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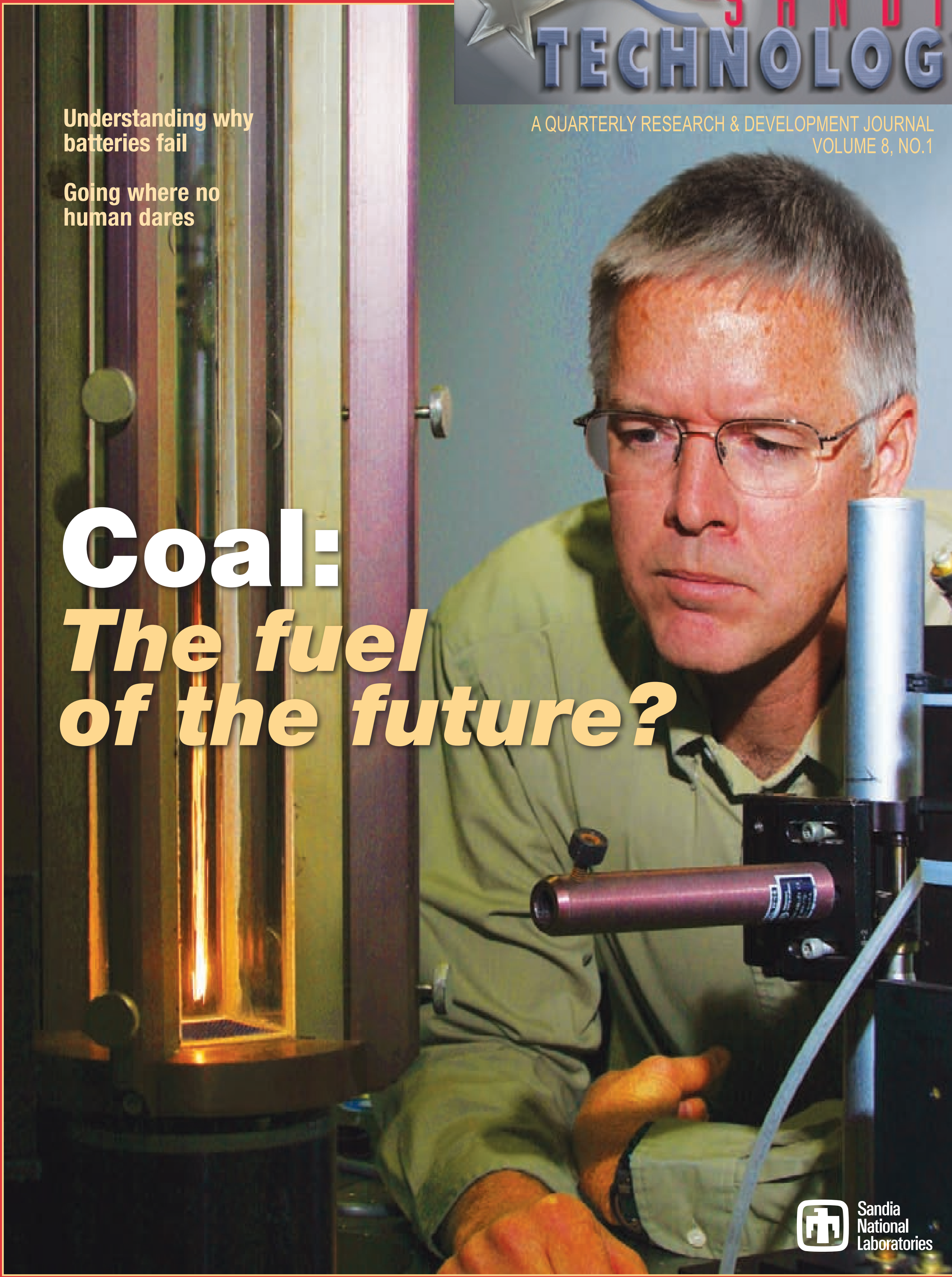
Understanding why batteries fail

Going where no human dares

Coal: *The fuel of the future?*



Sandia National Laboratories

What is LDRD

Sandia's world-class science, technology, and engineering work defines the Labs' value to the nation. These capabilities must remain on the cutting edge, because the security of the U.S. depends directly upon them. Sandia's Laboratory Directed Research and Development (LDRD) Program provides the flexibility to invest in long-term, high-risk, and potentially high-payoff research and development that stretch the Labs' science and technology capabilities.

LDRD supports Sandia's four primary strategic business objectives: nuclear weapons; nonproliferation and materials assessment; energy and infrastructure assurance; and military technologies and applications; as well as an emerging strategic objective in homeland security. LDRD also promotes creative and innovative research and development by funding projects that are discretionary, short term, and often high risk, attracting exceptional research talent from across many disciplines.

When the LDRD logo appears in this issue, it indicates that at some state in the history of the technology or program, LDRD funding played a critical role.

On the Cover:

Chris Shaddix studies an experiment to optimize the burning of coal at Sandia's Combustion Research Facility in Livermore, California. (Photo by Bud Pelletier)

Sandia Technology (ISSN: 1547-5190) is a quarterly magazine published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has broad-based research and development responsibilities for nuclear weapons, arms control, energy, the environment, economic competitiveness, and other areas of importance to the needs of the nation. The Laboratories' principal mission is to support national defense policies by ensuring that the nuclear weapon stockpile meets the highest standards of safety, reliability, security, use control, and military performance. For more information on Sandia, see our website at *http://www.sandia.gov*

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FROM THE *Editor*

Dear Readers,

Sandia National Laboratories is an institution that is about our national security.

When it comes to security, one of the most obvious places to look is along a nation's borders. Sandia's engineering research to better assess the security ramifications of the flow of commerce through our nation's bustling system of ports is featured in this issue. Another border success, the formation of the first bi-national laboratory, is also noted. This is an important step in what could be a model for international cooperation globally.

Much of the issue examines the Labs' work with energy security. Global energy consumption, along with population and economic production, continues to grow. While oil is expected to continue to dominate world energy use for some time, the potential downsides are numerous. Among them are global political unrest, severe environmental consequences, and a U.S. dependency on unstable sources.

Researchers are studying the fuel cell, crucial to making the hydrogen economy succeed. Using computer modeling and physical experiments, they are showing the way for others in industry in this important frontier effort. Other Sandia engineers are at work on longer-lived, more reliable batteries for the environmentally friendly FreedomCAR. At Sandia's Combustion Research Facility, in California, several researchers are focused on better ways of burning coal, a major energy resource that can provide electricity now and hydrogen in the near future. At a more basic level, research leading to better understanding of combustion and atmospheric chemistry is also showing some promising results.

It behooves a national laboratory to address these issues in a multidisciplinary way, and Sandia is doing just that.

