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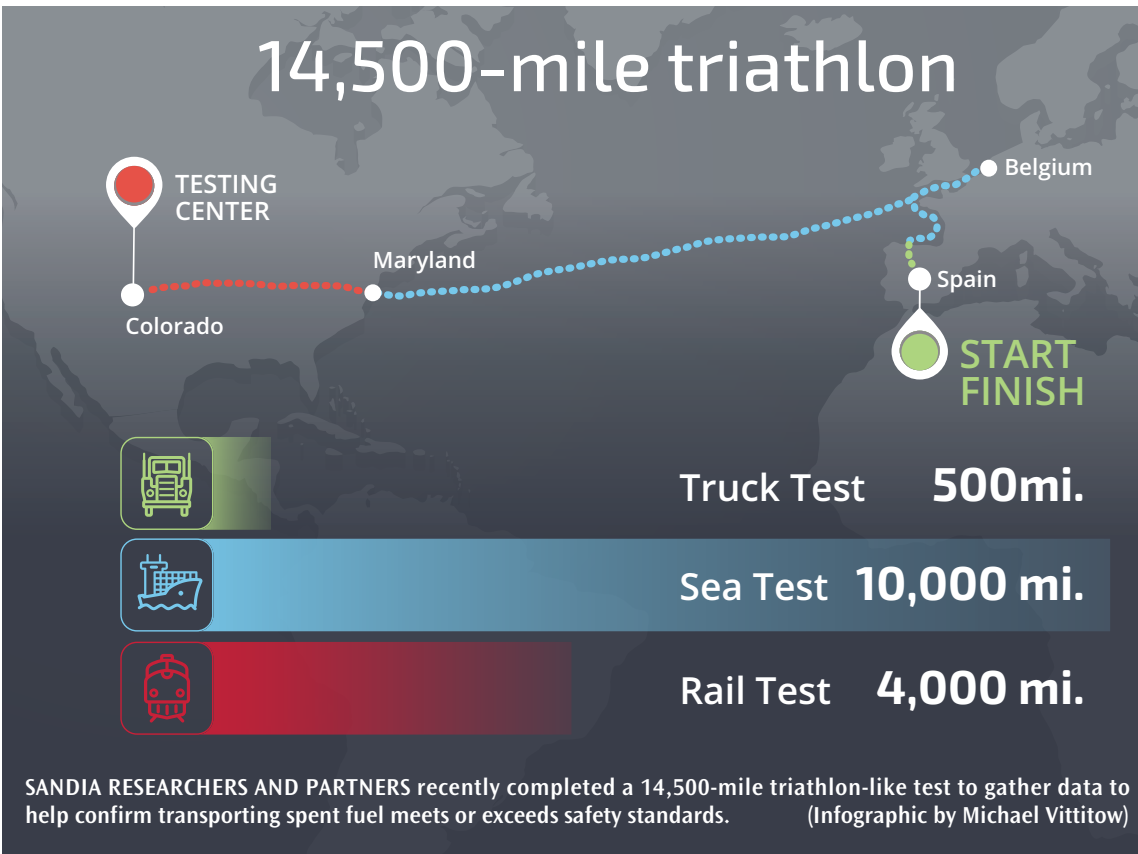
Sandia LabNews



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Road, rail, boat



Sandia transport triathlon puts spent nuclear fuel to the test

By Mollie Rappe

Spent nuclear fuel needs to be safely transported from the power plants where it is generated to interim storage locations or an eventual permanent geological disposal site.

“This test is more realistic than past tests and could result in a more reliable quantification of the transportation risks.”

— Sandia researcher Sylvia Saltzstein

Late last year, Sandia researchers completed an eight-month, 14,500-mile triathlon-like test to gather data to help confirm transporting spent fuel in specially designed and certified casks will meet or exceed safety requirements established by the Nuclear Regulatory Commission.

Nuclear power supplies almost 20 percent of US electricity and is the leading carbon-neutral power source. However, it produces between 2,200 and 2,600 tons of spent fuel in the US each year. Fuel rods become brittle and highly radioactive while powering the

(Continued on page 4)



