country over the explicit inclusion of Lawrence Livermore's Advanced Scientific Computing Research Program. The program was transferred from the Department of Energy's Office of Science to the new department's Science and Technology directorate.

With so much attention being directed at top-level issues such as transportation security and biodefense, the role of scientific computing in homeland security is often overlooked. All of the major homeland security issues have critical elements that require advanced computing. Advanced scientific computing is more than the world's fastest or largest computers, the aspect of computing for which Livermore is typically known.

In many cases, the homeland security computing challenges involve new modeling techniques, new algorithms for handling data, or even new ways of thinking about a problem. Once these techniques are in hand, they can often be implemented on ordinary desktop computers or palm-sized instruments, making it possible to deliver state-of-the-art computing capabilities into the field and even to first responders.

The advanced computing challenge most in the news is the intelligence problem of finding and connecting the critical pieces of information amidst mountains of data. Advanced scientific computing is key to developing the scalable information analysis techniques and large-scale data integration tools that are needed to solve this problem. In addition to developing new algorithms, we are also exploring novel computing architectures that could dramatically speed the discovery of relationships in large data sets.

The detailed simulations and scenarios required to improve emergency response planning and crisis management operations depend on advanced computing capabilities. Lawrence Livermore has long been a leader in computational fluid dynamics and other simulation technologies. This work forms the foundation of the National Atmospheric Research Advisory Center (NARAC) and is being applied to extend NARAC's capabilities to model the fate and transport of chemical and biological agents in the atmosphere. For example, we are applying expertise in adaptive mesh refinement and complex geometry modeling to simulations of aerosol dispersion in urban settings.

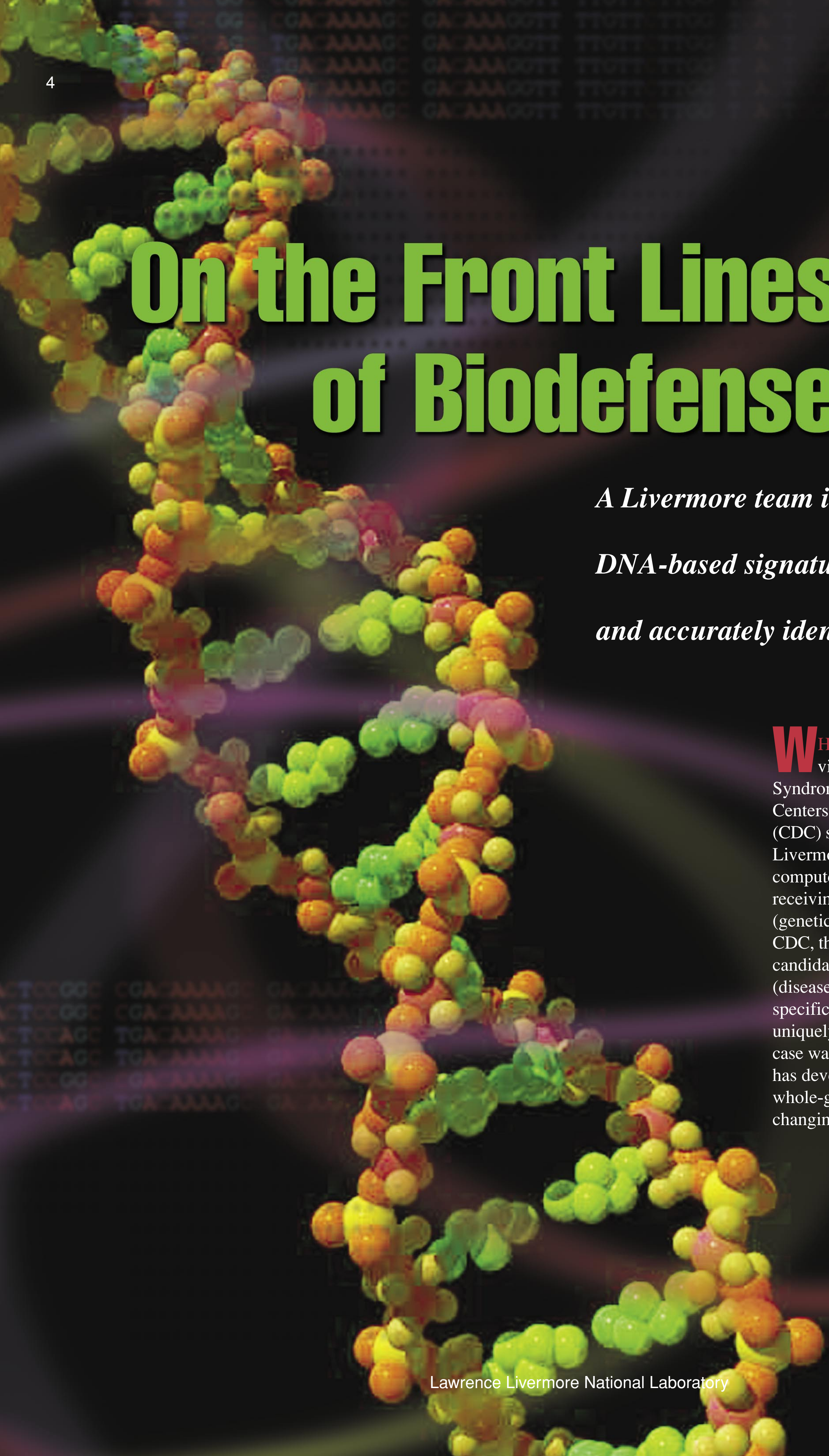
Advanced computing is also required for the comprehensive and dynamic risk-vulnerability-mitigation assessments and consequence analyses that are needed to develop strategies for protecting critical U.S. infrastructures. For instance, by combining the Laboratory's simulation strengths in shock physics and structural mechanics, we can understand the impact of explosions on buildings and other structures and then design appropriate countermeasures.

Advanced computing contributes to the development of better radiation detectors and biosensors. If we are to design detectors that exploit signatures that terrorists think are undetectable, we must first be able to model the physical and biological phenomena involved. In some cases, this requires first-principles simulations on supercomputers. Advanced computations also guide the micro- and nanoscale engineering required to miniaturize the devices.

As the article on p. 4 describes, advanced computing techniques are also being used to speed the development of the DNA and protein signatures that lie at the heart of biodefense. For example, biologists, computing scientists, and mathematicians collaborated to invent the first-ever algorithm for aligning draft genomes with finished genomes, making it possible to identify candidate signatures from incomplete data and thereby enable rapid responses to unexpected disease outbreaks. This kind of multidisciplinary teaming is a hallmark of the way Lawrence Livermore tackles tough problems. Other computing science advances have significantly reduced the time of a key step in the signature development process, and the algorithms involved are being scaled to permit work on organisms with larger genomes. Taken together, these computing advances will result in faster, less expensive, and more reliable biodetection capabilities for homeland security.

Lawrence Livermore is a leader in providing science and technology for homeland security. An important element of our success is our ability to integrate multiple scientific and technical disciplines to produce systems-level solutions to national security challenges. Advanced scientific computing is one of the keys to "being smart" about how we tackle homeland defense, enabling us to provide technologies and capabilities that significantly improve security.

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



On the Front Lines of Biodefense

A Livermore team is developing DNA-based signatures to quickly and accurately identify pathogens.

WHEN a sudden outbreak of a strange virus called Severe Acute Respiratory Syndrome (SARS) occurred last year, the Centers for Disease Control and Prevention (CDC) sought help from a team of Lawrence Livermore biologists, mathematicians, and computer scientists. Within three hours of receiving the first sequenced genome (genetic blueprint) of the virus from the CDC, the Livermore team produced several candidate signatures of the pathogen (disease-causing microbe). Signatures are specific regions of DNA or RNA that uniquely identify a pathogen. The SARS case was one of many in which the group has developed signatures using a novel whole-genome analysis approach that is changing pathogen diagnostic design.

Sensors Sniff City Air for Pathogens

The specter of terrorists attacking American cities with airborne pathogens has prompted federal agencies to develop systems that continuously monitor the air for biothreat agents.

The nation's first such monitoring system is the Biological Aerosol Sentry and Information System (BASIS). BASIS was developed by a team of researchers from Lawrence Livermore and Los Alamos national laboratories and involved extensive collaborations with emergency response, public health, and law-enforcement agencies. The system uses detection methods derived from DNA-based signatures designed by Livermore's bioinformatics group. BASIS was designed for the "detect to treat" mission, identifying a release quickly enough to permit effective medical treatment of those exposed.

BASIS was called into service after the anthrax attacks of October 2001. It was also deployed to Salt Lake City, Utah, as part of the overall security strategy for the 2002 Winter Olympic Games. (See *S&TR*, October 2003, pp. 6–7.) The system was later deployed in Albuquerque during the summer of 2002 and in New York City for the first anniversary of the September 11 terrorist attacks.

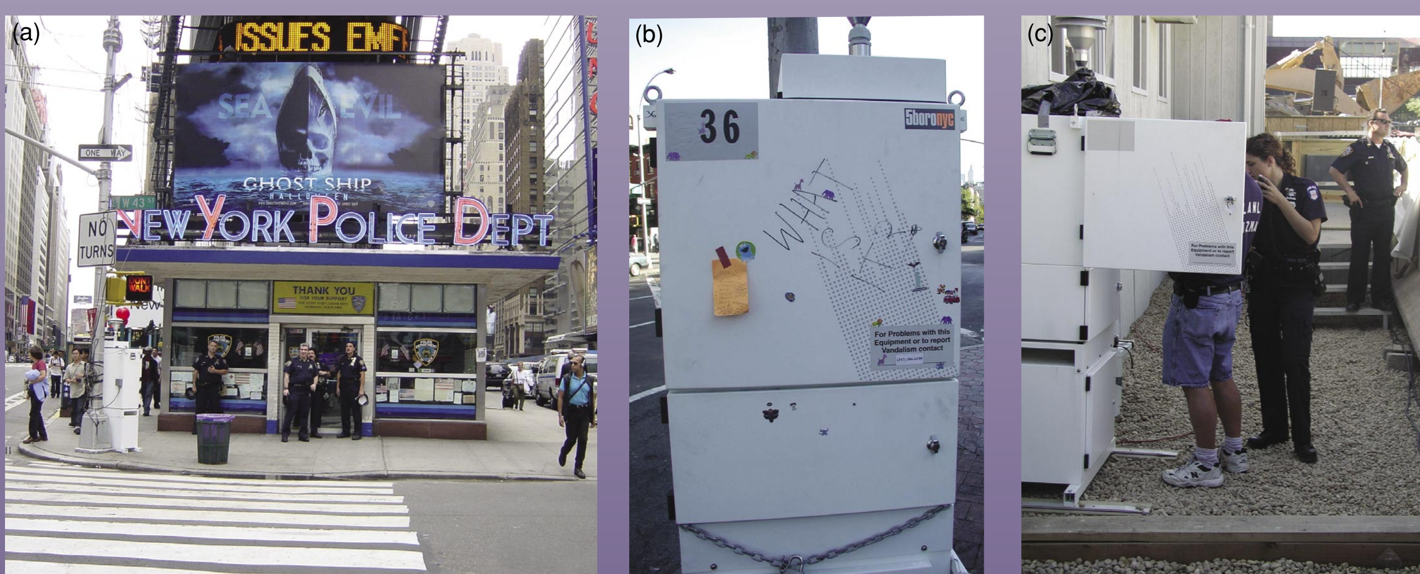
BASIS air-monitoring units collect aerosol samples at specific locations. A semi-automated mobile field laboratory rapidly analyzes DNA from the collected samples for evidence of potentially lethal bacteria and viruses. Safeguards built into the system ensure sample integrity. Should a positive identification be confirmed, the field laboratory immediately notifies the appropriate response agencies.