Will Keener
Editor

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Keeping points-of-entry safe **with systems-level modeling**

Sandia's Border Technologies Grand Challenge capitalized on a range of existing Sandia capabilities, including the Weapons of Mass Destruction Decision Analysis Center, the National Infrastructure Simulation and Analysis Center (a joint Sandia and Los Alamos National Laboratory program), and the Labs' expertise in robotics. Twenty-one Sandia researchers from both the California and New Mexico sites worked on the project.

Carolyn Pura is blunt in assessing the nature of her job. "Protecting our borders is difficult and expensive," she says.

Almost as quickly, however, she asserts that Sandia's recent work on border security is well on its way to providing an enormously valuable national asset. Sandia provides federal agencies with a reliable and comprehensive simulation capability that lets officials "test drive" various security solutions prior to investing in them, says Pura, who serves as program deputy for borders and transportation security at the Labs.

The focus of the Borders Grand Challenge, funded by a three-year, $6 million Laboratory Directed Research and Development LDRD project, was to develop simulation-based systems analyses for characterizing the security of the U.S. border system and the impact of new detection technologies.

Flow of people, goods

The interactive analysis that serves as the hallmark of the program has largely focused on the illegal smuggling of radiological material but can also be applied to other threats, such as explosives or chemical/biological attacks. The work uses detailed models that capture actual facilities and procedures and examines border operations of all kinds. Of utmost concern is the flow of people and goods through the various border choke points.

"There is a cost-benefit tradeoff associated with any technology that might be used in border security," Dan Horschel, project manager, explains. With commerce, for example, officials must consider the flow of people and goods crossing the border, any delays that might occur due to security provisions, and the operational costs that emerge as a consequence of the flow and delay. Sandia's

Sandia's models, can give decision-makers specific and reliable data to help make sound decisions about how and where to invest.

systems-level methodologies and tools address these complexities and allow homeland security officials to make data-driven decisions.

Economic impact is key

Sandian Mark Ehlen led the economic modeling effort. Ehlen points out that a unique feature of the program is its ability to project the economic impact that might be felt if a venue implements certain security options. A typical port, whose processing time increases due to a newly configured set of chemical detectors, for example, might expect to increase its on-site inventories and shipments by up to 15 percent, leading to increased business costs and decreased sales figures. In addition, says Ehlen, the firms that ship through the port will be affected by the delays and increased costs and may take their business elsewhere. Such consequences will fluctuate from venue to venue, depending on the security measures and operational plans.

Sandia's models, by simulating the effects of detector placement, the use of facial recognition software, or the impact of other technology devices and strategies, can give decision-makers specific and reliable data to help make sound decisions about how and where to invest.

Mid-fidelity vs. high-fidelity

The models themselves come in two primary forms. "Mid-fidelity" models offer a broader, bigger-picture look at a border location that might give users the ability, for example, to view personally owned vehicle and cargo vehicle flows at an actual facility, using that facility's own

Sandia researcher Andy Vaughn shows an example of how simulations developed at Sandia can help evaluate new sensor technologies and suggest ways to minimize impacts. In this case, cargo inspection equipment at a seaport increases the probability of detecting illicit materials but also disrupts operations and causes large delays when used in certain configurations.

(Photo by Bud Pelletier)

Analysis tools developed by Sandia can help evaluate the impact of technologies at border crossings in terms of throughput, security, and economic cost.

procedures. A "higher-fidelity" model, seen on the computer screen when the operator "zooms in" on the activity, might focus on security interrogation and feature detailed sensor modeling.

High-fidelity models, because of their visualization features and accurate geometries and motion, provide a sound environment for training and can be quickly reconfigured to address border concepts-of-operation.

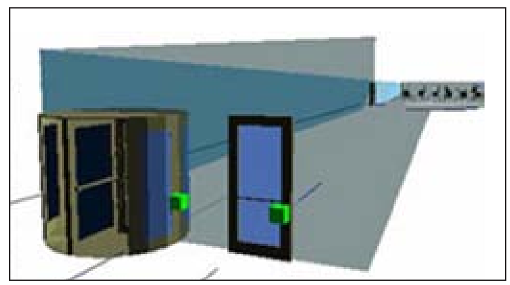
Sandia's models have been integrated to include multiple domains, including air, sea, and land. All of the domains have been built with the capability of analyzing the impacts of different types of sensing equipment, from radiation detection to x-ray equipment. Both a land crossing pedestrian model and an airport, for example, examine the movements of people and look at biometrics technology, while a seaport and land cargo port analyze cargo inspection equipment.

Sandia-developed simulations help officials identify the best approach within their facilities and the most "throughput-friendly" detector locations.

"Hot source" dilemma

One significant issue that security officials are known to face is the problem of "hot sources." These occur when multiple detectors sound alarms simultaneously due to benign radiation sources. Hot sources significantly disrupt port operations by causing long delays while the source is identified and, in most cases, determined to be nonthreatening.

Sandia's modeling work helps users of the system address the hot source problem by examining various detection scenarios and options to consider. An "in-situ" option, where traffic is stopped while threat sources are localized with a portable detector and removed from the primary traffic stream, might be suitable for certain venues, while others might choose to maintain a "self-identification pre-sort" lane of traffic that allows medical patients or known radioactive shipments to sort themselves out of traffic. Sandia-developed simulations help officials identify the best approach within their facilities and the most "throughput-friendly" detector locations.



Though Pura and Horschel say the work represents the most comprehensive modeling work available on border security, the research has the potential to go much further. Ideally, Sandia could extend the capability to all ports of entry across the country, creating a complete national model that is able to examine changing security measures and operations and their impact. "What we have now are high-quality, targeted studies," says Horschel.

"The value that a national model can offer decision-makers at the highest level could be immeasurable."

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"People around the world are interested in copying this model; even though we have only just started, it is a dream shared..."

Bi-National Sustainability Laboratory open for business

Four years in the making, the Bi-National Sustainability Laboratory is now a reality in a 4,000-square-foot facility at Santa Teresa, New Mexico, west of El Paso. Officials dedicated the lab at an opening ceremony November 18.

The BNSL is a collaboration initiated by Sandia's Advanced Concepts Group and financially supported by the United States, Mexico, and the State of New Mexico. The purpose of the fledgling enterprise is to create a "necklace" of research centers stretching from the Gulf Coast to the Pacific. Other states along the Mexico-U.S. border have expressed interest in the concept.

"This will be a wonderful opportunity for collaborative technical efforts to enhance border security," says Sandia vice president Gerry Yonas, who led the effort to create the BNSL.

Beyond border security, success for these labs will be defined by the number of research ideas its personnel can turn into functioning, profit-making companies, with better paying jobs on both sides of the border.