ON THE ROAD to cleaner, more efficient combustion . . . 3



SANDIANS WIN sustainability awards 5



JACQUELINE CHEN elected to National Academy . . . 6

The guns of shock physics find materials information through dynamic compression

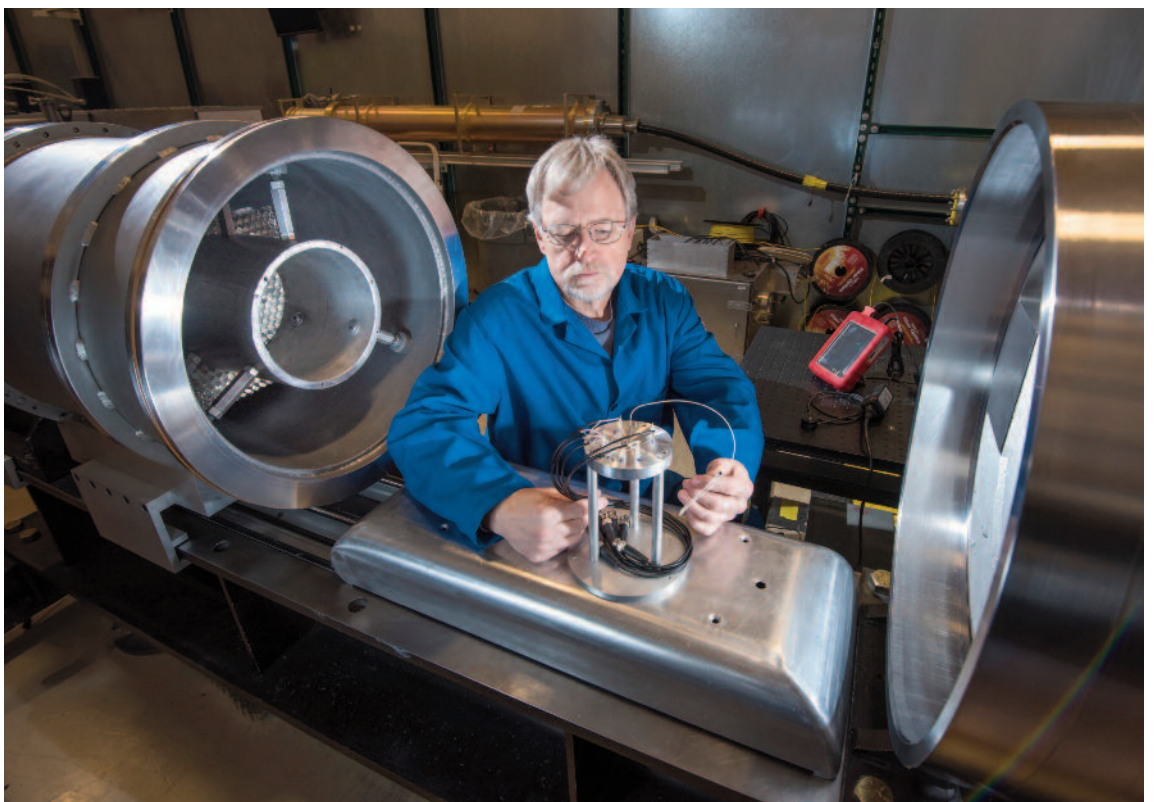
By Neal Singer

Sandia post-doctoral appointee Joshua Townsend, casually dressed in a dark green pullover and light brown pants, sits on what is effectively an aluminum saddle between the split components of a gas gun’s backstop.

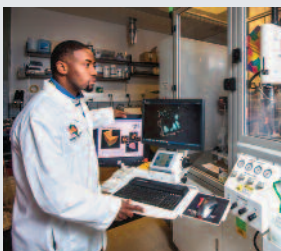
He’s absorbed in attaching wires to sensors embedded in a target about the diameter of a dinner plate. Once he’s done and moved out of the way, technicians will close the backstop so that the gun can fire a projectile into the plate.

A gas gun’s projectile is not a lightweight matter. A railroad shock absorber is needed to neutralize the impact of each shot, which originates in a cannon bolted to the floor about nine feet away. Impelled not by ignition but by the sudden expansion of helium gas

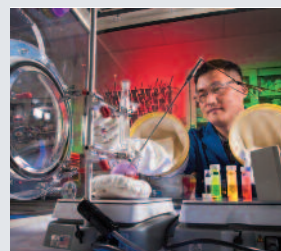
(Continued on page 5)



SANDIA RESEARCH TECHNOLOGIST Keith Hodge assembles an intricate gas gun target prior to a shock physics experiment. (Photo by Randy Montoya)



Enabling the workforce to accomplish the mission page 8



That's that

Have you heard about the incredible new building material that has captured the imagination of the global architectural community? It's called . . . wood. Over the past decade, it seems, there has been renewed interest in the construction industry and the environmental community in this most ancient of building materials. Why? For lots of reasons. New manufacturing processes have made wood-based construction products a very attractive and viable alternative to steel and concrete in high-rise buildings.

Using beams made of what is called cross laminated timber (CLT), which is as strong as steel, much lighter, more flexible, and faster and easier to assemble, architects and engineers are redefining the boundaries of what was thought possible with wood.

These wooden buildings are, counterintuitively, quite fire resistant, and because of the natural "give" of the material, stand up well to the forces unleashed in earthquakes. CLTs can be molded into novel shapes, meaning that building designs are not bound by the limitations of steel and concrete. It seems that 21st century skylines may look striking different than those of today.

If architects like the creative options afforded by CLTs, environmentalists love the new building trend.

"If we built a 20-story building out of cement and concrete, the process would result in 1,200 tons of carbon dioxide," said architect Michael Green in a TED Talk (as quoted in an online *Popular Science* story). "If we did it in wood . . . we'd sequester about 3,100 tons, for a net difference of 4,300 tons. That's the equivalent of about 900 cars removed from the road in one year."

The *PopSci* story goes on to note that "According to a 2014 study from researchers at Yale and the University of Washington, as much as 31 percent of global carbon dioxide emissions could be avoided by building with wood instead of steel and concrete."

So where is the edge of the envelope with this material? Japan's Sumitomo Forestry Co. Ltd. has announced plans to construct a 350-meter, 70-story high-rise built mostly of wood. That project, still just a paper exercise, is slated to be completed in 2041 to coincide with the company's 350th anniversary. In the nearer term, a 265-foot-tall high-rise tower in Norway called Mjøstårnet is under construction today and is expected to be completed in 2019. When it opens it will be the world's tallest wooden building, a record it isn't likely to hold for long.

While the renaissance in giant-scale wood construction is exciting, let's not forget the remarkable accomplishments of engineers and architects from the pre-industrial era. To cite just one example, the earthquake-proofing engineered into Japan's Horyu-Ji Temple, a 120-foot-tall wood structure built in 670 AD, is simply brilliant.




Speaking of unique wooden structures, that's a subject Sandia knows something about. One of the biggest (some sources say the biggest) wooden structure in the world is housed at Sandia/New Mexico, practically right under our noses.

Some background: during the Cold War, the military considered it imperative to understand how the electromagnetic pulse generated by a nuclear explosion might affect front-line aircraft. EMPs were known to knock out advanced electronics of the kind our aircraft were crammed with. To test those avionics in as near to real-world circumstances as possible, the idea was to zap an aircraft with millions of volts of electricity from a couple of super powerful Marx generators and then study the resulting data.