In late 2002, the U.S. Department of Homeland Security, the Environmental Protection Agency, and the Centers for Disease Control and Prevention implemented the national BioWatch program.

Some BioWatch sensors resemble a phone booth topped with an air intake and radio antenna. Couriers collect air filters from the sensors and deliver them to military facilities or public health laboratories. There, technicians use Livermore-developed signatures to detect the presence of target pathogens. If a pathogen were detected, officials would examine wind patterns in the area of the contaminated sensor and take action to protect the population.

In summer 2003, BioWatch sensors in Houston detected fragments of *Francisella tularensis*, a bacterium found in rabbits, prairie dogs, and rodents that can spread to humans and cause tularemia. Health officials concluded there had been no attack. Instead, the sensor had detected tiny amounts of *F. tularensis* naturally present in the environment. Although *F. tularensis* was known to be endemic in Texas, this was the first time it was detected in an aerosol sample.

The Department of Homeland Security announced that the incident marked the first time the BioWatch network had detected such a serious airborne threat, one that in this case was naturally occurring. Tom Slezak, leader of Livermore's bioinformatics group, notes that in more than 700,000 uses of Livermore-developed signatures, the BASIS/BioWatch network of sensors has never raised a false-positive alarm, that is, concluded that pathogens were present when they were not.



(a) Air samples are collected by this BASIS sensor installed outside a New York Police station. (b) Another sensor resides in a New York City borough neighborhood. (c) New York City Department of Public Health officers accompany a Department of Energy employee retrieving air samples from a sensor located near the former World Trade Center. Air samples are tested by Livermore technicians at a nearby laboratory.

The team, part of the Laboratory's Biology and Biotechnology Research Program (BBRP), has been on the front lines of the nation's biodefense effort since 2001. Eleven computer scientists, biologists, and mathematicians led by computer scientist Tom Slezak comprise one of the largest pathogen bioinformatics groups. Their work spans the full spectrum of effort, from identifying signature candidates to developing DNA-based signatures and deploying validated assays in the field. Team members have traveled throughout the nation, often with only a few hours' notice, to support the national effort to defend against bioterrorism.

Biological weapons could include bacteria (anthrax, plague), DNA viruses (smallpox), RNA viruses (ebola, SARS, foot-and-mouth disease), fungi (soybean rust, corn rust), protozoa (giardiasis), and toxins (ricin). Pathogens such as these and many others could be used to sicken or kill urban populations, livestock, or crops. Early detection and unmistakable identification are crucial to limiting the potentially catastrophic human and economic costs of a bioattack.

Many types of signature requests are received by the team. One request may be for all strains of a normally pathogenic species, including its nonpathogenic and vaccine strains. Another request may be for all of the pathogenic strains of a particular species. Fulfilling these requests can be difficult because while there may be hundreds of strains of a particular species, genomic sequences may exist for only a few. Strains may also vary in pathogenicity, and their genetic near-neighbors may or may not be virulent or may affect hosts other than humans. In addition, RNA viruses have extremely high mutation rates, so it may be difficult or impossible to find adequate stable regions suitable for use as a signature.

The Livermore bioinformatics team has developed DNA-based signatures of virtually every biothreat pathogen (the organisms identified by the CDC as high-priority threat agents) for which adequate genomic sequences are available as well as for several other human and livestock pathogens. Signature requests come from agencies such as the Department of Energy (DOE), the CDC's Laboratory Response Network and BioWatch Program, the Department of Agriculture, the Food and Drug Administration, and the Department of Defense. Livermore signatures are part of the nation's public health system and have been in use for homeland defense since fall 2001. (See the box on p. 5.)


Livermore researchers try to sleep on a U.S. Air Force C-130 transport plane on their way to deploy a pathogen-detection system.

Pipeline Called KPATH

Livermore's signature pipeline, called KPATH, is used to develop the signatures of bacterial and viral pathogens. This Livermore-designed system is a fully automated DNA-based signature "pipeline," able to deliver signature candidates (spanning 200–300 base pairs of DNA) in minutes to hours. In simplest terms, KPATH works by comparing the genome of the target pathogen to a library of microbial genomes, searching for those areas that are unique to the target organism. (See the box on p. 8.)

KPATH uses the software programs Multiple Genome Aligner (MGA) and Vmatch, which were developed by collaborators in Germany. MGA aligns the multiple genomes of a target pathogen, and Vmatch uses efficient algorithms to quickly compare the genome of interest with all other sequenced microbial genomes. "These software tools allow the pathogen genomes themselves to show us which regions of DNA are important," Slezak says. The DNA regions that are significant to the pathogen are conserved among all strains of the pathogen sequenced to date and are unique when compared to all other organisms sequenced to date. That is, they are present in every strain of the pathogen and absent in all other organisms.

The algorithms work by locating those portions of the genome that are not unique and eliminating them from consideration. "In this way," says Slezak, "we define regions of apparent uniqueness and mine them for candidate signatures."

Candidate signatures must then be verified in the laboratory. "It's a long path from candidate signature to validated assay," notes Slezak. Hundreds of thousands of candidate signatures are computationally screened. Wet-chemistry procedures reduce that number to hundreds and then dozens. Much of the laboratory testing takes place at the CDC and other organizations that are certified to work with virulent pathogens. Once a signature is verified, the final step is optimizing the signature for a specific detection chemistry or instrument using a specific protocol. When that process is complete, the signature is called an assay.

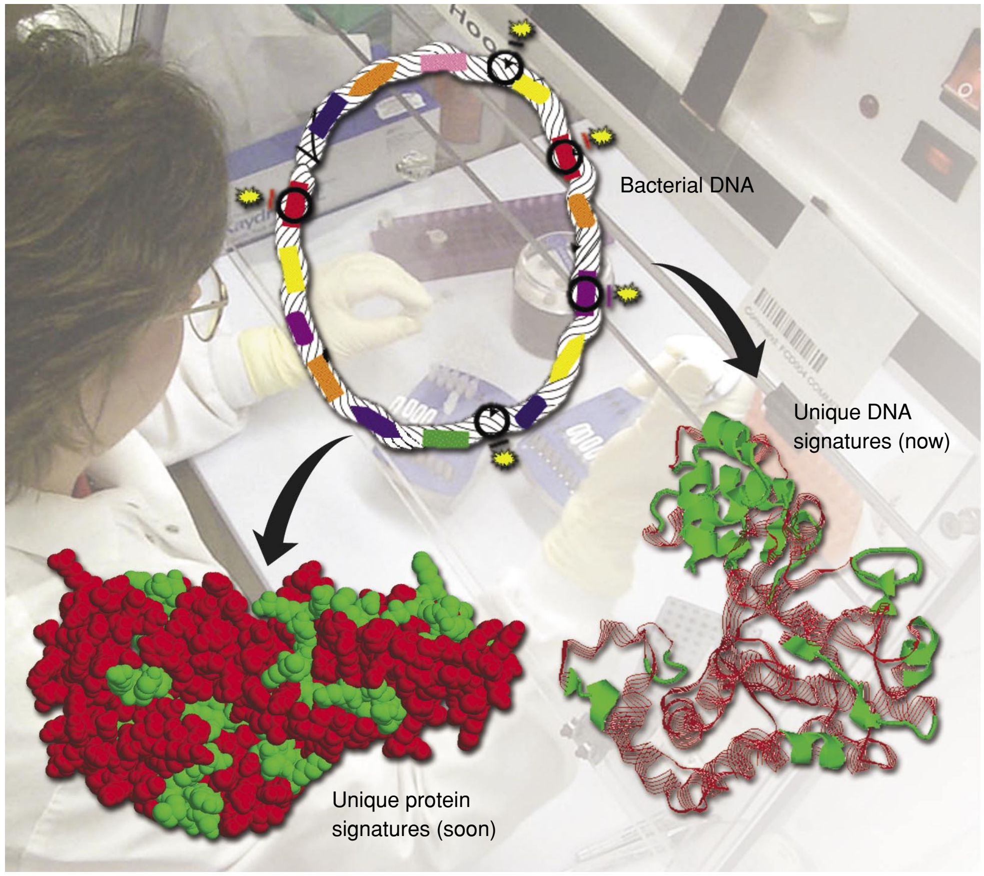
One of KPATH's important features is that it automatically downloads newly sequenced pathogen genomes from all major public databases, and all validated and fielded assays are verified weekly as the new sequence data are acquired. "As known strains evolve and new strains are discovered and their genomes sequenced, some of the 'unique' regions will erode," says Slezak. "We'll then need to refine the signature."

Olympic Games Motivate

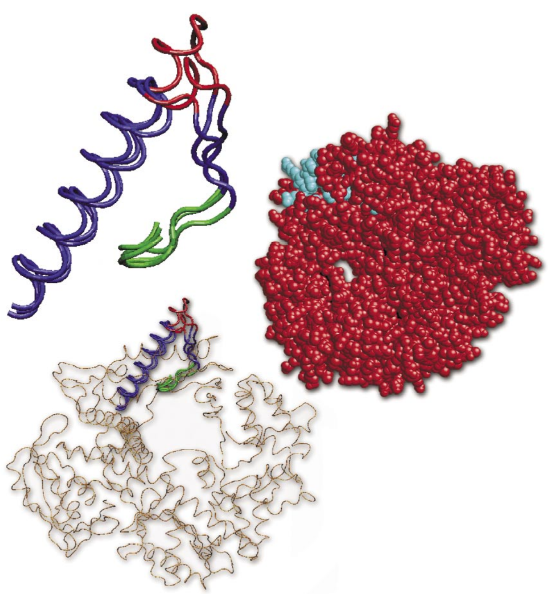
In early 2000, the DOE's Chemical and Biological National Security Program (CBNP) began a national pathogen-detection effort following the announcement by then-Secretary Richardson that DOE would be providing biosecurity at the 2002 Winter Olympic Games in Salt Lake City, Utah. Lawrence Livermore was assigned the task of developing reliable and validated assays for a number of the most likely bioterrorism agents. (See the box on p. 5.)

The bioinformatics team reasoned that a whole-genome analysis approach—that is, comparing a target pathogen genome against all other sequenced microbial genomes—would reveal which regions of the DNA were unique. They also believed the process could be automated to get results more quickly. Until the Livermore approach, signature design was a time-consuming, expensive process done largely by hand and guided heavily by intuition. Analysis was generally limited to sequences from a few genes thought to be important. Traditional approaches to DNA-based signature development started with the assumption that a particular gene was vital to an organism's virulence, host range, or other factor. The resulting assay would then be tested with the available strain. This approach would at times yield good results, but it frequently resulted in failure. Computational support for diagnostic development was rare. "The time was ripe for radical changes in this field," says Slezak.