"People around the world are interested in copying this model; even though we have only just started, it is a dream shared. . . . We hope this will change the way borders are looked at," says a spokesperson for the Mexican National Council of Science and Technology.

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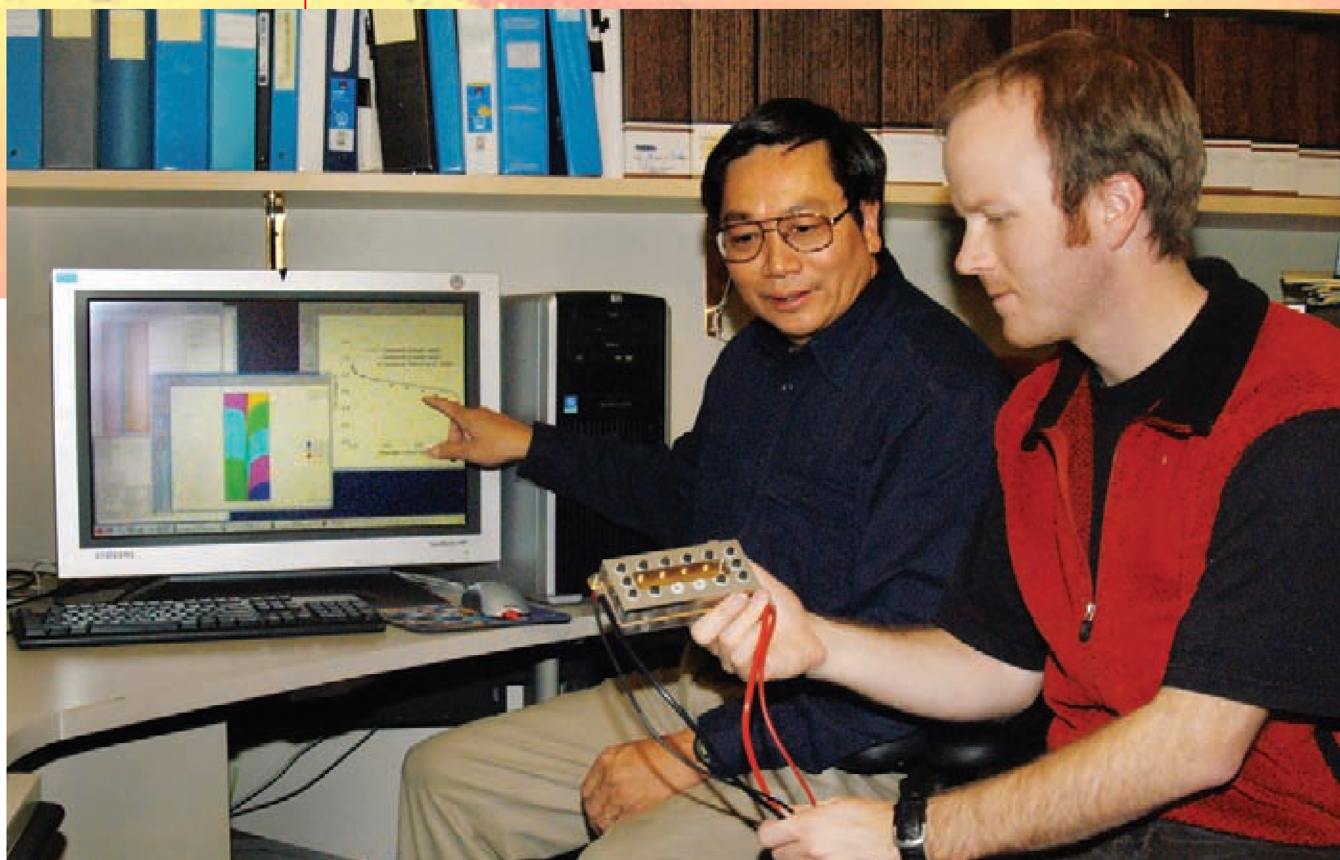
Sandia vice president Gerry Yonas speaks during BNSL opening ceremonies.

Understanding PEM fuel cell performance and durability



Sandia researchers Ken S. Chen (left) and Mike Hickner are collaborating to study PEM fuel cells. Ken is developing computational models to describe the phenomena, while Mike is performing physical experiments.

(Photo by Michelle Fleming)

Two Sandia researchers are working to understand several key phenomena that control hydrogen-fueled PEM (proton exchange membrane or polymer electrolyte membrane) fuel cells. Ken S. Chen is developing computational models to describe the phenomena, while Mike Hickner is performing physical experimentation.

The work is internally funded through a three-year LDRD project to tackle key technical challenges.

Proper water management and performance degradation, or durability, must be addressed before PEM fuel cells can be used to routinely power automobiles and homes.

"A natural byproduct of using hydrogen and oxygen to produce electricity in a PEM fuel cell is water [with waste heat being the other]," Chen, project principal investigator, says. "One challenge is maintaining the proper amount of water in a PEM fuel cell. Sufficient water in the membrane is needed to maintain its conductivity, but too much liquid water can result in flooding the cathode gas diffusion layer. This prevents reactant oxygen from reaching catalytic sites and causes performance deterioration."

The work of two Sandia researchers is leading to better understanding of how liquid water is produced, transported, and removed efficiently in PEM fuel cells and how PEM fuel cell performance degrades. These understandings are keys to finding ways to maintain the cells' long-term performance during normal and harsh (such as freezing) conditions and improving their durability.

Better understanding

The close teaming between Chen's modeling and Hickner's experimental efforts has been quite helpful in meeting project objectives. "Our approach in combining computational modeling with experiments is unique," Chen says. "Typically, Mike would perform discovery experiments to gain physical insights. I would then develop a model to describe the observation or data that Mike has obtained. Mike would perform further experiments so I can validate the model I have developed."

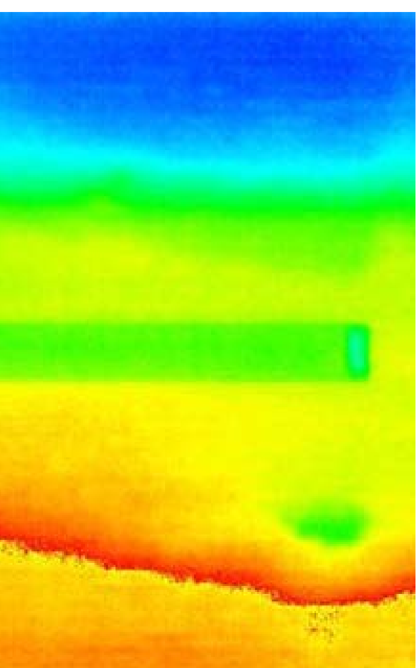
Hickner says they've obtained some positive feedback between the experiments and analyses. The intent is to build a computational tool that can be used in designing fuel cells, eliminating the need to experiment on every single part of them.