The catch was that the aircraft test stand where the zapping was to be done could have no metal parts. The metal would skew the results. What to do? During the Cold War, it seems, no project was too big, no undertaking too daunting. You need an all-wood test stand big enough to hold a B-52? Consider it done. The end result was the so-called Sandia Trestle, a 6.5 million-board-foot structure, 12 stories tall and more than 1,000 feet long. Built by the Air Force and operated by Sandia, the trestle was in use from 1980 right through the end of the Cold War in 1991. Mission accomplished.

For all of the wonders of modern wood construction, though, to me, the most memorable wood structures were those that soared into the sky in our own back yards. Did you and your friends, like me and mine, scrounge around behind garages and sheds, looking for the odd pieces of scrap wood that you could cobble together into tree houses? If we weren't playing baseball, we were in the trees, hammering away, working 20 feet up without a net. And oh, were those rickety things beautiful! We were decades ahead of the "tiny house" movement and we built ours for free out of recycled materials.

See you next time.

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Retiree deaths

Doyle Frasier (age 84).....	Dec. 22
Stanley Ewen (72).....	Dec. 23
Bruce Caskey (83).....	Dec. 26
Tom Takahashi (97).....	Dec. 26
Warren Siemens (80).....	Dec. 28
Violet Burnam (93).....	Dec. 29
Connie Baca (93).....	Dec. 29
James Hoffman (88).....	Dec. 31
James Constant (81).....	Dec. 31
Josephine Sandoval (84).....	Jan. 1
Edward Ratliff (83).....	Jan. 1
Eugene Byron Lopp (91).....	Jan. 5
G. Ronald Hadley (71).....	Jan. 9
Donald Hinman (92).....	Jan. 9
William Purcell (86).....	Jan. 10
Charles Burks (86).....	Jan. 11
Secundino Baca (98).....	Jan. 13
Tony Chavez (94).....	Jan. 15
Carol Garcia (76).....	Jan. 16
Frances Paulos (91).....	Jan. 19
Wayne Corbett (88).....	Jan. 31

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Albuquerque, New Mexico 87185-1468

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Bill Murphy, Editor 505/845-0845

Randy Montoya, Photographer 505/844-5605

Patti Koning, California site contact 925/294-4911

Michael Lanigan, Production 505/844-2297

Contributors: Michelle Fleming (Ads, Milepost photos, 844-4902),

Neal Singer (845-7078), Stephanie Holinka (284-9227), Darrick Hurst

(844-8009), Michael Baker (284-1085), Troy Rummeler (284-1056),

Valerie Larkin (284-7879), Lindsey Kibler (844-7988), Tim Deshler

(844-2502), Mollie Rappe (844-8220), Kristen Meub (845-7215),

Michael Padilla (925-294-2447), Julia Bernstein (925-294-3609),

Jim Danneskiold, manager (844-0587)

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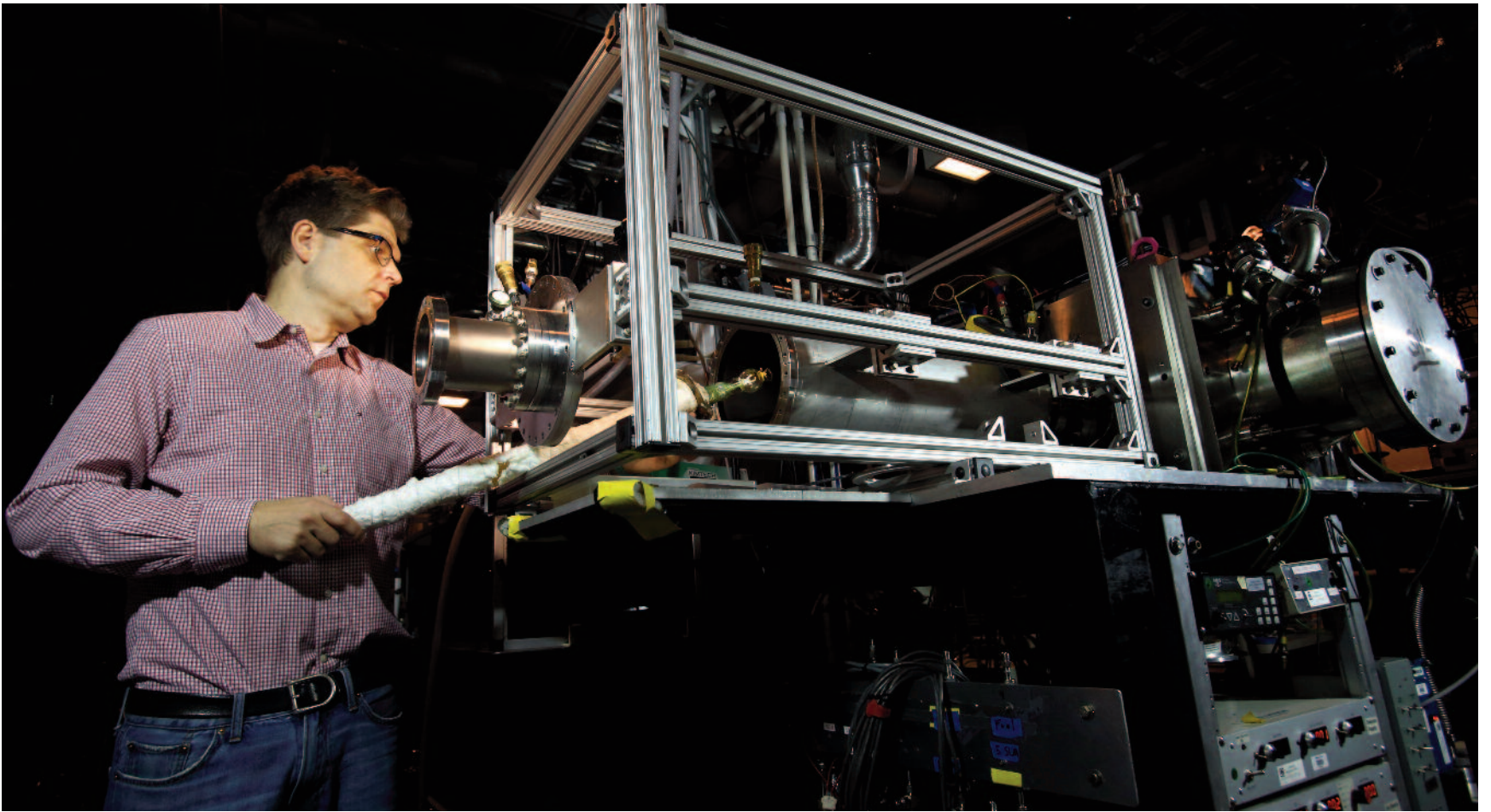
Sen. Heinrich releases Solar Toolkit