In August 2000, the team began building a set of tools that would accomplish these goals. Slezak says, "We used techniques and mindsets from our many years of experience working on the Human Genome Project (HGP)." Slezak formerly led Livermore's HGP bioinformatics effort and later the



There are two major ways to detect pathogen signatures. One involves finding specific regions of DNA (or RNA) that uniquely identify a pathogen. The other (still under development) involves finding specific regions of a unique protein whose production is specified by that pathogen's DNA (or RNA).



DNA-based signatures are often the part of a pathogen's genome that reflects the code of a particular protein or enzyme unique to the pathogen. This model depicts one such pathogen protein. Blue represents the part of the protein that is conserved (present) in all strains of the pathogen's DNA. Red represents the portion of the protein that is unique to the target strain. Green depicts the most highly conserved portion across multiple organisms. The DNA-based signature of this target strain, therefore, combines those portions of DNA that code for both the blue and red regions.

On the Road to KPATH: A Short Timeline

In 2000, a crude test on *Bacillus anthracis,* the causative agent of anthrax, demonstrated that a computer-based approach to pathogen-signature development would work. The test took summer student Marisa Lam several days to process more than 4 billion bytes of information from analysis of the *B. anthracis* genome. The roughly 4,000 resulting candidate signatures were narrowed down to a handful and forwarded to the Centers for Disease Control and Prevention (CDC) for formal validation. These optimized signatures became the assays used for the nation's Biological Aerosol Sentry and Information System (BASIS) and BioWatch environmental monitoring networks. By comparison, earlier methods of signature design had yielded zero successes among more than 1,000 candidates. Buoyed by this successful test, a team led by computer scientist Tom Kuczmarski began work on an automated signature pipeline.

In February 2001, foot-and-mouth disease was devastating the cattle and sheep industry in the United Kingdom. The Livermore team analyzed the tiny (8-kilobase) genome of the foot-and-mouth disease virus (FMDV) and found that viral genomes, although tiny compared to the typically 3- to 5-megabase bacterial genomes, can be troublesome to analyze because of their high mutation rate. The team determined that only one region of the FMDV genome is capable of supporting a signature assay. In the spring, the team began collaborating with Sharon Hietala of the University of California at Davis to detect agricultural pathogens that are common to California cattle and cause symptoms that mimic those of FMDV.

Livermore computer scientist Tom Slezak was attending a conference in Maryland when the September 11 terrorist attacks occurred. During the five days it took him to return to California, he conceived of a fully automated DNA-based signature-design-and-maintenance system that would download all new and updated genomic sequences weekly from the major public databases. The system would then compare those sequences with the existing, fielded DNA-based signatures to determine if any new sequences had invalidated them. Slezak named the system KPATH. "I was inspired by radio-station call signals," says Slezak. "KPATH, all pathogens, all the time. Bringing you the pathogen hits of the 50s, 60s, and today." To achieve the desired speed and capacity, KPATH would require a large server with multiple central-processing units (CPU), a powerful database server, and more advanced algorithms.

The Livermore signature development team includes (from left) Nisha Mulakken, Carol Zhou, Adam Zemla, Ed Miller, Tom Slezak, Tom Kuczmarski, Jason Smith, Marisa Lam, Clinton Torres, Shea Gardner, Mark Wagner, and Beth Vitalis. The Livermore team collectively has expertise in biology, mathematics, systems science, and computer science.

In October 2001, when the anthrax attacks occurred, BASIS was the only system in the country capable of taking on pathogen monitoring duties. "The anthrax attacks resulted in the first real awareness of bioterrorism by most of the U.S. general public," notes Slezak. A few months later, BASIS also took on monitoring duties at the 2002 Winter Olympic Games.

In June 2002, supplemental funding was obtained from the Department of Energy to purchase a 24-CPU server, an 8-CPU database machine, and a 3-terabyte file server and to hire six summer students to help build KPATH. The team also adopted the new Multiple Genome Aligner (MGA) program, which was developed by collaborators in Germany to dramatically speed up signature development.

In fall 2002, three of the team's summer students who had graduated—Clinton Torres, Jason Smith, and Lam—were hired to complete the KPATH system. Meanwhile, Kuczmarski and Shea Gardner handled the constant demands for new pathogen signatures using the original pipeline.

In December 2002, Livermore's smallpox and related signatures were evaluated by the CDC. A year earlier, Livermore had anticipated the need for smallpox assays and had developed candidate signatures. Just after KPATH signatures passed extensive testing in January 2003, the CDC requested that the team process several new smallpox and near-neighbor genomes in anticipation of world events.

In March 2003, the CDC requested assistance in analyzing the newly sequenced Severe Acute Respiratory Syndrome (SARS) virus. The Livermore team processed both a Canadian genome and a CDC genome and returned a set of signature candidates within three hours. The U.S. Army later tested these signatures, and the CDC is considering several for validation.

"SARS presents a special situation," says Slezak. "We don't really know what near-neighbor species are like, so it is very hard to be sure which signatures will work when near-neighbor viruses are eventually discovered. At this time, 77 percent of the genome appears to be highly unique, but this clearly will not be the case once other related organisms are discovered and sequenced. However, the automated KPATH approach will be capable of capitalizing on new data, and within 30 minutes we should be able to know which regions of SARS still appear to be unique and therefore which signatures will continue to work."

In June 2003, an unexpected outbreak of monkeypox in the U.S. occurred as a result of exotic animals being imported from Africa as household pets. Ironically, although the team had developed candidate signatures of monkeypox in 2002, the CDC had not tested these because monkeypox had never occurred in the Western Hemisphere. Following the U.S. outbreak, the CDC supplied Livermore with sequenced monkeypox from both a human and a prairie dog. The genomes, which turned out to be identical, were used by the Livermore team to refine the monkeypox signatures.

"These naturally occurring situations provide us with real-life training experiences for rapid emergency response," says Slezak. "It is a distinct honor that our team has earned the privilege of being the bioinformatics team assisting the CDC on major pathogen emergencies."

Joint Genome Institute's informatics effort. BBRP scientist Paula McCready led Livermore's HGP sequencing effort for several years and was the first leader of the sequencing effort at DOE's Joint Genome Institute.

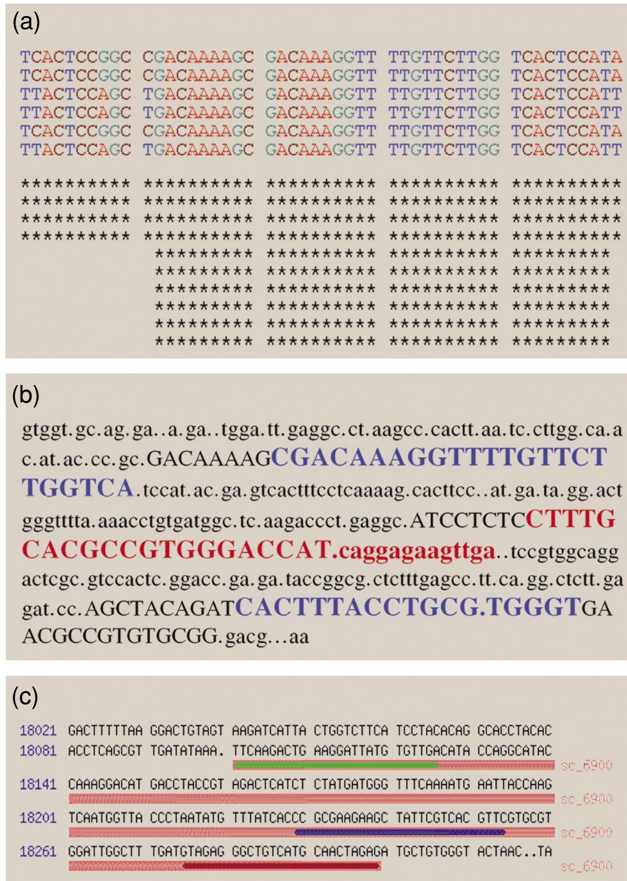
The concept of an automated signature-design system began with a crude algorithm and a proof-of-principle test that took about one week. The goal was to develop a signature for *Bacillus anthracis*, the bacterium that causes anthrax. When the test proved successful, Slezak began to search for more efficient algorithms.

"In October 2000," says Slezak, "we began building a preliminary pipeline based on this approach with funding obtained from the Laboratory Directed Research and Development Program. In May 2002, we were funded by DOE to build the current KPATH pipeline. We continued to use the first pipeline until about January 2003, when KPATH was shown to be functionally equivalent and much faster."

New Features on the Horizon

The bioinformatics team is developing additional features for KPATH, including the capability to generate multiple types of signatures to support different detection chemistries and machines, better algorithms to improve processing efficiencies, and improved capabilities for developing signatures of RNA viral genomes. Signature development of RNA viruses is particularly difficult because they mutate so rapidly. To overcome this difficulty, the team is building a pipeline of protein signatures—the other major approach to pathogen detection.

Protein signatures are commonly used in diagnostic kits, such as commercially available home-use pregnancy tests. Slezak notes that the sequence of amino acids that make up a protein tends to be conserved (unchanged) because altering the protein sequence is likely to change the protein's shape, which in turn would alter its function. Using this approach, the team has found conserved and unique signature regions in the glycoprotein of the West Nile virus (an RNA virus) and has mapped



KPATH uses computers and efficient algorithms to compare genomes and identify those portions that are unique to a particular pathogen or family of related pathogens. (a) A small part of the genome (50 DNA bases out of 8,000) of six strains of a pathogen are aligned and arranged in five columns for comparison. (The letters T, C, A, and G represent thymine, cytosine, adenine, and guanine, the four nucleic acids that make up all DNA.) The stars are a rough visual indicator of the degree of similarity or "consensus" among the six strains in each column. (b) A "consensus genome" is derived from those regions that are common to the six strains, indicated by the upper case letters. (c) The consensus region is mined to obtain a unique signature of the pathogen, which corresponds to the colored sequence.

these regions to three-dimensional protein structure models created by Livermore mathematician Adam Zemla. Antibodies derived from these regions are being tested at the University of California at Davis to verify that the identified regions are indeed unique.

The team also plans to develop fungi signatures. However, fungal DNA is more difficult to analyze than bacterial DNA because of the larger genome size of fungi. Because of funding constraints, only a few fungi genomes have been sequenced. As a result, it is difficult to know what genomic regions are common to fungi and thus are not useful for signatures.

Another ongoing task for the team is building and maintaining relationships with partners in various agencies and universities. Slezak explains, "Much of the data we need are not in the public domain."

In the meantime, researchers worldwide are regularly publishing the sequences of new and updated genomes. As additional pathogens are sequenced, the Livermore team will continue to provide rapid computational analysis and develop DNA-based and protein signatures to help thwart bioterrorists.

—*Arnie Heller*

Key Words: BASIS, bioinformatics, bioterrorism, BioWatch, Centers for Disease Control and Prevention (CDC), DNA, foot-and-mouth disease, Human Genome Project, KPATH, microbe, pathogen, protein signature, RNA, Severe Acute Respiratory Syndrome (SARS), smallpox.

For further information contact Tom Slezak (925) 422-5746 (slezak1@llnl.gov).

Defending against Corrosion

A Livermore-designed engineered barrier system for the proposed Yucca Mountain nuclear waste repository works with natural barriers to keep radioactive waste in its place.