Larger issues

"We want to have all the small pieces worked out in the modeling process so we can concentrate on the larger issues with experiments," he says.

Chen has been using GOMA, a Sandia-developed multidimensional and multi-physics finite-element computer code, as the basic platform to develop 2-D performance models for PEM fuel cells. With the assistance of Nathan Siegel, a postdoctoral researcher with Sandia's Solar Technologies department, he is also exploring the development of quasi-3D PEM fuel cell models using FLUENT, a commercial computational fluid dynamic computer code.

Chen emphasizes that the focus of this LDRD project is on understanding the key phenomena using experimental means and computational models, both simplified and multi-dimensional.



Liquid water content of an operating PEM fuel cell. Red color means more water, blue less.

"Sandia's state-of-the-art multiphysics codes, like GOMA, form the backbone from which simplified phenomena-centric models can be developed to explore complex behavior, such as occurs in operating PEM fuel cells," says Joel Lash, manager of Sandia's Multiphase Transport Processes department.

For the past couple of years, Chen and Hickner have focused mainly on liquid water transport, developing a PEM fuel cell model that can be employed to simulate fuel cell performance, and performing diagnostic tests on fuel cells for phenomena discovery and model validation. Next, Chen says, they will tackle the technical issues of performance degradation or durability.

Publishing results

To date, the team has reported portions of its work in three refereed publications, four proceedings papers, and half a dozen technical presentations. "Our validation method is new and exciting and leading us to learn some things not well known previously," Hickner says.

Bruce Kelley, project manager for the PEM fuel cell LDRD, says the project was developed specifically to leverage Sandia's capabilities in multiphysics modeling and membrane materials to develop broader capabilities with applicability to fuel cells and other related technology areas. In doing so, Kelley says, "We have attracted significant industrial interest in the work."

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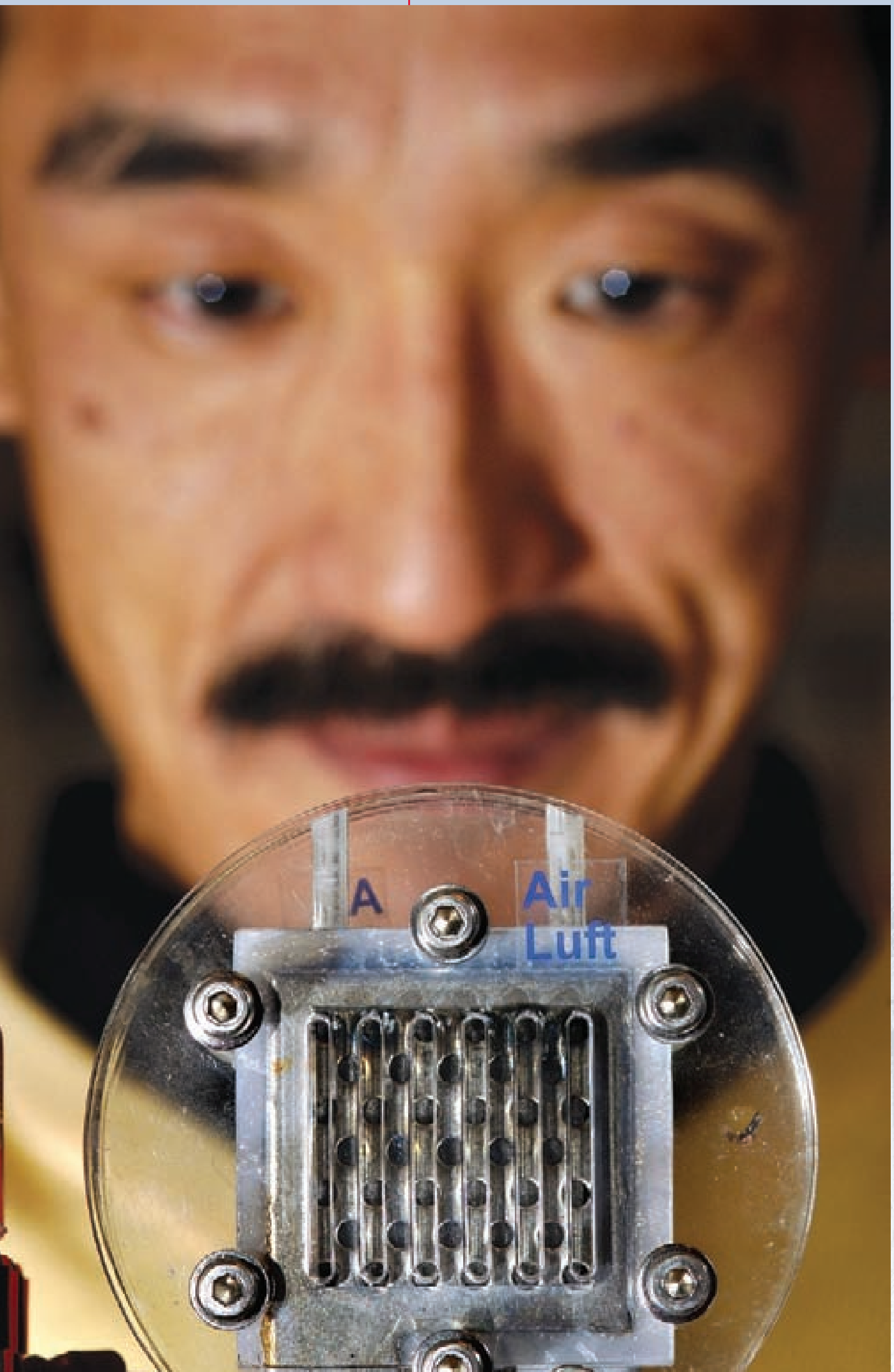
Sharp and Sandia join forces to study fuel cell technologies



Sharp Corp. researcher Akimasa Umemoto examines a prototype miniature fuel cell stack.

(Photo by Randy Montoya)

Sandia National Laboratories and Sharp Corp. have signed a Cooperative Research and Development Agreement (CRADA) to work together on renewable and alternative energy technologies, including advanced fuel cells for portable power applications.

Jeff Nelson, Sandia manager of the CRADA, says the agreement is one of Sharp's first interactions with a U.S. laboratory. Nelson says Sandia will contribute novel membrane and catalyst capabilities to the fuel cell project, while Sharp will lend its system and application-level experience.

"Our hope is that we're successful and that success will expand our collaboration into solar photovoltaics and other areas," Nelson says. Sharp is the world's largest producer of photovoltaic modules.

The broader partnership between Sandia and Sharp will involve research and development of Sharp's solar photovoltaic technologies, including tests and improvements on reliability, durability, calibration of solar modules, inverters, and other advanced applications. Sandia's immediate focus is on portable power applications, such as the use of direct methanol fuel cells to power consumer electronics like laptops, cell phones, and PDAs.