CNM PHOTOVOLTAICS INSTRUCTOR Janet Hughes, left, Albuquerque City Councilor Pat Davis, Albuquerque Mayor Tim Keller, Sandia Labs Tribal Energy program lead Sandra Begay, Sen. Martin Heinrich, and Environment New Mexico Director Sanders Moore celebrate the release of Heinrich's Solar Toolkit, created to connect communities to solar energy resources and information. "It is my hope that this solar toolkit provides a launching point for local governments, tribes, schools, power providers, rural businesses, policymakers, and educational institutions to consider whether solar can meet their needs," said Heinrich in a statement introducing the toolkit on his website.

New chemical mechanisms identified on road to cleaner, more efficient combustion

Sandia researchers unravel chemistry of organic compounds



JET-STIRRED REACTOR – Sandia researcher Nils Hansen uses a device called a jet-stirred reactor to conduct chemical research that adds to the fundamental knowledge of combustion. (Photo by Dino Vournas)

Sandia researchers have identified key chemical mechanisms for the first time that add to the fundamental knowledge of combustion chemistry and might lead to cleaner combustion in engines.

By Michael Padilla

Sandia researcher Nils Hansen and former post-doctoral appointee Kai Moshhammer focused on low-temperature oxidation of hydrocarbons and other alternative fuels. They identified key chemical intermediates, which are relevant for oxidation reactions at temperatures in the range of 400 to 600 K (260 to 620 degrees Fahrenheit). The chemical nature of the intermediates and their concentrations provides new details on the chemical processes involved in autoignition.

Autoignition is a chemical process in which a fuel-air mixture spontaneously ignites. It is commonly explained by theory through a set of self-sustaining and accelerating chain-branching reactions. It is most important for understanding knock in spark-ignition engines.

Nils and Kai were among a multi-institution team of researchers whose work was published in a paper titled, “Unraveling the structure and chemical mechanisms of highly oxygenated intermediates in oxidation of organic compounds.” The researchers focused on deepening the insights into low-temperature oxidation chemistry of hydrocarbons and other alternative fuels.

“We can run an internal combustion engine today without knowing the details of the chemistry,” Nils says. “However, this research provides new insights that should be targeted by new combustion models. It eventually should allow for the development of more clean and efficient combustion strategies in the future.”

Nils and Kai used molecular-beam mass spectrometry

to discover the chemical intermediates. The molecular beam freezes the chemistry and can be compared to the German autobahn.

“In the molecular beam, all the molecules are sucked into a vacuum to fly in the same direction and at the same speed, so there are no collisions just like on the autobahn,” says Nils. “When we isolate the molecules this way, it allows us to separate them by their weight and thus their molecular makeup.”

Extracting detailed information from nature

Extracting detailed molecular information directly from igniting mixtures is a difficult and challenging task, especially because of large temperature swings and the low molecular concentrations of key intermediates.

“Even after a few decades of research on this topic, these highly oxygenated molecules had never been seen before,” Nils says.

Yiguang Ju, professor and director of Sustainable Energy at Princeton University, says this work clearly reveals the formation of oxygenated intermediates through the multiple oxygen molecules addition processes. “The oxygenated intermediates are critical to affect low-temperature ignition, cool flame, mild flame and knocking formation in internal combustion engines,” Ju says.

Jet-stirred reactor designed to conduct research

Nils stresses that these discoveries were made by experiments that focus on chemistry while minimizing the effects of mixing, turbulence, and large temperature and concentration gradients.

To conduct the work, the Sandia researchers designed a device called a jet-stirred reactor, which is best described as a quartz reactor into which unburned fuel-oxidizer mixtures are continuously added through four small nozzles to create a homogenous mixture which is then ignited with external heat. With this approach, the researchers avoid large spatial and temporal changes in the concentrations of the key intermediates and temperatures and the reactor can be readily modeled. The researchers then used molecular-beam sampling and high-resolution mass spectrometry to identify gas components from the reactor.

“Our persistent interest in low-temperature oxidation processes led to this research,” Nils says. “While the first studies focused around small fuels such as dimethyl ether (CH₃OCH₃), we eventually moved to larger, more practically relevant fuels, such as heptane, and ‘accidentally’ detected a signal that was not explainable through the known chemical mechanisms. We wanted to provide

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validation targets for model developments in the form of molecular identification and concentration.”

Previous research identified reactions and intermediates that helped predict ignition characteristics of individual fuels. Sandia’s work has shown that the scientific community’s understanding of these processes is not complete and that additional reactions and intermediates must be considered. This work will help to develop models with better predictive capabilities, and has implications beyond combustion. “This is fundamental chemical kinetics research that can also impact climate-relevant tropospheric aerosol formation,” Nils says.