Years of scientific study have been devoted to designing a proposed underground nuclear waste repository at Yucca Mountain in the Nevada desert.

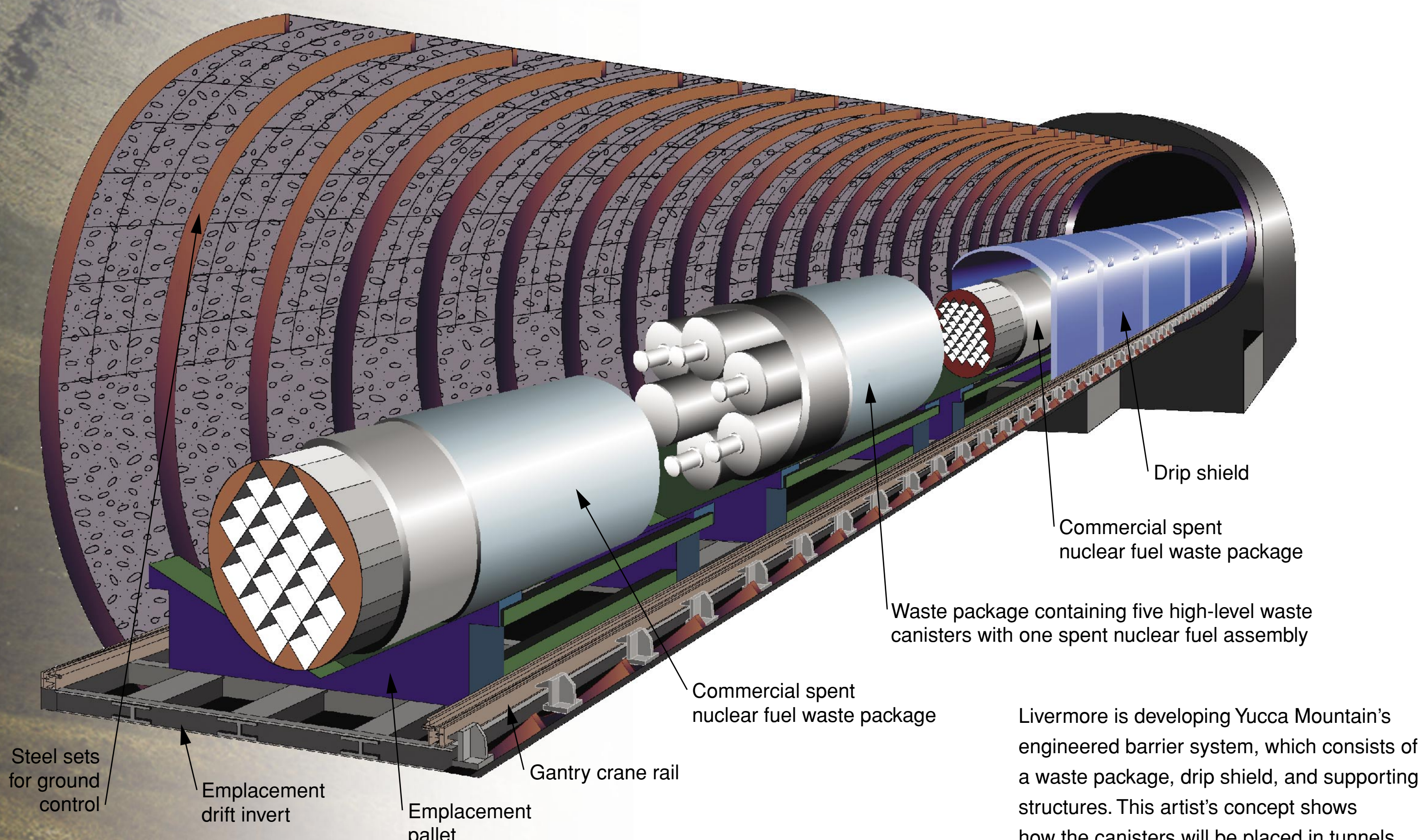
LAWRENCE Livermore researchers thrive on challenging assignments. Few assignments have been as demanding as designing a waste package system to keep high-level radioactive waste packages essentially intact for at least 10,000 years. A team of Livermore researchers—engineers, metallurgists, chemists, microbiologists, and computer scientists—are testing and refining the design and materials for what will eventually be 12,000 waste packages. These efforts are an integral part of a national program to design, license, and build an underground nuclear waste repository in Yucca Mountain, Nevada.

Yucca Mountain was selected by the Department of Energy (DOE) as a highly promising repository site. (See the box on p. 14.) In 1987, Congress directed the DOE to focus on Yucca Mountain as the candidate location to safely store about 70,000 tons of waste from civilian nuclear power plants and highly radioactive waste from defense-related activities at DOE facilities. As part of the DOE's Yucca Mountain Project, Livermore scientists have made major contributions in characterizing the proposed underground site, determining the effects on the site from storing high-temperature radioactive wastes, and selecting and characterizing corrosion-resistant materials.

Livermore's largest effort is developing Yucca Mountain's engineered barrier system, which consists of a waste package, drip shield, and supporting structures. The engineered barrier system is designed to work with the natural barriers of Yucca Mountain to contain the repository's radioactive wastes and prevent them from seeping into the water table which lies about 300 meters below the planned repository.

"We need to show that our design will substantially contain the waste inside the canisters for at least 10,000 years under extreme and varying conditions of temperature, radiation, and corrosion," says Dan McCright, Livermore metallurgist and Yucca Mountain Program senior scientist. According to McCright extensive analyses have shown that even if waste were to eventually leak from the canisters, additional barriers, both natural and engineered, are expected to keep the waste far from the water table and humans.

No direct information exists about how modern materials will behave over thousands



Livermore is developing Yucca Mountain's engineered barrier system, which consists of a waste package, drip shield, and supporting structures. This artist's concept shows how the canisters will be placed in tunnels about 300 meters underground. The waste packages will rest on a strong corrosion-resistant pallet and supporting steel frame.

of years under a range of conditions. The Livermore research is based on accelerated aging tests of materials that are proposed to make up the engineered barrier system and on computer models that simulate how a repository built at Yucca Mountain would perform over thousands of years.

Defense in Depth

The current repository design calls for waste to be stored in a package consisting of a set of two nested canisters—an outer canister made of a highly corrosion-resistant metal (Alloy 22) and an inner canister made of a tough, nuclear-grade stainless steel (316NG). An overhanging drip shield made of titanium will provide additional protection to the waste package from dripping water and any falling rocks from the repository ceiling. "Because the waste package and the drip shield are made of different corrosion-resistant materials, they form corrosion defense in depth," says McCright.

Storing the waste packages horizontally and commingling the different kinds of waste packages will create a relatively uniform temperature in each underground drift, or tunnel, carved inside the mountain. The waste packages have a common diameter (1.8 meters), but their lengths vary according to the type of waste—from about 3.6 meters for the defense waste to 5.7 meters for the spent nuclear fuel.

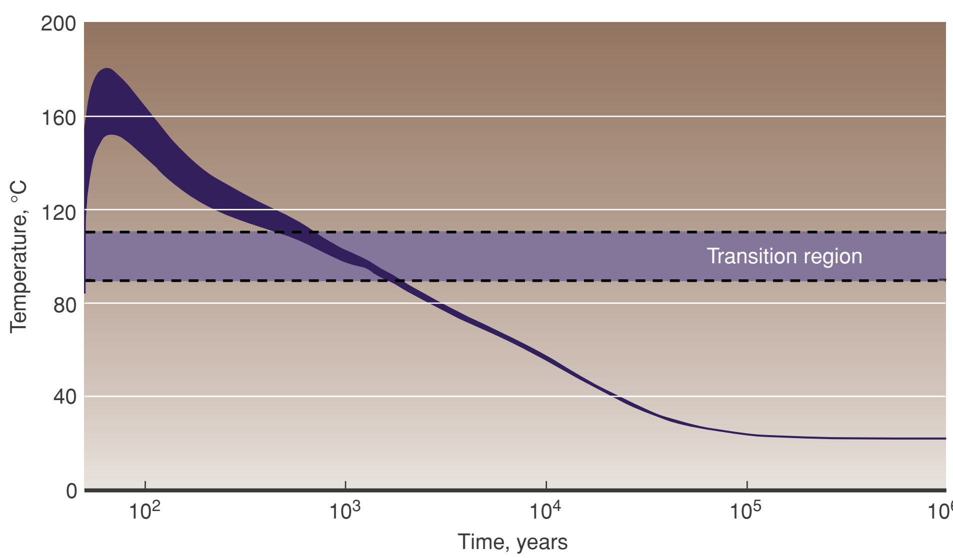
The most critical element of the engineered barrier system is the 20-millimeter-thick outer canister made of Alloy 22, which consists of about 60 percent nickel, 22 percent chromium, 13 percent molybdenum, and 3 percent tungsten. Alloy 22 is highly resistant to fractures and is easier to weld than alternative materials such as titanium. It is also extremely corrosion resistant under the conditions of high temperature and low humidity expected to prevail for hundreds to thousands of years in a repository. In addition, it is resistant under conditions of either low or high humidity at the lower temperatures expected in the repository when radiation levels decrease. Hence, the selection of Alloy 22 would provide containment over a range of environmental conditions. "It's the best engineered material available for the job," says McCright.

Nuclear-grade stainless steel (316NG) was chosen for the 50-millimeter-thick inner canister to add strength and bulk to the waste package. It is corrosion resistant, more compatible with Alloy 22 than carbon steel, and more economical than more complex steel alloys.

The titanium drip shield, which McCright compares to a sturdy awning, would be fabricated from grade 7 titanium. This material contains a small amount of palladium to provide greater corrosion resistance. The drip shield, however, is not considered essential to containing the wastes. Earlier projections of Alloy 22's corrosion performance assumed that there would be no drip shields and that drips from the repository walls would fall directly on the canisters.

The waste packages will rest on a pallet fabricated from Alloy 22 clad onto steel.

Livermore scientists are testing the design of the waste packages to be used in the Yucca Mountain repository. The waste packages will have a common diameter (1.8 meters), but their lengths will vary according to the type of waste—from about 3.6 meters for defense waste to 5.7 meters for spent nuclear fuel. The scientists work on prototypes like the one above that have the full-scale diameter but shortened lengths.



Once the repository is sealed, it will take hundreds of years before waste-package surface temperatures drop below boiling because of the slow decay of the radioactive waste. This graph shows the projected decline of temperatures on waste canisters' surfaces over 1 million years. The range of temperatures corresponds to uncertainty about heat-transfer modes, variation among the heat output of individual waste packages, and the location of waste packages in the repository. The dotted transition region marks where temperatures fall below boiling. At this point, water may come into contact with the containers.

The pallet, in turn, will sit on a steel frame and crushed gravel. The waste packages will be placed close together (about a meter apart) so that by design their surfaces will reach a maximum surface temperature of 160°C (caused by radiation levels of up to 180 rads per hour) once the repository is sealed. “It may take hundreds of years before surface temperatures cool below boiling because of the slow decay of radioactive components in the waste,” says McCright. Keeping the canister surfaces above the boiling point will ensure they are dry, with the intention to prevent corrosion.