Sharp has asked Sandia to fabricate fuel cells using Sandia's proprietary membranes and catalysts. Sandia researchers, led by principal investigator Chris Cornelius, have begun designing the materials and membrane electrode assemblies for Sharp's specific application target. They will fabricate and test the fuel cells during the 12- to 18- month project.

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Understanding why batteries fail

"Batteries are a necessary part of hybrid electric-gasoline powered vehicles and someday, when the technology matures, will be part of hybrid electric-hydrogen fuel cell powered vehicles," says Dan Doughty, of Sandia's Advanced Power Sources Research and Development Department. "Current hybrid vehicles use nickel-metal hydride batteries, but a safe lithium-ion battery will be a much better option for the hybrids."

Doughty notes that a lithium-ion battery has four times the energy density of lead-acid batteries and two to three times the energy density of nickel-cadmium and nickel-metal hydride batteries. It also has the potential to be one of the lowest-cost battery systems. His department receives about $1.5 million a year from the FreedomCAR program to improve the safety, lengthen the lifetime, and reduce the costs of lithium-ion batteries.

As part of the Department of Energy-funded FreedomCAR program, Labs researchers are studying ways to make lithium-ion batteries work longer and safer.

Hybrid vehicles, like the Honda Insight above, will benefit from research being done by Sandia's Power Sources Technology group.

The FreedomCAR program, initiated by President Bush in 2002, focuses on developing hydrogen-powered electric vehicles to help free the U.S. from dependence on foreign oil supplies. Five national laboratories — Sandia, Argonne, Lawrence Berkeley, Idaho, and Brookhaven — are involved in the program, each researching different aspects of making hybrid electric-hydrogen vehicles a reality.

Graceful failure

Sandia's FreedomCAR work centers on the areas of battery abuse tolerance and accelerated lifetime prediction, with abuse tolerance receiving most of the focus. "We want to develop a battery that has a graceful failure — meaning that if it's

Sandia researcher Brad Hance examines a lithium-ion battery that may someday be used in a hybrid car or one powered by a fuel cell.

(Photo by Michael Overstreet)

damaged, it won't cause other problems," Doughty says. "We have to understand how batteries fail and why they fail."

The technical goal is to comprehend mechanisms that lead to poor abuse tolerance, including heat- and gas-generating reactions. Understanding the chemical response to abuse can point the way to better battery materials. But, Doughty says, there is no "magic bullet" for completely stable lithium-ion cells. "Fixing the problem will come from informed choices on improved cell materials, additives, and cell design, as well as good engineering practices.

"You won't want batteries to fail if you're driving just a little too fast, so we take batteries to conditions they're not designed for and see how they fail," Doughty says. Researchers overheat the batteries, simulate a fuel fire, crush or penetrate batteries, and drop them on hard surfaces. They also charge them too much, perhaps to twice the limit, or short-circuit them.

"The idea is to see what the response of it is, to characterize the magnitude of the response, how severe it is" so engineers can figure out how to overcome the problem, Doughty says. Work in abuse tolerance is beginning to shed light on mechanisms that control cell response, including effects of the anode and cathode, electrolyte breakdown, and battery additives.

Accelerated life test

The other area of work — accelerated life test — involves developing a method to predict lithium-ion battery life. Researchers have been improving the lithium-ion battery for a decade; what's needed now is testing and analysis to validate the battery's life and performance in hybrids and its real cost, says Ted J. Miller, who works on advanced battery technology for the Ford Motor Company.

Miller, speaking on behalf of the U.S. Advanced Battery Consortium, which has worked closely with Sandia on a lithium-ion battery, said he expects the technology to be introduced in hybrids before the end of the decade.

The Sandia research team uses two models, Doughty says. "The empirical model generates life prediction from accelerated degradation test data, while the mechanistic model relates life prediction to changes in battery materials. Our approach provides an independent measure of battery life so we don't have to rely on what battery manufacturers tell us."

Improved test procedures developed at Sandia have led to lithium-ion test standards that the battery team has developed and recently published in a Sandia research report. Doughty anticipates that the Society of Automotive Engineers will soon adopt these test procedures as national standards, just as they adopted in 1999 the abuse test procedures Sandia developed for electric vehicle batteries.

"There has been substantial progress in making batteries more tolerant to abusive conditions," Doughty says. "It won't be long before these batteries will be used in gasoline-electric hybrid vehicles. And the great thing is this technology will be able to transfer over to the electric-hydrogen fuel cell powered hybrid vehicles of the future."

Doughty agrees battery life and cost are linked. If a battery is cheap enough, it could be replaced more frequently; if it lasts a long time, a customer might be willing to spend more money for it, he says.

"The battery has to last 150,000 miles, which is the life of a car. That is no small feat," says Doughty. "Durability becomes a cost issue if you have to change your several-thousand-dollar battery twice in the life of the car. That significantly changes the economics of a hybrid vehicle."

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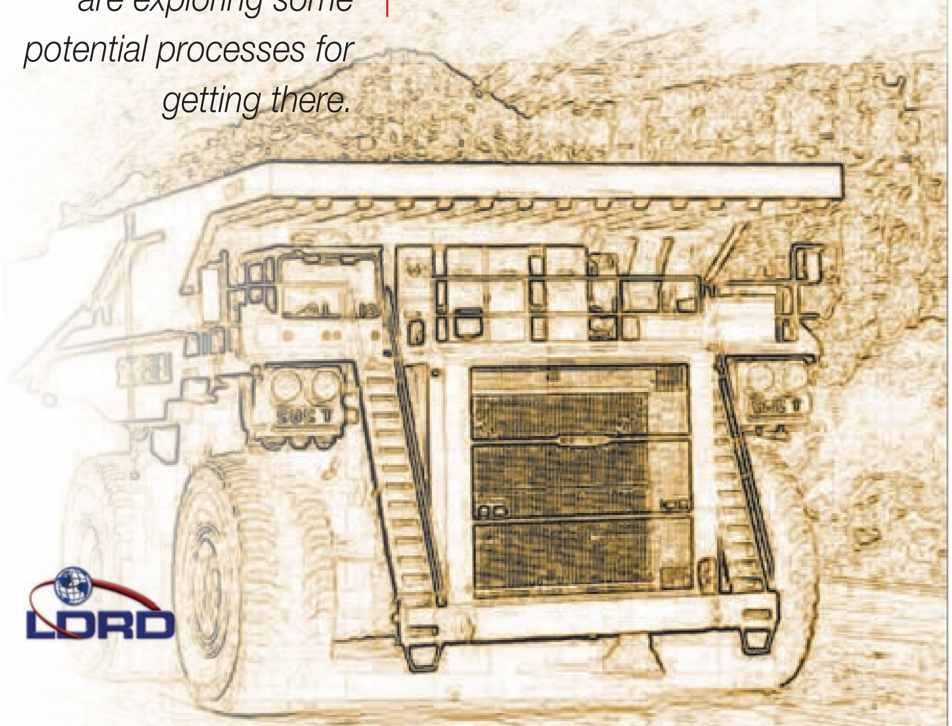
The path to the hydrogen economy leads through some familiar territory. Although there are many long-term options for providing hydrogen as a future fuel, coal is a leading contender to supply hydrogen in the near term. Researchers at Sandia's Combustion Research Facility in Livermore, California, are exploring some potential processes for getting there.