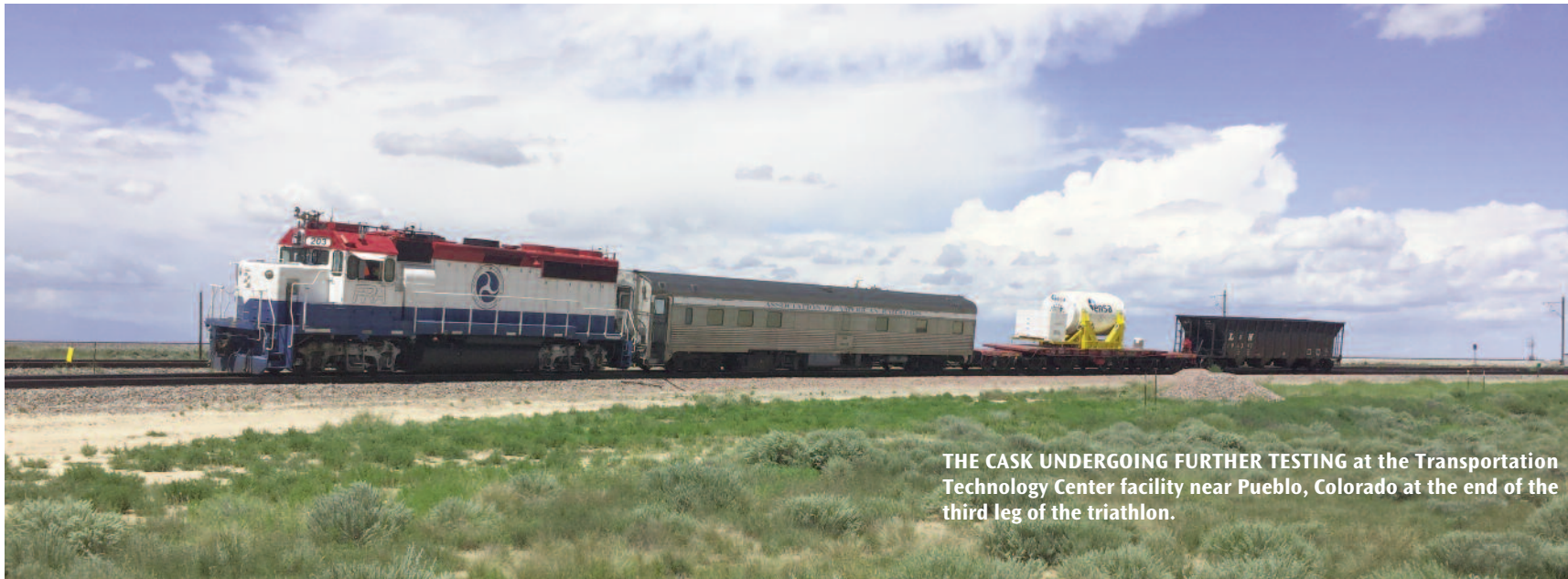
“In the future, we will need to develop new experimental techniques and capabilities that would allow for an unambiguous assignment of the molecular structure.” —Nils Hansen

Paul Wennberg, the R. Stanton Avery professor of Atmospheric Chemistry and Environmental Science and Engineering at Caltech, says this research also provides a wealth of new data and insight into the oxidation processes involved in the oxidation of organic molecules in the atmosphere. For example, the knowledge of how many oxygens are added following the formation of the first radical, how the structures of the organic substrates alter the pathways, and whether this chemistry can compete with bimolecular processes is essential for predicting if this chemistry is important at the much colder temperatures relevant for the atmosphere.

“The final impact of these discoveries in autoxidation on our understanding of air pollution is unclear,” Wennberg says. “We know that breathing particulates is a public health threat, but how toxic the particulates created via autoxidation are and how long these compounds persist in the atmosphere is simply not known at this time.”

The use of mass spectrometry to detect these intermediates is only the first step in this research.

“In the future, we will need to develop new experimental techniques and capabilities that would allow for an unambiguous assignment of the molecular structure,” Nils says. “We will test two-dimensional mass-spectrometric techniques and microwave spectroscopy as analytical tools to find the exact chemical structures.”



THE CASK UNDERGOING FURTHER TESTING at the Transportation Technology Center facility near Pueblo, Colorado at the end of the third leg of the triathlon.

Road, rail, boat

(Continued from page 1)

nuclear reactor, making safe transportation important.

A nuclear waste transportation and storage cask fresh off the assembly line was loaded with three surrogate fuel rod assemblies from the US, Spain, and South Korea and then traveled from Spain to Colorado and back again by truck, ship, and train. Zirconium alloy tubes filled with lead or molybdenum pellets imitated the uranium oxide pellets inside a spent nuclear fuel rod.

A more reliable quantification of risks

“All of our preliminary data suggests that the likelihood of a fuel rod breaking during routine handling and transportation is low. This test is more realistic than past tests and could result in a more reliable quantification of the transportation risks,” says Sylvia Saltzstein, manager of the transportation projects.

Sandia collaborated on the triathlon with Equipos Nucleares S.A. (ENSA), the Spanish cask designer manufacturer, and Empresa Nacional de Residuos Radiactivos S.A. (ENRESA), the corporation responsible for the management of nuclear waste in Spain. The Korea Radioactive Waste Agency (KORAD) and Korea Atomic Energy Research Institute (KAERI) also participated in the triathlon.

A grid of almost 300 rods makes up a fuel assembly, and the cask used in the test can hold 32 assemblies in a specially designed basket. The mock fuel rods within the three assemblies were outfitted with tiny accelerome-

ters and strain gauges before they went into the cask. The cask and basket were similarly equipped.