Getting a Close-up View

A major effort is under way to understand and characterize the environments closest to the drip shield and the waste package because these environments will determine the potential for corrosion and how fast it could proceed. Surface conditions will be characterized by the temperature, humidity, and composition of gases in the repository; the contaminants in the dripping water from repository walls; and the mixture of minerals and salts that may eventually be deposited on the drip shield and canisters. As temperatures cool, for example, moisture and dust in the atmosphere will settle on the canisters’ surfaces despite the presence of the drip shield. If a drip shield is eventually breached, water seeping through rock fissures could contact the canisters directly and cause more minerals or salts to precipitate on their surfaces, thereby increasing the potential for corrosion.

Limiting corrosion is the paramount objective. Corrosion can be general, occurring more or less uniformly over the entire surface, or localized, occurring in specific areas such as in pits or crevices on a metal’s surface. Corrosion can also be assisted by cracking from stresses in a metal or weld, a phenomenon called stress corrosion cracking.

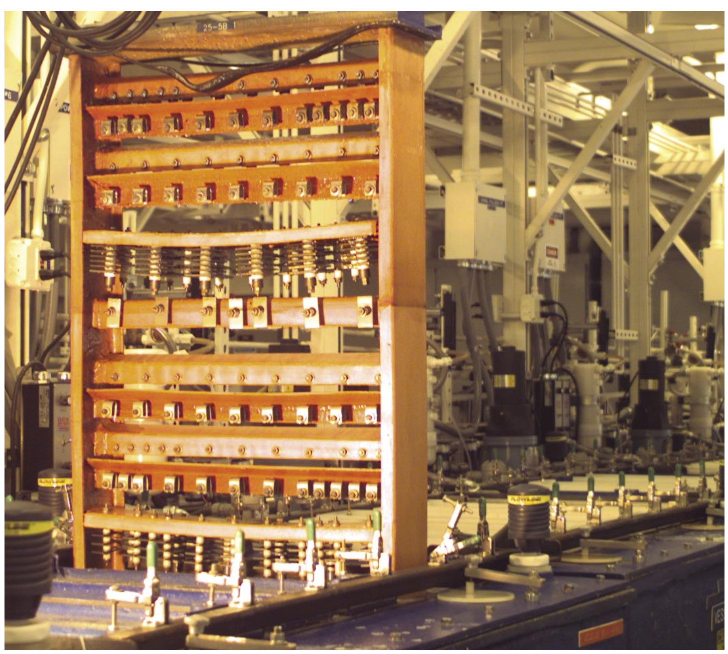
The materials chosen for the waste package are among the most corrosion resistant of engineering materials. They are used routinely under harsh conditions in the chemical process industry and at nuclear power plants and are expected to perform well in the expectedly more benign conditions within Yucca Mountain. Both titanium and Alloy 22 gain their corrosion protection from the natural, extremely fast growth of thin films (about 3.5 nanometers or 10 atomic layers thick) of metal oxides caused by oxygen in the environment. When these stable, chemically unreactive films consolidate, the corrosion rate decreases. One Livermore research effort is studying the growth of metal-oxide thin films on Alloy 22 and titanium under the expected environmental scenarios at Yucca Mountain. The observed compositions and structures of the films are compared with model predictions of film growth.

It is essential to demonstrate that Alloy 22 will survive all anticipated repository conditions. In particular, scientists must show that corrosion rates, both general and localized, are extremely low and that welds will not crack over time. Materials performance tests are conducted at Livermore’s Long-Term Corrosion Test Facility (LTCTF) to provide assurance that the waste packages will maintain their integrity and corrosion resistance for thousands of years.

Aging 18,000 Metal Coupons

The corrosion tests at the LTCTF are designed to rapidly “age” metal samples, called coupons, by subjecting them to much harsher conditions than would be expected in the repository. More than 18,000 alloy coupons are being tested, each of which measures about 5 centimeters square or less. Fourteen alloys are being tested to compare the corrosion resistance of Alloy 22, stainless steel, and titanium with other materials.

Four kinds of coupons are used to test the various forms of corrosion. Crevice coupons consist of metals tightly pressed against Teflon washers to determine the extent of corrosion from liquid trapped between the metal and washer. Weight-loss coupons measure general corrosion. Galvanic coupons measure corrosion that occurs when two dissimilar alloys are pressed against each other. Finally, U-bend coupons are metals bent under continuous stress to try to induce stress corrosion cracking. Many of the coupons are welded to determine the effects, if any, of welds on corrosion.



Corrosion tests of metal samples, called coupons, are carried out at Livermore’s Long-Term Corrosion Test Facility. Four types of coupons are kept in 24 tanks, each filled with about 1,000 liters of one of the three aqueous solutions that are likely to be found in the underground Yucca Mountain environment. In this photograph, a rack containing several hundred coupons is pulled out of solution for inspection.

The coupons are kept in 24 tanks, each filled with about 1,000 liters of one of three different solutions derived from those likely to be found in the Yucca Mountain environment. One solution is a concentrated mixture of salts and minerals common to Yucca Mountain. The second solution is a diluted version of this mixture. The third solution is an acidified version of the concentrated mixture. Solutions are heated to either 60°C or 90°C. The coupons are mounted on vertical racks and are either submerged in solution, suspended over the solution, or partially submerged.

Coupons were removed from the tanks six months, one year, two years, and five years after mounting. (Most of the coupons are still in the tanks awaiting longer-term tests.) When a coupon is removed, it is analyzed to determine whether corrosion has occurred, and if so, where it is, and how much damage it caused.

Corrosion activity is evaluated by weighing the coupons after they are cleaned

Yucca Mountain Project Eyes Licensing

In 1982, Congress passed the Nuclear Waste Policy Act, which made the Department of Energy (DOE) responsible for finding a suitable site and designing, building, and operating a permanent underground radioactive-waste disposal facility, called a geologic repository. The search identified several possible locations for the nation's first long-term waste repository. In 1987, Congress amended its earlier act to focus solely on the Yucca Mountain site in Nevada, about 145 kilometers northwest of Las Vegas. On July 23, 2002, President George W. Bush signed House Joint Resolution 87, allowing DOE to proceed in establishing a safe repository in which to store nuclear waste.

Yucca Mountain is located in a remote desert on federally protected land within the secure boundaries of DOE's Nevada Test Site. Hundreds of scientists and engineers have studied Yucca Mountain's geology, hydrology, chemistry, climate, and other physical aspects that could affect a repository's safety. The U.S. is not the only country facing the disposal issue. Around the globe, virtually all nations that use nuclear power are exploring approaches to safely dispose of radioactive waste.

DOE is preparing an application to obtain a Nuclear Regulatory Commission license to proceed with construction of the repository. DOE has set 2010 as Yucca Mountain's opening date, that is, when the first waste will be placed in canisters and moved inside.

The Yucca Mountain repository would house more than 70,000 metric tons of spent nuclear fuel from civilian nuclear power plants and highly radioactive waste from defense-related activities at DOE facilities across the U.S. Currently, spent nuclear fuel is stored in ponds or silos near operating commercial nuclear plants, while high-level nuclear waste from defense programs and experimental reactors is stored as liquid in tanks or as glass logs at several DOE facilities.

Homeland Security Concerns

The vulnerability of this waste, dispersed in so many locations, to potential terrorists is of concern to homeland security experts. The government's plan is to dispose of this waste in a centralized, well-monitored, and highly secure repository.

Nearly 90 percent of the waste will be spent fuel, which consists of solid pellets of enriched uranium oxide sealed in a cladding of corrosion- and heat-resistant zirconium alloy. The spent nuclear fuel from power plants would be delivered to the Yucca Mountain site "as is." The waste from DOE defense programs would first be vitrified, that is, converted into a borosilicate glass, before delivery to the repository.

The Yucca Mountain repository would be constructed in a layer of rock called tuff about 300 meters below the surface and about 300 meters above the permanent water table. Yucca Mountain is unique among potential sites under consideration in the waste disposal programs throughout the world because waste would be emplaced above the water table in an environment that is oxidizing in nature (that is, has plenty of oxygen).

Applying the principle of "defense in depth," the repository would incorporate multiple protective barriers, both natural and engineered. The engineered barriers include a canister and an overhanging drip shield. Emplaced waste would be monitored for the first 100 years of operation, and then the repository would be permanently closed. Scientists believe the dry conditions within the tuff will minimize the prospects for water to contact the canisters and that the waste will be sufficiently isolated for thousands of years.

The Yucca Mountain Project falls under the purview of the DOE Office of Civilian Radioactive Waste Management. The prime contractor is Bechtel SAIC Company, LLC, which is a joint venture between Bechtel National and Science Applications International Corporation. The project is one of the most closely reviewed programs ever undertaken by the federal government. Reviewing organizations include Congress, the General Accounting Office, the Nuclear Regulatory Commission, the State of Nevada's Nuclear Waste Project Office, Nye County Nuclear Waste Repository Office, the Nuclear Waste Technical Review Board, and the National Academy of Sciences.

Scientists at Yucca Mountain's Drift Scale Test Facility are acquiring a better understanding of the thermal, mechanical, hydrological, and chemical processes that occur deep underground at the site.

of compounds that have precipitated on their surfaces and by using an electron microscope and an atomic force microscope to scrutinize their surfaces.

LTCTF manager Dave Fix notes that the corrosion detected in the coupons in the various solutions is generally so slight that it resides at the limit of what is measurable. The average corrosion rate is about 20 nanometers per year. At this rate, a 20-millimeter-thick barrier of Alloy 22 would be effective for more than 100,000 years before general corrosion would provide a means for water to contact the underlying stainless-steel layer. In addition, the extremely low corrosion rates appear to be nearly the same for all the water chemistries and temperatures tested.

Significant corrosion is measured only when coupons are subjected to extreme, unrealistic conditions. For example, the basic metallurgical structure of Alloy 22 is transformed over long periods of time at temperatures of more than 500°C (100°C is the boiling point of water at sea level). Several hundred millivolts of electrochemical potential are necessary to make the test solution extremely corrosive. "These extreme testing conditions are totally unrealistic for the Yucca Mountain repository setting," says McCright, "but our models consider them."

Assessing Microbes' Effects

Livermore microbiologist Joanne Horn leads a team assessing the potential damage microbes can cause to the engineered barrier system. Some bacteria and fungi, both those indigenous to Yucca Mountain and those introduced by construction activities, could cause corrosion of the engineered barriers. Horn notes that an abundance of microbes exists in the Yucca Mountain repository setting. Microbial activity is expected on the canisters when adequate moisture is present. Some bacteria, for example, are expected to form patchy, thin films over the metal-oxide films covering the waste packages and drip shields.

Horn notes that microbes have been found in the most inhospitable environments on Earth, such as the scalding vents at the ocean's floor. Some bacteria have very efficient DNA repair mechanisms that might enable them to survive high radiation levels.