Coal: The fuel of the future?

While some day we may be able to produce hydrogen by breaking up water molecules in association with the high-temperature heat from nuclear power reactors, or through renewable energy technologies, right now the most cost-effective way to produce hydrogen is with coal. That's the view of Chris Shaddix of Sandia's Combustion Research Facility (CRF) in Livermore, California.

Shaddix and his colleagues are involved in a number of experiments to optimize the combustion of coal to produce the most energy and the least possible pollution. While traditional coal combustion produces many harmful emissions, modern plants can meet environmental regulations for burning coal cleanly, Shaddix says. This can be costly to utility companies, but the cost of competing fuels — particularly natural gas — have climbed to the point where burning clean coal is competitive.

Figure in the potential benefits of storing carbon dioxide emissions, stripped from the smoke stacks, in geologic repositories, such as old oil fields, and coal looks very promising for generating both electricity and hydrogen to provide a bridge to that future technology. "Utilities are starting to invest in coal," says Shaddix.



Two approaches

Two different approaches to burning coal are now under study. One, called oxy-combustion, combines coal with pure oxygen. The second, called gasification, burns coal only partially to create a fuel-gas. The first approach is driven by concern over emissions of CO_2 and other

Chris Shaddix (left) and Alejandro Molina discuss an experiment to determine the best proportion of oxygen and CO_2 for oxy-combustion of coal. Molina's small-scale experiments have established the groundwork to bring two other larger reactors into the research.

(Photo by Bud Pelletier)

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pollutants. The burning of coal in oxygen is a near-term solution that with current knowledge can produce exhaust streams that are close to pure CO_2, says Shaddix. Harmful pollutants like nitrogen oxides, sulfur compounds, and mercury are virtually eliminated.

Companies in Japan, Canada, Germany, and other countries favor the oxy-combustion approach, and several pilot plants are under construction. "Because the U.S. didn't sign the Kyoto accord, companies here are not as interested," says Shaddix. "They tend to favor gasification technologies, which offer higher efficiency and lower pollution formation."

DOE has already demonstrated gasification technology in two pilot projects. The next step is for the U.S. to combine coal gasification with hydrogen production and CO_2 sequestration. At the same time, several commercial proposals are afoot in the U.S. for private utilities to build these plants without government support.

Working with the National Energy Technology Lab, Morgantown, West Virginia, the CRF is focused on understanding the chemistry and physics of coal combustion using its state-of-the-art diagnostic capabilities and modeling expertise. "We apply computational models of reacting particles to the data to understand why we see the results we see," says Shaddix.

Modeling, experiments

Shaddix and researcher Andy Lutz developed a model of key components in the system in an LDRD project begun last year. The concept (see diagram) basically calls for burning coal with oxygen to create a syngas, or fuel-gas, that is cleaned of contaminants and stripped of hydrogen with the carbon-rich remainder being used to generate power through a turbine.

As experimental results are used to adjust the model, researchers can get a better idea of some of the limitations on the system when hydrogen is extracted. "No one has looked at the operational limits of this type of system yet," says Shaddix. Data on CO_2 produced from the process will also be valuable to studies on carbon sequestration, or storage of CO_2 in geologic repositories such as depleted oil fields. "We will work to coordinate the outputs from our model for use in carbon sequestration modeling," says Lutz.

Alejandro Molina, a Sandia postdoctoral student working with Shaddix, lights a flat-flame burner plate in the CRF's small-scale lab for coal studies and adjusts the amount of coal particles fed through the burner. A two-foot-tall chimney around the burner protects against air disturbances inside the lab and enables researchers to analyze the combustion.

He points out a bright zone, just above the burner, where initial combustion occurs. A longer vertical track of flame is known as the char oxidation zone. "To optimize coal combustion for carbon sequestration, it is very important to understand how fast it burns and releases energy," Molina says. Burning coal with air, which is predominantly (79 percent) nitrogen,

Sandia staff member Al Salmi examines a gasification test reactor at the Combustion Research Facility being developed to help study the behavior of coal gases under pressure.

(Photo by Bud Pelletier)

One type of gasification, called steam reformation, combines the coal with steam in a hot environment to produce a "syngas," composed mostly of CO and hydrogen. Once the syngas is produced, it can be burned directly in a combustor — such as a turbine — to produce power or can be further reacted with more steam to shift the remaining CO to CO_2 and to produce more hydrogen. The CO_2 can be sequestered and the hydrogen can be used to power a car in an engine or fuel cell, to power a turbine to produce electricity, or even to fly an airplane.

creates the problem of separating CO_2 and nitrogen before sequestration. "If you use pure oxygen instead of air, you get water and CO_2, so you only have to condense the water and you have 100 percent CO_2."

One problem with this oxygen approach has been a high flame temperature, he continues, which could rapidly destroy the metal burner materials. One solution is to recycle cooler CO_2 into the burner to cool the flame temperature. "The question is: what is the right proportion of oxygen and CO_2?"