The accelerometers and strain gauges measured each bump, rattle, and jolt the mock fuel experienced during the trip, yielding data that could confirm transporting spent nuclear fuel is safe.

Though Sandia has thoroughly tested the robustness of nuclear waste casks during decades of simulated catastrophic transportation accidents, another challenge is the stress from everyday transportation on the fuel rods inside the cask. Sylvia and her colleagues hope that repeated jostling won't lead to a fuel rod snapping, like bending a soda can tab one too many times.

Though Sandia has thoroughly tested the robustness of nuclear waste casks during decades of simulated catastrophic transportation accidents, another challenge is the stress from everyday transportation on the fuel rods inside the cask.

The triathlon is actually Sandia's fourth test to measure routine transportation strains.

The first used a large shaker table to test Sandia's sensor-studded mock fuel assembly, with lead rope in zirconium alloy tubes to mimic the weight of uranium

pellets. A shaker table is just that, a table that vibrates up and down in a controlled manner. The researchers programmed the table to reproduce the shocks and vibrations from traveling by truck and measured the strain experienced by the fuel rods. Although a reasonable initial test, the table only went up and down, so more testing was needed.

The second test placed the same assembly on a truck trailer loaded with 50,000 pounds of concrete, the same as a transportation cask, and took it on a 38-mile trip on highways, city streets and dirt roads. This test showed similar, very low, levels of strain on the mock fuel. However, since spent nuclear fuel mostly will travel by train, the third test looked at the shocks and vibrations experienced riding the rails.

Sandia researchers took shock and vibration data provided by the Association of American Railroads to set up a shaker table that could move in six directions instead of just up and down, simulating the strain and acceleration of train travel. They also replaced the lead rope in some of the rods with lead and molybdenum pellets for a better approximation of spent fuel. This test agreed with two earlier tests: The stresses from normal transportation are about 100 times lower than the stresses calculated to damage nuclear fuel rods.

Tests boost confidence

The three tests gave Sandia researchers confidence, but they needed a yet more realistic test. For the triathlon, they moved an actual spent fuel cask from one mode of transportation to another to obtain data closer to real world conditions.

The triathlon started in northern Spain, where the cask traveled by heavy-haul truck for about 250 miles through main roads and highways. After a layover to download data from the sensors, the cask was transferred to a barge, which skirted along the coast of France to Belgium, sailing more than 1,000 miles over four days. After a layover in Belgium, the cask was transferred to a cargo ship. Then the ship crossed the Atlantic to Baltimore — almost 4,000 miles — through sometimes rough seas. This took two weeks.

In Baltimore, the cask was transferred to a dedicated flatbed train car and traveled west about 2,000 miles through 12 states, which took seven days. There, in partnership with the Association of American Railroads, the cask and fuel assemblies were tested at the Transportation Technology Center Inc. facility near Pueblo, Colorado. The center has almost 50 miles of test track, permitting such controlled scenarios as joining two railcars together or rumbling over a track crossing. After these trials, the cask with its sensors reversed course and returned to Spain.

8 terabytes of data

In addition to the logistical challenges, the biggest technical challenge was building a data acquisition system that could collect all the shock and vibration data robustly and unsupervised, says Paul McConnell, project manager for the tests. A Sandia contractor, Bill Unca-pher, designed the system and Sandia technologists Carissa Grey and Wes Chilton built the system.

The rail cask test generated about 8 terabytes of shock and vibration data. Sylvia expects the full analysis will take nearly a year. The data from the test also will be used to validate computer models of the stresses experienced by spent fuel during normal transportation.

“Preliminary results show very low shock and vibration levels, which we will compare to the mechanical properties of fuel that's come out of a nuclear power reactor,” Paul says. “Ultimately, we want to understand if the fuel can withstand the accumulation of shocks and vibrations during the journey that could potentially cause a fuel rod to break.”

The test was partially funded by the DOE Office of Nuclear Energy's Spent Fuel and Waste Science and Technology program. Pacific Northwest and Argonne national laboratories also took part in the triathlon.

Job shadowing at Sandia



SANDIA HOSTED A CLASS OF SOPHOMORES from Manzano High School at this year's Groundhog Job Shadow Week. The job shadow week, presented by Junior Achievement of New Mexico and Mission: Graduate, offered students the opportunity to visit various professional work environments in the community and learn about career preparation, interview skills, and professionalism in the workplace. Students took a tour of the Technology Training and Demonstration Area and participated in mock interviews with Sandia human resources and business professionals. Communications Center 3600 Director Frederick Bermudez spoke to the students about Sandia's work and the many job opportunities the Labs offers to include STEM-related fields as well as business support and operations. In the photo above, Sandia Community Involvement manager Amy Tapia helps two Manzano High School students with their Smile Tower project. The engineering activity teaches team work, financial responsibility and problem solving skills to students, who must design and construct a tower that can survive an earthquake using materials like straws, toothpicks, and tape.

(Photo by Katrina Wagner)

Gas gun

(Continued from page 1)

released into the barrel from a side pocket behind the projectile, it will scuffle forward like an NFL lineman to hit with the impact of more than 500 pounds per square inch. An exhaust valve downstream releases pressure before it builds high enough to be dangerous.

The guns of shock physics at Sandia have been used to explore everything from the properties of new materials to the 2003 *Columbia* shuttle disaster. Says Randy Hickman, test operations engineer at Sandia's gas gun center, "The piece of foam that struck the shuttle's heat tiles and caused the crash would not normally be considered [hard enough to be] an issue, but anything moving that fast can damage a vehicle. Similarly, we've studied debris shields for the space station and satellites, armor materials for the military, and even potential meteor impacts on earth and other planets. For anyone who needs an understanding of the mechanical properties of a material, we have the ability to probe it at various pressures and temperatures to obtain conditions of failure or uniformity."