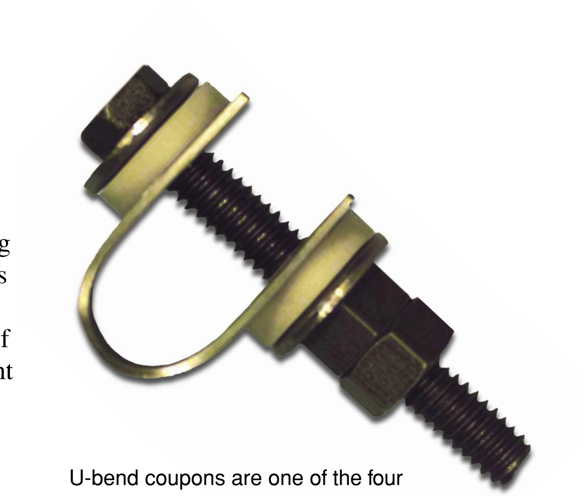
Horn's team has identified more than 65 species and subspecies of bacteria living in the Yucca Mountain rock. The team has also identified the different growth requirements for these bacteria. One set of laboratory experiments analyzes the extent of corrosion on metal coupons caused by bacteria contained in crushed Yucca Mountain rock and fed with simulated groundwater. Another set of experiments determines the extent of corrosion caused by specific species of bacteria that have potentially corrosive activities, such as a species that oxidizes sulfur compounds. The results of these experiments are compared with the corrosion that occurs under identical conditions but in environments that have been presterilized to kill all microbes. The team also analyzes the solutions to determine if bacterial metabolic products could change the repository chemistry.

"The findings of the bacterial experiments parallel those of the long-term corrosion facility," says Horn. "To date, our results show that over 10,000 years, the corrosion rate from bacteria would not penetrate beyond 1 millimeter. Alloy 22 is a very tough metal."

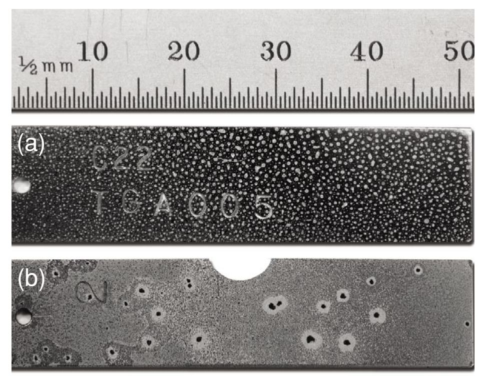
Overcoming Weld Stresses

How the waste packages are manufactured, especially the required welds, can affect their resistance to corrosion as well as their structural integrity. Residual stresses are a common by-product of manufacturing, especially welding, and if left untreated could lead to stress corrosion cracking. Livermore metallurgists plan to treat the canister welds in the repository with an annealing process that reduces the residual tensile stress and produces instead a compressive stress on the canisters' surface. Stress corrosion cracking does not occur under compressive stress.

The annealing process involves subjecting the welds to 1,100°C and then quenching



U-bend coupons are one of the four types of coupons being tested for corrosion resistance. U-bends are metals kept under continuous stress to try to induce stress corrosion cracking.



Coupons of (a) Alloy 22 and (b) Alloy 825 (which contains less nickel and molybdenum than Alloy 22) show many precipitates when subjected to high concentrations of minerals and salts. However, Alloy 22 has no localized corrosion whereas Alloy 825 has permanent pits caused by corrosion.

the metal in a water bath to produce a small overall compressive stress on the exterior surface. The canisters would then be shipped from the factory to the repository for storage until they are ready to be filled and sealed.

The canister lids would be fabricated offsite and then welded on after the canister was filled at the repository. Annealing would not work as a technique to lessen the stresses that will unavoidably occur in the final closure welds because the high heat generated during the process would damage the contents. "The nuclear waste will be in a relatively inert form when it is placed in the canisters," says McCright. "Subjecting the waste to the temperatures required by annealing might compromise that inertness."

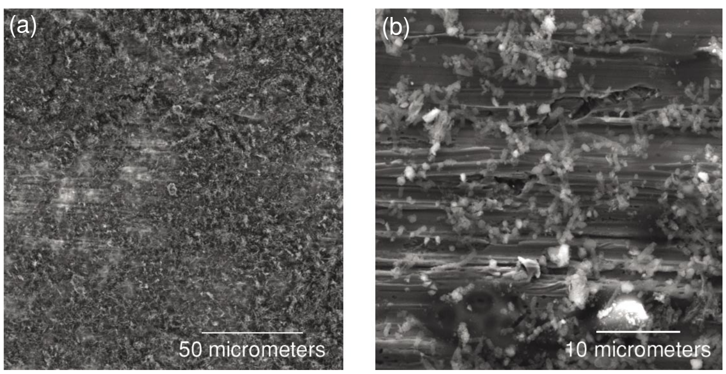
One promising alternative to annealing is laser peening, a process developed at Livermore, in which a laser produces a shock wave on a weld to form a compressive stress. (See *S&TR*, March 2001, pp. 26–28.) Laser peening can produce a compressive layer about 3 millimeters deep in the metal to strengthen the final closure welds. Livermore experts are characterizing structural changes of peened Alloy 22 samples using transmission electron microscopy, x-ray diffraction, and other techniques.

Favorable Testing Results

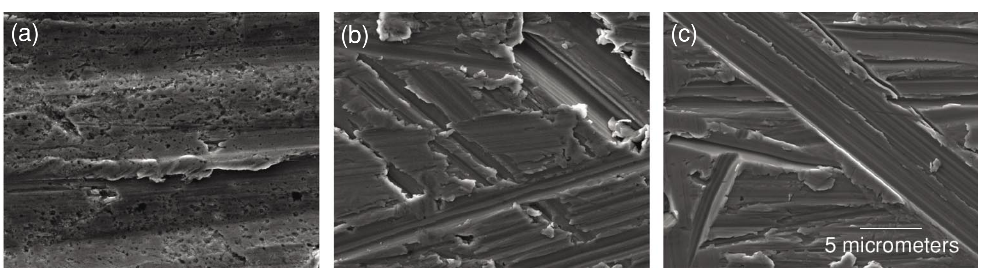
Attempts to accelerate corrosion with solutions representing the waters that could eventually contact the metal canisters have thus far indicated an extremely low general corrosion rate. The tests also have shown that the canister metals have extremely high resistance to all forms of localized corrosion and stress corrosion cracking in environments relevant to the repository. Also, no appreciable differences have been noted in corrosion rates obtained from the various water compositions and temperatures. The testing results support Livermore's models for long-term prediction of the waste packages' performance and strongly confirm the selection of Alloy 22 for the outer canister.

Testing and modeling at Livermore will proceed for several more years. In the meantime, McCright and others are refining the engineered barrier design to make components more efficient and economical to manufacture. "The plan is to manufacture 12,000 waste packages over 25 years, the equivalent of manufacturing more than one canister a day," he says. "We want every one to be as corrosion resistant as we can practically make them."

—*Arnie Heller*



Thin films of bacteria form on the surface of metal coupons tested in a solution containing nonsterile crushed Yucca Mountain rock. Bacteria that have colonized on an Alloy 22 coupon are shown magnified (a) 1,200 times and (b) 5,000 times.

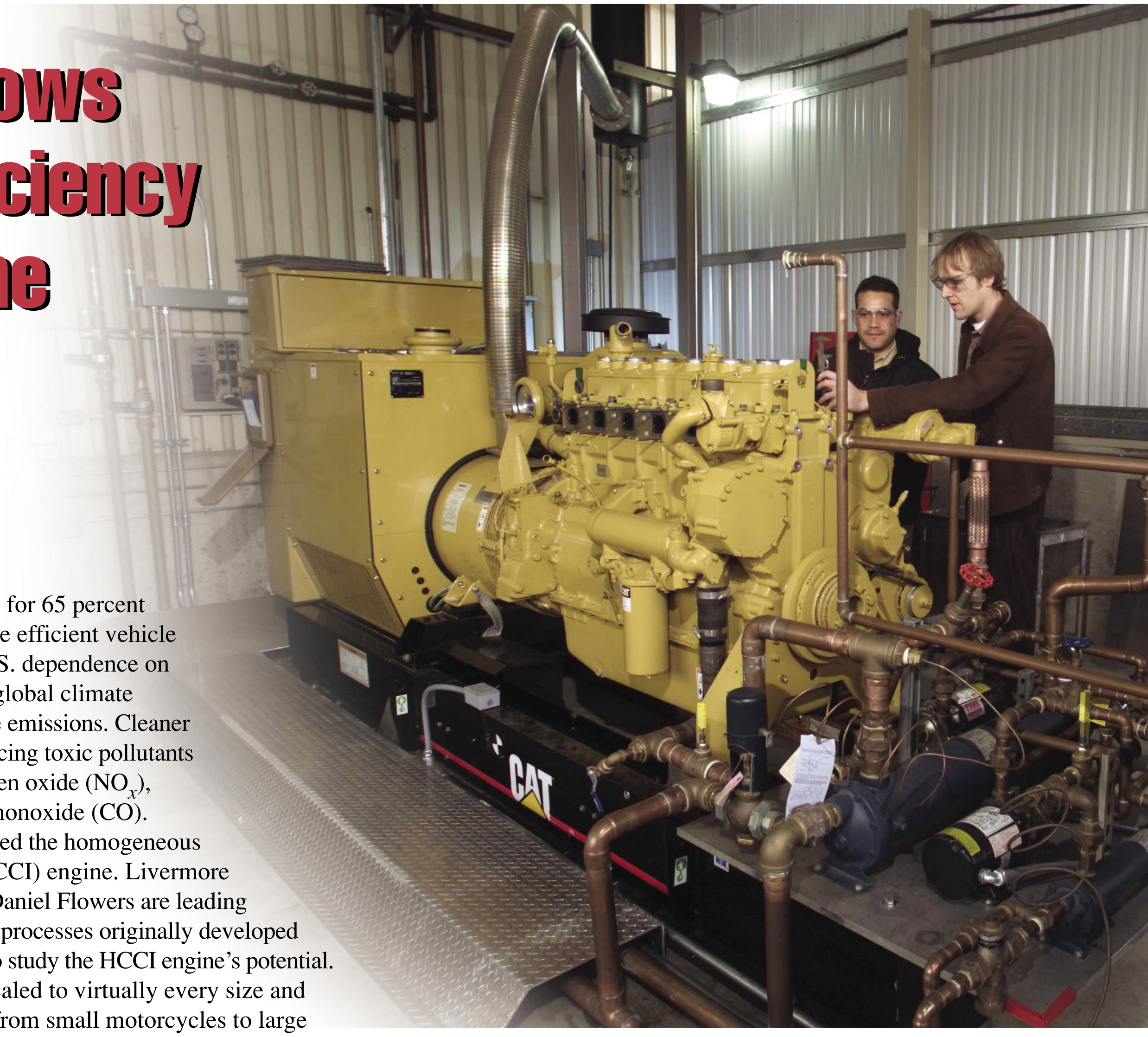


Electron micrographs (8,000 times magnification) show the extremely limited corrosion on an Alloy 22 coupon caused by bacteria after (a) 57 months in a solution containing nonsterile crushed Yucca Mountain rock compared to (b) a coupon that has been in a solution with presterilized rock (to kill all microbes) for 43 months, and (c) the same coupon at the start of the experiment.

Key Words: Alloy 22, engineered barrier system, laser peening, Long-Term Corrosion Test Facility (LTCTF), Nevada Test Site, Nuclear Regulatory Commission, nuclear waste repository, Yucca Mountain.

For further information contact Dan McCright (925) 422-7051 (mccright1@llnl.gov).

Engine Shows Diesel Efficiency without the Emissions



Livermore engineers Francisco Espinosa-Loza and Daniel Flowers work on the stationary homogeneous charge compression ignition engine.