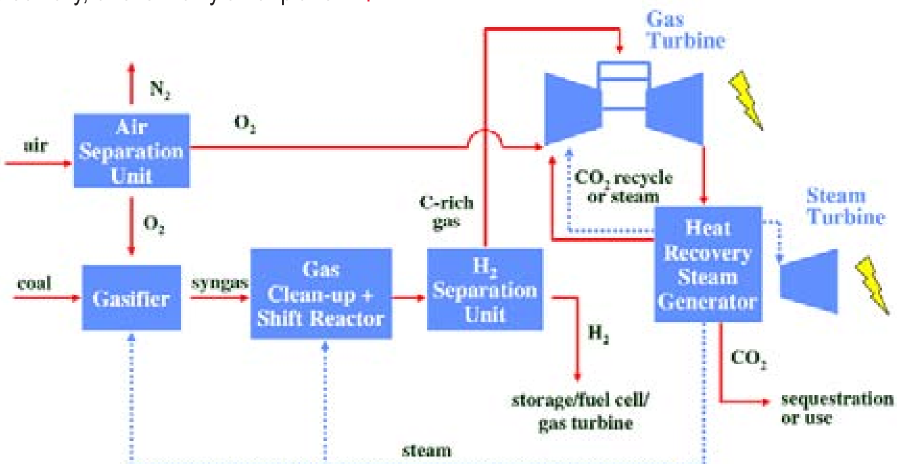
Two new labs

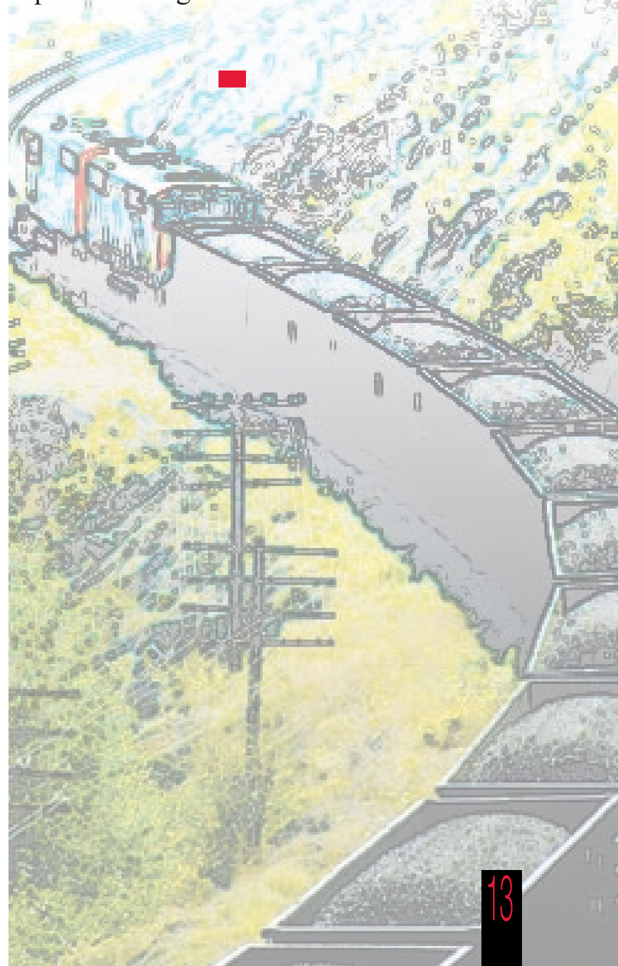
Molina has been working on these experiments for about two years in the small-scale lab, but work is now under way to bring two other CRF facilities into the research. A gasification lab will help the researchers study the behavior of coal gas under pressure. While the small-scale work was focused on particle behavior and fundamental-scale measurements, a large-scale lab will focus on gas issues within the reactor.

The gasification lab, expected to be operational by this summer, includes a two-inch tube within a pressure vessel. "Gasification is slower than combustion, so it is done under pressure to increase the reaction rates," Shaddix explains. The new apparatus is instrumented for laser diagnostics and sample collection and includes electrical heaters to preheat the gases so they flow through a vertical center section where data can be collected.

The third reactor is a two-story flow reactor that will help the team study the oxygen-coal combustion with recycled CO_2. The unit includes a six-inch-diameter reactor tube running downward below a 75-kilowatt thermal heater. Specially designed hardware injects highly refined coal particles into the top of the reactor tube. As the reaction moves down the tube, equipment allows sampling and laser diagnostic testing.

A key effort will be to measure the concentrations of ammonia and hydrogen cyanide, precursors to nitric oxide formation, says Shaddix. The coal char phase of burning can eliminate nitric oxide, creating the possibility that in actual operations more NO is consumed than is produced, leading ultimately to a commercial application. Large-scale tests in this reactor are expected to begin in a few months.





'Riding the dimer' to understand NO splitting

By straddling twin molecules, a Sandia physicist — working with an international team — obtains a unique view of their breakup. The detailed experimental results are expected to provide tests for computational methods used by chemists to describe complex chemical processes in combustion and atmospheric chemistry involving the nitric oxide molecule.

Imagine you are standing, John Wayne style, on the backs of two runaway horses pulling a stagecoach. You try to bring the horses to a stop but instead the harnesses break, the horses separate, and an unlucky passenger gets thrown from the stage.

You learn, first, that you are not John Wayne (because he always succeeded). But because you were standing at the heart of the action, you alone of all the bystanders saw exactly how the breakup occurred and how the passenger was ejected.

In work published in a January issue of *Science*, a team of researchers from Sandia, the National Research Council in Ottawa, Canada, and elsewhere accomplished this trick scientifically. In effect, they stood on pair after pair of joined nitric oxide molecules (called NO dimers) and watched as each pair split after being excited by an ultra-short laser pulse.

They not only measured the direction of each separating NO molecule, but also the direction and energy of an electron spat out as each breakup occurred. The electron revealed the quantum energy levels of the dimer as it separated — a key factor in analyzing the process.

Calculating back

By using a computer to calculate back from the final speeds and angles, the researchers could reconstruct the event to "see" the exact path the electron and each dimer fragment had taken, exactly as though they had ridden on the dimers as they split. With previous experimental techniques, scientists usually watched these events from the sidelines, their points of view external to the reactions — the so-called "laboratory frame of reference." Such methods can only average the results obtained from molecules oriented in all different directions, thus obscuring details of the reaction.

The new experiments reconstruct action from the molecules' perspective — the molecular frame of reference — and yield a more detailed view. This provides a stringent test of theoretical calculations.

"For those using computing to predict what happens in chemical reactions, without actually doing the experiments, the NO dimer is a very challenging system to calculate," says Sandia's Carl Hayden.

Results showed that the dimers don't come apart smoothly, as had formerly been thought, but go through an intermediate step. About 150 femtoseconds after the initiating pulse, a more diffuse but definite configuration, known as a Rydberg state, appears. That state dissociates in about 600 femtoseconds. (A femtosecond is one millionth of a nanosecond, or 10^{-15} second in scientific notation. It is a measurement used in laser technology.)

Understanding the dissociation process is not simple. "The number of possible electronic states is very large," says Hayden. One purpose of the work is to determine which of these states are important during the dissociation.

The results were obtained by firing femtosecond laser excitation pulses at a beam of NO molecules made cold enough to allow NO dimers to form (about 20 degrees Kelvin). Firing only enough energy to disrupt one dimer with each laser pulse, researchers performed the experiments until as many as 500,000 dissociations had been observed.