One problem for students interested in entering the field, however, is finding hands-on practice. Because of the complicated nature of shock physics, the science of dynamic compression — the way a material behaves when impacted — is taught at only a few top universities, and even there the subject matter is almost entirely theoretical.

"Hardware is hard to come by," says Randy.

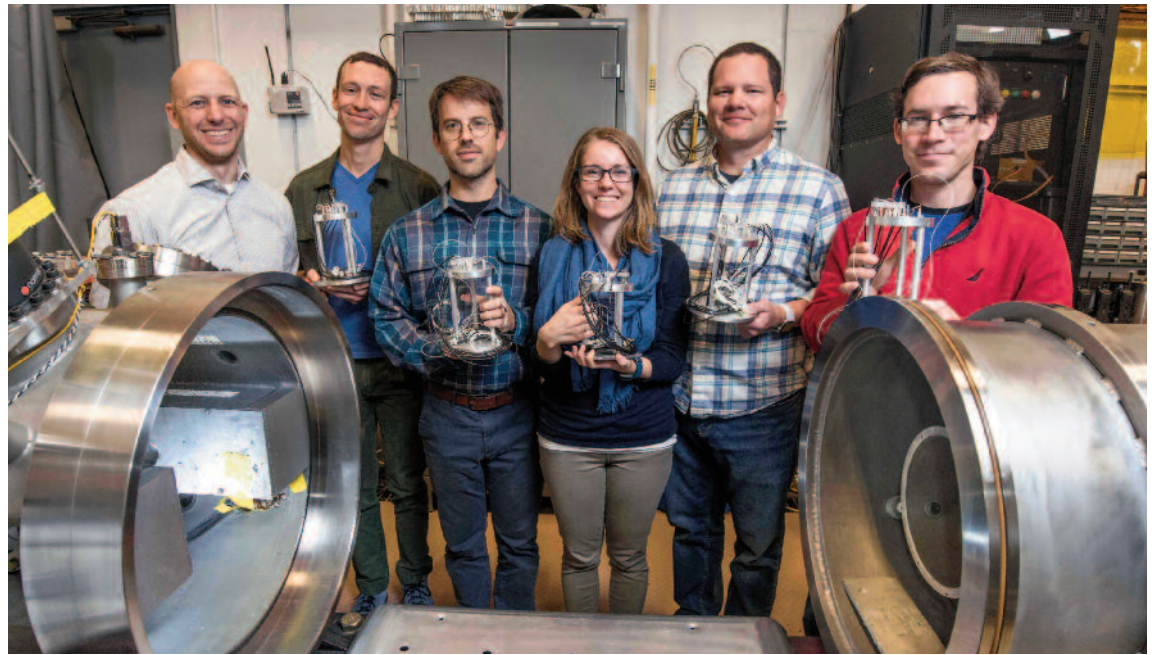
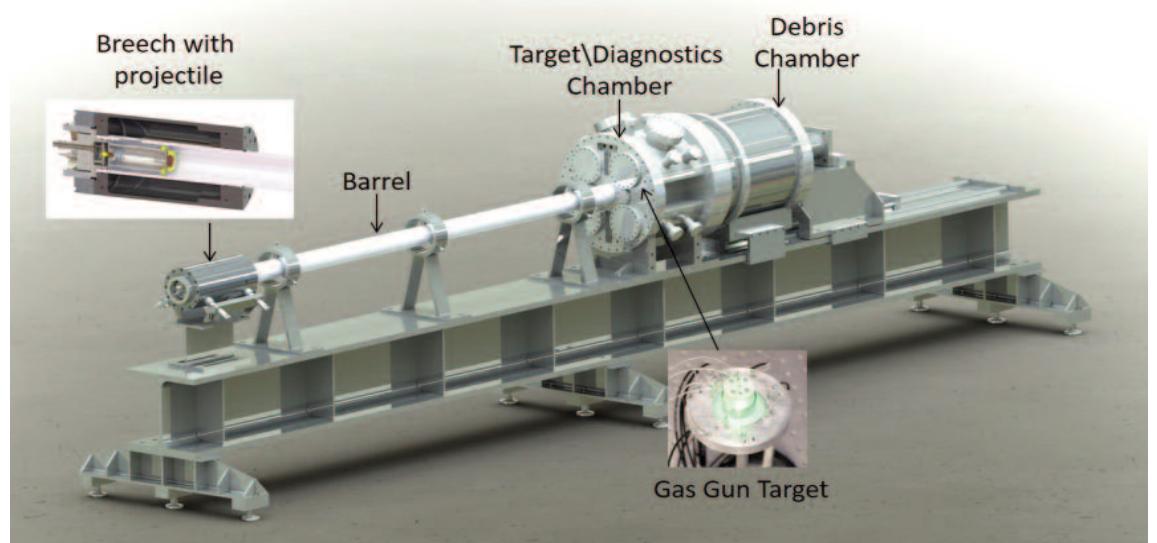
Theory + experiment = better science

But because the subject has so many applications, Sandia management believed that time spent providing students hands-on experience with real shock physics experiments could improve their modeling skills, and so Sandia provides a program to supplement theoretical university courses with projectiles and real shocks.

Says Josh, normally involved in high-energy-density physics theory, "I had never encountered [the field of] shock compression of materials before Sandia. Then, through the program, I got my hands on materials and realized it's useful for me to know how the experiments are done. Then I can work more efficiently with experimentalists. I realize up front why they can't just go out and measure something I would think, from calculations alone, could be easily done. So, we improve our combination of experiment and theory to do better science than could be done separately."