TRANSPORTATION accounts for 65 percent of U.S. oil consumption. More efficient vehicle engine designs would reduce U.S. dependence on foreign oil and help to mitigate global climate change caused by carbon dioxide emissions. Cleaner engines would contribute to reducing toxic pollutants in the atmosphere, such as nitrogen oxide (NO_x), hydrocarbon (HC), and carbon monoxide (CO). One promising technology is called the homogeneous charge compression ignition (HCCI) engine. Livermore engineers Salvador Aceves and Daniel Flowers are leading a team that is applying modeling processes originally developed by nuclear weapons researchers to study the HCCI engine's potential.

HCCI technology could be scaled to virtually every size and class of transportation engines, from small motorcycles to large ships. Stationary HCCI engines could replace the spark-ignited and diesel engines currently used for backup-power generation and in businesses such as hotels where recovered exhaust heat is used for swimming pools and other facilities. Caterpillar Inc. has donated a six-cylinder stationary engine for the Livermore team to verify modeling results experimentally.

In the HCCI engine, fuel is homogeneously premixed with air, as in a spark-ignited engine, but with a high proportion of air to fuel. When the piston reaches its highest point, this lean fuel–air mixture autoignites (spontaneously combusts) from compression heating, as in a diesel engine. A feature of the HCCI engine is that it burns cooler than spark-ignited and diesel engines. Lower temperature combustion considerably reduces the emissions of nitrogen oxide. In addition, premixed combustion in HCCI engines reduces particulate matter emissions to very low levels. An HCCI engine can operate using any fuel, so long as the fuel can be vaporized and mixed with air before ignition.

Although the advantages of the HCCI engine are clear, significant challenges must be overcome before the engine is commercially viable. Once engineers resolve these issues, HCCI engines could achieve approximately 40 percent peak efficiency versus 30 percent for spark-ignited engines. Diesel engines can achieve high efficiency similar to HCCI engines, but diesel engines are major sources of NO_x and particulate matter emissions. The Department of Energy's Office of Energy Efficiency and Renewable Energy and the California Energy Commission are funding the Livermore research. Professors Karl Hedrick, Robert Dibble, and J. Y. Chen at the University of California at Berkeley are collaborating with Livermore researchers to address some of the engine combustion control challenges.

Combustion Counts

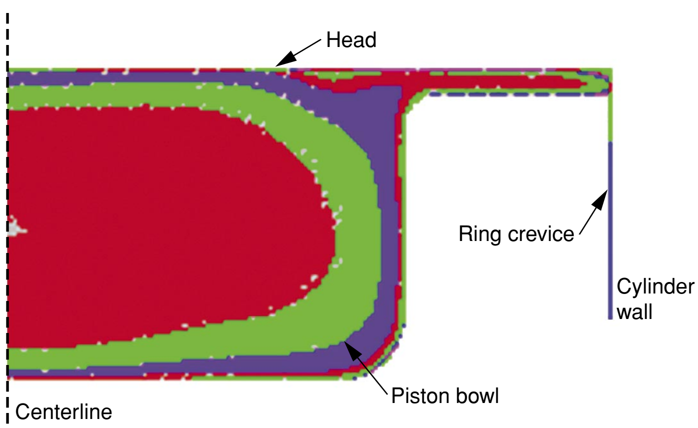
The greatest challenge is controlling the HCCI engine's ability to operate under a wide range of speeds and loads. The HCCI engine does not have a combustion trigger such as a spark plug or fuel injector found in conventional engines. Instead, combustion is achieved by controlling the temperature, pressure, and composition of the fuel–air mixture so that it spontaneously ignites at the proper time. The required control system is fundamentally more challenging than conventional engines because the ignition is sensitive to very small changes in temperature. When a load is suddenly added, as when a vehicle goes from idle to cruising speed, the control system must adjust the temperature, pressure, and composition rapidly enough to maintain stable combustion.

"Because HCCI engines lack traditional combustion-control systems, understanding the chemical kinetics of combustion is key to addressing its challenges," says Aceves. Livermore's chemical kinetics code, known as HCT, and Los Alamos National Laboratory's fluid mechanics code KIVA, used in combination, have allowed Laboratory researchers to make critical contributions to HCCI technology.

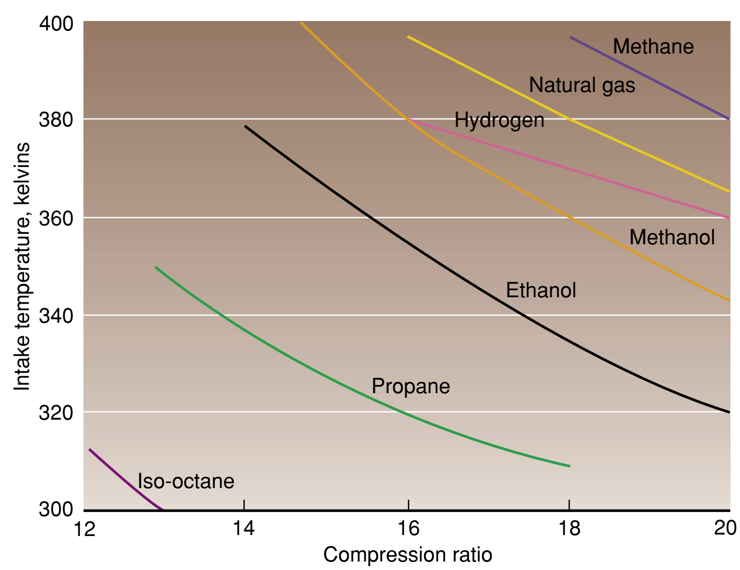
HCT calculates problems involving gas hydrodynamics, transport, and chemical kinetics (how molecules react). The code has been used to study the combustion properties of many compounds. The Livermore team has modified HCT by incorporating models for heat transfer, a turbocharger, and exhaust-gas recirculation, which are all required for engine analysis.

KIVA is a three-dimensional fluid mechanics code that simulates liquid and gaseous flow under steady-state and transient conditions. Livermore researchers use KIVA to simulate flow in a model of the HCCI cylinder divided into spatial zones. This multizone approach allows temperature and charge velocity distributions to be calculated separately from the much more computationally intensive chemical kinetics processes, which are solved using only a few zones. These codes allow engineers to visualize the inner workings of the combustion process.

Because combustion in HCCI engines is mainly controlled by chemical kinetics and minimally by turbulence effects, the Livermore team developed a two-step process to analyze combustion. The effect of turbulence is first considered by running KIVA to obtain a temperature distribution within the cylinder. The results from KIVA are then used in HCT, which calculates the combustion parameters related to HCCI. This two-step process makes it possible to obtain accurate predictions for the turbulent combustion inside an HCCI engine, within a reasonable computational time for the Laboratory's computers. The significance of this computer-based analysis is that for the first time, researchers can accurately predict combustion rates, emissions, and performance of HCCI engines.



KIVA, a three-dimensional code, is used to simulate gaseous flow in a model of the HCCI engine divided into spatial zones. Together with the HCT code, researchers determine where and when in the combustion chamber the hydrocarbons and carbon monoxide are formed.



Intake temperatures necessary for various fuels to operate a heavy-duty engine running at maximum power. The intake temperature required for proper ignition is shown as a function of the compression ratio (the ratio of the volume of the combustion space in the cylinder at the bottom of the piston stroke to the volume at the top of the stroke).

Finding the Optimal Fuel

In 2003, Livermore researchers used the HCT and KIVA codes to evaluate fuels and additives that might improve HCCI engine performance. Engineers analyzed several fuels, including propane, methane, natural gas, ethanol, iso-octane, and a variety of additives.

Modeling and experiments have shown that operating conditions for satisfactory HCCI combustion are, in part, dictated by the characteristics of the fuel. Fuels with a relatively low octane number, such as n-heptane or diesel fuel, require lower intake temperatures, and fuels with a high octane number, such as methane and natural gas, require higher intake temperatures. Understanding the limitations of each fuel leads to specific engine design options. Flowers notes, “Certain engine features will work better depending on the type of fuel. We can make any given fuel work with HCCI, but we’re still defining the characteristics that work best.”

Computer simulations were conducted using small amounts (10 parts per million) of 913 additives to determine if one additive might better control combustion. Some of the peroxides showed the most promise, considerably advancing ignition timing. Although this finding is significant, the benefit of using additives to control combustion must be compared to other potential control mechanisms, such as adjusting the intake temperature to obtain satisfactory ignition timing and combustion. Using an additive may increase the engine’s complexity because additional systems would be needed to store and deliver the additive to the combustion chamber.

HCCI’s low-temperature combustion also affects its emissions. Although the engine produces lower NO_x and particulate emissions, it releases higher amounts of hydrocarbon and carbon monoxide than spark-ignited or diesel engines. At very low loads, CO levels can reach as high as 60 percent of the total fuel carbon because of incomplete combustion. Fortunately, CO and unburned HC are easily controlled with commercially available oxidation catalysts.

Laboratory researchers used the two-step KIVA–HCT method to investigate when and where in the cylinder the HC and CO are formed. The simulations showed that CO reaches its maximum level immediately following the main heat release during combustion. CO then decreases and slowly rises again during the expansion stroke of the piston. This increase happens because fuel is not completely consumed in the lowest temperature regions of the combustion chamber. Aceves says, “There is enough time during the expansion stroke for unburned fuel to migrate from the crevices and boundary layer into the hot core of the cylinder, where it can react and produce additional CO and CO_2.”

Because HCCI is a thermal autoignition process, temperature sensitivity is an important issue. Controlling cylinder temperatures will help not only to address the emissions issue but also to control combustion itself. “A few degrees in temperature,” says Aceves, “can make the difference between combustion and no combustion. HCCI needs a control mechanism that detects ambient temperature and adjusts the mixture of air to fuel in the cylinders to obtain ignition at the right time, and the controller has to be fast enough to handle the adjustments.” One possibility is for gases coming into the cylinder to be warmed by heat recovered from exhaust gas.