A critical second pulse

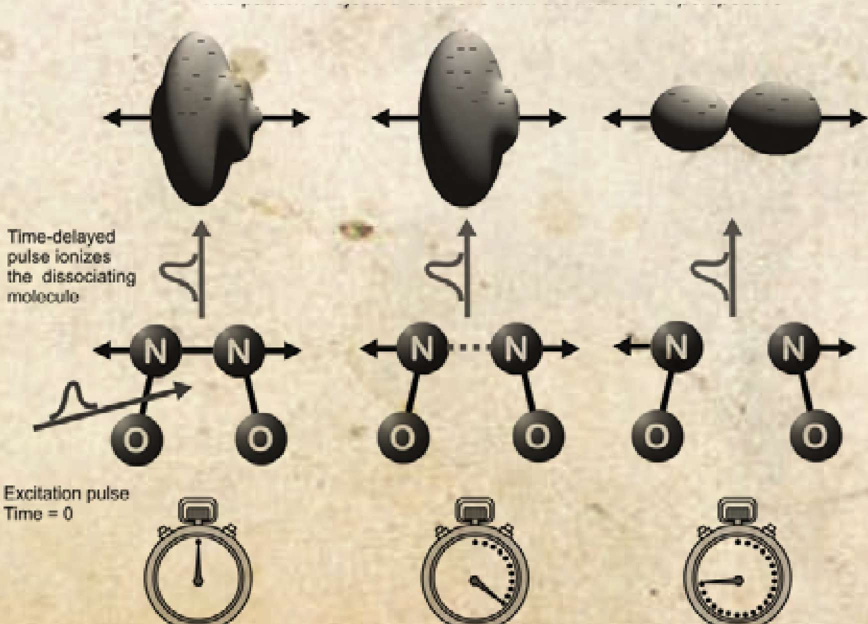
A second femtosecond probe pulse, sent with a variable time delay after the excitation, ejected an electron from each dimer as it broke up, providing a "snapshot" of the progress of the dissociation. The dimer fragments were analyzed by a tool developed at Sandia/California called a time-resolved, coincidence-imaging spectrometer. The spectrometer, which uses a flat detector, is able to capture electrons flying off in three dimensions through use of an electric field that bends the electron flight toward the detector. "The ones that arrive latest have traveled the farthest from the point of ejection," says Hayden. "The energy and angle is what we're looking for."

A similar process is used to simultaneously measure velocities of the ions and hence the NO molecular fragments produced. DOE's Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences funded the work.

Results were the product of an international collaboration. The measurements from the molecular perspective were done at Sandia, with complementary work to measure dimer intermediate state lifetimes achieved at the Steacie Institute for Molecular Sciences, at the National Research Council of Canada. Other groups in Canada and at the University of Southern California did quantum mechanical calculations. The Open University in the United Kingdom performed some of the modeling of the 3-D electron distributions.

Carl Hayden (right) prepares to image dimer molecules very rapidly as they split and emit electrons.

Drawing below illustrates ejection pattern from NO molecule's perspective.



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Going where no human DARES

Facing a tough situation at the White Sands Missile Range in New Mexico, a Sandia robot recently withstood deadly radiation to free a stuck radiation source and render a test facility useable once again. The source… was safely returned to its insulated base at a 3,000-square-foot Department of Defense lab in southern New Mexico. The robot, for its successful efforts, was unofficially dubbed "M2" for the cartoon character Mighty Mouse.

Bob Anderson demonstrates the capabilities of the robot affectionately known as M2. (Photo by Randy Montoya)

Alarms were blaring, warning lights flashing, and personnel were monitoring the stricken site around the clock in late October at the Gamma Irradiation Facility at White Sands Missile Range in southern New Mexico. The cause was a cylinder, the size of a restaurant salt shaker but considerably more deadly: Gamma rays from the cobalt-60 it contained could kill a human in 30 seconds. Its radiation field was too deadly even in a protective suit to get near enough to free it.

The cylinder — used to irradiate circuit boards and

Because high radiation levels can kill a robot's electronics, Sandia robotics manager Phil Bennett estimated M2 could withstand intense radiation for only 50 minutes.

vehicles to see how their electronic circuits stand up to radiation — normally arrived and departed for tests through a metal sleeve, driven by pneumatic air. (The method is similar to that used by drive-up banks, where pneumatic air drives a cylinder containing transaction paperwork and money through a tubing system.)

But this time the cylinder became stuck. From the safety of their control room, White Sands technicians increased air pressure in steps until they had reached 50 times normal, but they could not budge the cylinder. They speculated it had jammed into a signal switch in the sleeve's pathway. Increased air pressure would only push the switch's edge more deeply into the cylinder.

White Sands management decided to call the local NNSA RAP team — the Radiological Assistance Program — headquartered at Sandia in nearby Albuquerque.

Richard Stump, Sandia RAP leader, explained the problem to robotics manager Phil Bennett, who suggested a robot that might do the job. The 600-pound, five-foot-long robot, which became unofficially known as M2, rolled on treads, could maneuver around obstacles, and had a long, multijointed gripper arm with the dexterity to reach into awkward places and apply force to drills and screwdrivers. Intended as a bomb-disabling unit, M2 could remember positions, important in starting with tools at the right height and depth.

No trigger finger

The team's plan called for the robot to reach up and drill a hole through an oddly angled steel plate, insert a wire through the drilled hole, and nudge the switch to a more appropriate position.

Because the robot lacked a trigger finger to depress and release a drill control, the Sandia team stalked the aisles of local hardware stores, buying cordless equipment to modify into remotely operated drills, hooks, and grippers. Sandians Bob Anderson and Jim Buttz tested M2 on a mock-up of the stuck container and switch until it performed perfectly.

But the October trip to White Sands revealed that reality was more complex than the dry run. Anderson steered the robot around two radiation shields and stopped it at the work site. The robot drilled through the steel plate, opening a space for a probe to pass through and push down one side of the switch. It didn't budge.

A hole at the switch's fulcrum failed to dislodge the obstacle. After an hour and a half, the robot's lower portion, damaged by radiation, was no longer responding to commands. Using a long pole, a safety rope, and a winch, the RAP team carefully pulled the trapped robot out of the radioactive lab.

After a day of tool redesign, trips to local hardware stores, repairs, rebooting the robot and performing other maintenance, Anderson and Buttz found they could reactivate it. On the third day of work, M2 succeeded in removing a plate covering the switch. A blast of air blew the entire switch out of the cylinder's pathway, and the radiation source at long last was blown back to its storage position.

"The warning lights and horns that could be heard for miles away finally stopped after 21 straight days of annoying personnel at White Sands," says Stump. An inspection revealed the problem: forceful early attempts to blow the cylinder back apparently had bent the straight switch into a right angle. "It would have been impossible to return the source to storage without removal of that switch," says Stump.

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"We want to develop a battery that has a graceful failure — meaning that if it's damaged, it won't cause other problems. We have to understand how batteries fail and why they fail. Fixing the problem will come from informed choices on improved cell materials, additives, and cell design, as well as good engineering practices. You won't want batteries to fail if you're driving just a little too fast, so we take batteries to conditions they're not designed for and see how they fail."

Dan Doughty
Manager, Advanced Power Sources R&D

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