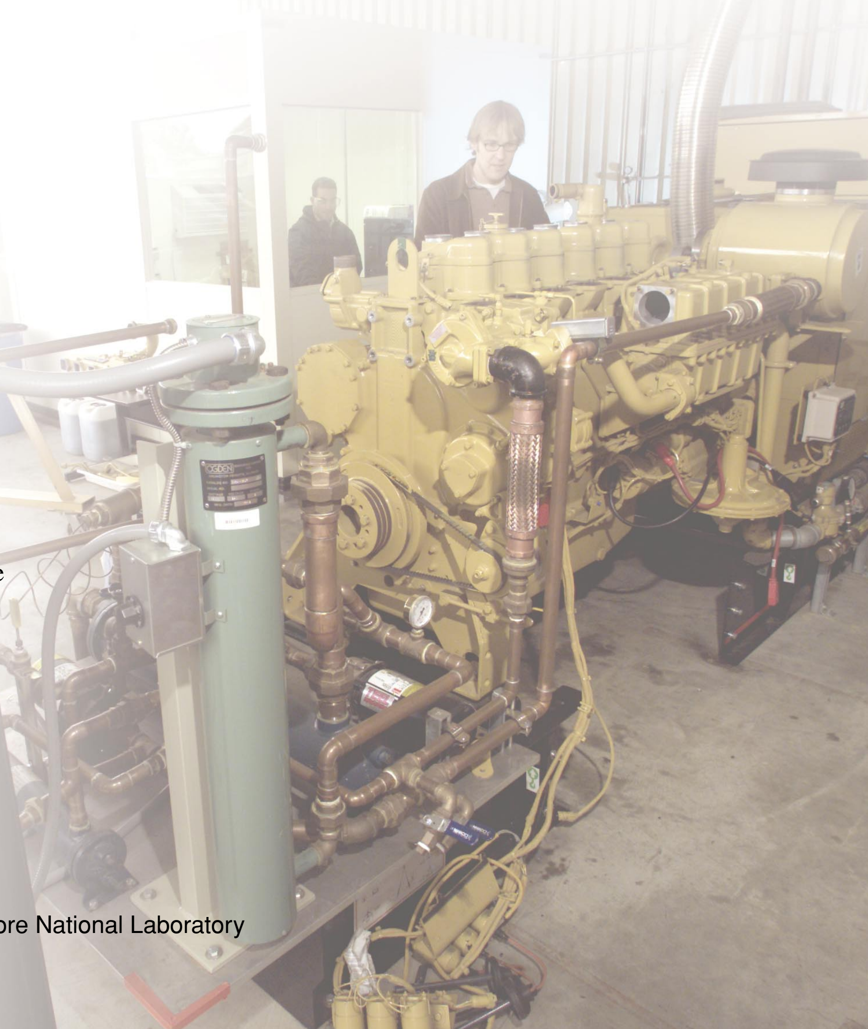
Controlling the temperature is also an important factor for enabling multiple cylinders to work together efficiently. Flowers explains, “Because HCCI is very sensitive to temperature changes, the interactions and differences between cylinders have a greater effect in an HCCI engine than in a spark-ignited or diesel engine.”

The Livermore team projects that a stationary HCCI engine will be commercially available in the next five years. Nissan currently sells a hybrid HCCI–diesel automobile in Japan and in Europe. Laboratory engineers are hopeful that in a decade or so, HCCI engines will be powering the transportation industry in the U.S.

—*Gabriele Rennie*

Key Words: combustion; homogeneous charge compression ignition (HCCI) engine; hydrodynamics, chemistry, and transport (HCT) code; KIVA code.

For further information contact Salvador Aceves (925) 422-0864 (aceves6@llnl.gov) or Daniel Flowers (925) 422-0529 (flowers4@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 and System Using Power Modulation and Velocity Modulation Producing Sputtered Thin Films with Sub-Angstrom Thickness Uniformity or Custom Thickness Gradients

Claude Montcalm, James Allen Folta, Christopher Charles Walton
U.S. Patent 6,668,207 B1
December 23, 2003
A method and system to determine a source flux modulation recipe for achieving a selected thickness profile of a film to be deposited over a flat or curved substrate (such as concave or convex optics). The substrate is exposed to a vapor deposition source operated with time-varying flux distribution. Preferably, the source is operated with time-varying power applied thereto during each sweep of the substrate to achieve the time-varying flux distribution. Preferably, the method includes the steps of measuring the source flux distribution (using a test piece held stationary while exposed to the source with the source operated at a number of applied power levels), calculating a set of predicted film-thickness profiles (each film-thickness profile assuming the measured flux distribution and a different one of a set of source flux modulation recipes), and determining from the predicted film-thickness profiles a source flux modulation recipe that is adequate to achieve a predetermined thickness profile. Aspects of the invention include a computer-implemented method using a graphical user interface to facilitate convenient selection of an optimal or nearly optimal source flux modulation recipe to achieve a desired thickness profile on a substrate. The method enables precise modulation of the deposition flux to which a substrate is exposed and thus provides a desired coating thickness distribution.

Glass-Silicon Column

Conrad M. Yu
U.S. Patent 6,670,024 B1
December 30, 2003
A glass–silicon column that can operate in temperature variations between room temperature and about 450°C. The glass–silicon column includes large-area glass, such as a thin Corning 7740 boron–silicate glass bonded to a silicon wafer with an electrode embedded in or mounted on column glass and a self-alignment silicon post-glass hole structure. The glass–silicon components are bonded, for example, by anodic bonding. In one embodiment, the column includes two outer layers of silicon each bonded to an inner layer of glass, with an electrode embedded between the layers of glass and with at least one self-alignment hole-and-post arrangement. The electrode functions as a column heater, and one glass–silicon component is provided with a number of flow channels adjacent to the bonded surfaces.

Pre-Loading of Components during Laser Peen-Forming

Lloyd A. Hackel, John M. Halpin, Fritz B. Harris
U.S. Patent 6,670,578 B2
December 30, 2003
A method and apparatus for forming shapes and contours in metal sections by prestressing a workpiece and generating laser-induced compressive stress on the surface of the metal workpiece. The step of prestressing the workpiece is performed with a jig. The laser process can generate deep compressive stresses to shape even thick components without inducing unwanted tensile stress at the metal surface. The precision of the laser-induced stress enables exact prediction and subsequent contouring of parts.

Method of Fabrication of Electrodes and Electrolytes

Alan F. Jankowski, Jeffrey D. Morse
U.S. Patent 6,673,130 B2
January 6, 2004
Fuel-cell stacks contain an electrolyte layer surrounded on top and bottom by an electrode layer. Porous electrodes are prepared, enabling fuel and oxidant to flow to the respective electrode–electrolyte interface without the need for high temperatures or pressures to assist the flow. Porous anodes, cathodes, and electrolytes are fabricated using rigid, inert microspheres and thin-film metal deposition techniques. Microspheres contained in a liquid are randomly dispersed on a host and dried so that the microspheres remain in position. A thin-film deposition technique is subsequently used to deposit a metal layer on the microspheres. After the metal layer is deposited, the microspheres are removed. Voids (that is, pores) are left in the metal layer, forming a porous electrode. Successive repetitions of the fabrication process result in the formation of a continuous fuel-cell stack. Stacks may produce power outputs ranging from about 0.1 to 50 watts.

Awards

David Chambers has been elected a **Fellow** of the **Acoustical Society of America** (ASA) for his contributions to time-reversal processing methodology. The award will be presented during a recognition ceremony at the ASA meeting in May 2004.

Chambers was initially hired at the Laboratory as a physicist but later moved to the Electronics Engineering Department and worked on ocean acoustics and broadband acoustic beam design for ocean applications. That work led to research in acoustic tomography, imaging, and acoustic time reversal. He is now applying time-reversal imaging techniques to radar imaging in highly cluttered environments.

The Laboratory's **Transportation Systems Management Program** (TSMP) received the **2003 Federal Energy and Water Management Award**, which was awarded jointly by the Department of Energy (DOE) and the Federal Interagency Energy Policy Committee, and the **2003 Departmental Energy Management Award**, awarded by DOE.

Energy Secretary Spencer Abraham says the Laboratory's "excellent performance in supporting the Energy Management Program is an example for others to emulate." The Secretary cited the TSMP's success in reducing fleet- and commuter-fuel operating costs by an estimated $1.4 million annually. The Livermore program is designed to develop effective methods to reduce traffic-related air-quality and congestion problems at the Livermore and Tracy sites and in the surrounding communities. An important part of TSMP's activities is keeping Laboratory employees informed about convenient and cost-effective commuting alternatives, such as buses, carpools, and vanpools. Another related mission is educating employees and the public about the hazards of air pollution.

Abstracts

On the Front Lines of Biodefense

Livermore's pathogen bioinformatics group is developing DNA signatures (specific regions of DNA or RNA that uniquely identify a pathogen) and deploying validated assays in the field. The signatures were used at the 2002 Winter Olympics, are included in the nation's public health system, and have been in continuous use for homeland defense since autumn 2001. Early detection and unmistakable identification of pathogen outbreak (natural or intentional) are crucial for limiting their potentially catastrophic human and economic cost. The team has developed DNA signatures for virtually every major pathogen for which there is adequate genomic sequence information available. The team uses a Livermore-designed, automated system called KPATH to develop signatures for bacterial and viral pathogens. This system, the world's only fully automated DNA signature "pipeline," delivers signature candidates (spanning 200 to 300 base pairs of DNA) in minutes to hours. KPATH also automatically downloads newly sequenced pathogen genomes from all major public databases to ensure that existing signatures are still effective.

Contact:
Tom Slezak (925) 422-5746 (slezak1@llnl.gov).

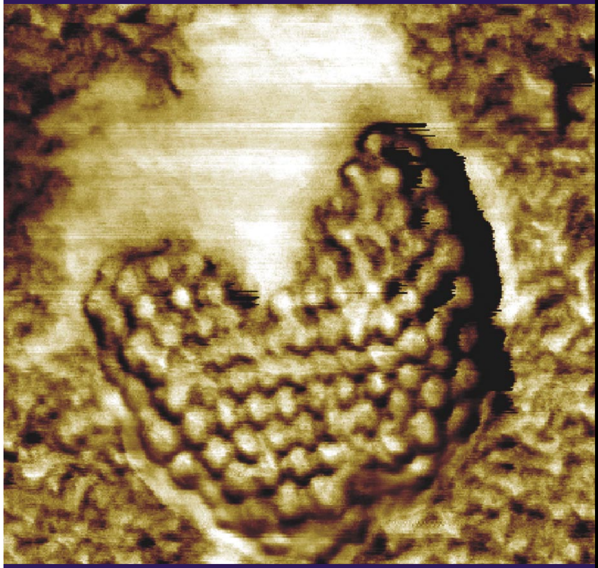
Defending against Corrosion

A team of Livermore researchers is testing and refining the design and materials for what may eventually be 12,000 nuclear waste packages as part of a nationwide program to design, license, and build an underground nuclear waste repository in Yucca Mountain, Nevada. Livermore is focusing on developing the engineered barrier system, which consists of a waste package, drip shield, and supporting structures. The engineered barrier system is designed to work with the natural barriers of Yucca Mountain to contain the repository's radioactive wastes and prevent them from seeping into the water table, which lies about 300 meters below the planned repository. Information is needed about how modern materials will behave over thousands of years under the range of conditions expected to occur in the repository. As a result, the Livermore research is based on accelerated aging tests of materials that are proposed for use in the engineered barrier system as well as on computer models to simulate how a repository built at Yucca Mountain would perform over thousands of years. In the current repository design, waste will be stored in a package consisting of a set of two nested canisters—an outer canister made of a highly corrosion-resistant metal (Alloy 22) and an inner canister made of a tough, nuclear-grade stainless steel (316NG). An overhanging drip shield made of titanium will give added protection from dripping water and any rocks falling from the repository ceiling.

Contact:
Dan McCright (925) 422-7051 (mccright1@llnl.gov).

U.S. Government Printing Office: 2004/683-056-70057

Biosecurity and Nanosciences



Livermore's BioSecurity and Nanosciences Laboratory is pioneering new ways to study pathogens and biomolecules at the nanoscale level.

Also in May

- *Laboratory researchers are developing a system to detect nuclear materials in cargo containers.*
- *Improved algorithms speed up the calculations being run on the nation's supercomputers.*
- *Ocean sequestration is one possible approach to stabilize the amount of carbon dioxide in the atmosphere.*

Coming Next Month

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