Says Sandia shock physicist Seth Root, "To help our post-docs learn the technical aspects of shock physics, we designed experiments involving the complete assembly of a shock physics target. Post-docs assemble the target sample, attach optical fiber and electrical signal diagnostics, and make all the measurements. Then they learn how a target is installed in the gun, how the optical diagnostics work, and even participate in the post-experiment clean-up. Then, with data from the experiment, students determine characteristics of the target sample. Combining the theoretical class with our hands-

This Solid Works rendering of the DICE Facility Light Gas Gun depicts the major components of the system.



HANDS ON — Posing next to a gas gun open for servicing are, left to right, Sandia shock physicist Seth Root and post-docs Matthew Hudspeth, Joshua Townsend, Bethany Chidester, Jim Williams, and Ray Clay, who are holding the targets they created. (Photo by Randy Montoya)

on practice helps our post-docs transition faster and more confidently to the specialized work we do in dynamic compression."

The gun's relatively inexpensive mechanism (when compared with the costs to do experiments on pulsed power machines, like Z, which achieve far higher pressures) means projectiles can be sent with a variety of velocities against targets. This creates a series of data points charting the behavior of a material under increasing pressure.

To realize this data accurately, pins of varying lengths are inserted in the target. The time difference between electrical signals from the longer ones, struck first by the incoming projectile, and signals from the shorter ones, struck last, allow researchers to calculate the projectile's velocity. Meanwhile, a fiber optic probe

measures the shock wave's arrival time and profile.

Says Sandia research technologist Keith Hodge at the close of one test, "Manual dexterity is improved by work at constrained spaces the site provides."

Joshua is one of four Sandia post-docs recently to get hands-on training in the program. They take theoretical coursework at the Institute for Shock Physics at Washington State University, which offers an introductory class that covers theoretical aspects of shock wave propagation, equation of state, and other topics important for dynamic compression.

"I think we post-docs all knew basic thermodynamics before going into the experiment," says Joshua. "But we had no clue about how to produce a set of experimental measurements. In this respect, it is the hands-on experience that is novel and most important."

Sandians honored for sustainability efforts

Sandia staff members garnered a pair of 2017 DOE/NNSA Sustainability Awards for their efforts to reduce waste and stop pollution stemming from the Labs' operations.

NNSA officials presented two awards: the Life Cycle Management Award for Waste Reduction and Pollution Prevention to a team led by Justin Griffin, ES&H technologist for the neutron generator organization; and the Life Cycle Material Management Award that recognized Sam McCord of Sandia Waste Management as a Change Agent.

Members of Justin's team included Rick Elliott and Bill Lucy.

The first award honored a green team in the neutron generator organization that looks for opportunities to make environmental and process improvements. Among their successes were a series of waste assessments on their buildings that measured the pounds of waste per person generated and identified ways to reduce waste for each building. They also developed a pilot project that replaced water coolers with built-in, bottle-refilling-capable water fountains in the same buildings, and measured the positive environmental impact and return on investment.

The NNSA award also recognized the same team for identifying, conducting pedigree research, and then safely disposing of a large inventory of obsolete classified equipment, freeing up additional classified storage, reducing nearly 3,000 classified holdings, and eliminating associated security risks. That work also captured a Sandia Environmental Management System Award.

Sam's change agent award recognized his tireless



GREEN TEAM — Officials from NNSA headquarters recognized Sandia's work in reducing waste and preventing pollution with 2017 Sustainability Awards. Pictured, from left, are Nick Logotheitis, NNSA Sandia Field Office; Jessica Arcidiano, director of NNSA's Office of Environment and Sustainability-NA-533; Sandia winners Samuel McCord of Sandia waste management, and Justin Griffin, ES&H technologist for the neutron generator organization; and Ahmad Al-Daouk, deputy associate administrator for Enterprise Stewardship, NNSA NA-53. (Photo courtesy of Infrastructure Services)

efforts leading Labs-wide the Zero Waste 2025 program and helping to inspire organizations large and small to recycle and insitute a wide range of creative programs that cut down on the waste that Sandia sends to land-

fills. He also was recognized for adding computer automation to several key processes and customer communication to improve accuracy, turn-around time, and user satisfaction.

Sandia researcher Jacqueline Chen elected to National Academy of Engineering

By Michael Padilla

Jacqueline Chen, a distinguished member of the technical staff at Sandia, has been elected to the National Academy of Engineering. Jacqueline is among the 83 new US members and 16 foreign members in the 2018 class.

Election to the National Academy of Engineering is the highest professional distinction for an engineer in the United States. Those in the new class will be formally inducted Sept. 30 during a ceremony in Washington, D.C.



JACQUELINE CHEN

Jacqueline, who has spent her entire career working at Sandia's world-renowned Combustion Research Facility, was chosen for her contributions to the computational simulation of turbulent reacting flows with complex chemistry. She believes her election recognizes the importance of chemically reacting flows in many important applications, such as combustion engines and the atmosphere, and the rise of computation to an equal status with theory and experimentation in the science trifecta.

"Computation at extreme scales requires interdisciplinary teams of physical scientists and computer scientists pushing computing's limits to achieve scientific discovery," she says. "Hence, this honor is really shared with the many graduate students, postdoctoral researchers and collaborators — from both combustion and computer science fields — who have contributed to a common goal of gleaning new understanding in combustion science through advanced computation. It was made possible through sustained sponsorship from the Department of Energy's Office of Science, both from the

Basic Energy Sciences (BES) and Advanced Scientific Computing Research (ASCR) Offices."

Jacqueline actively works to lead this integration of high performance computing and engineering research through her involvement on both the ASCR Advisory Committee and the Board of Directors of the Combustion Institute.

Out of her numerous research achievements, Jacqueline takes the most pride in understanding intricate turbulence-chemistry interactions, exemplified by a recent simulation of a turbulent jet of a complex hydrocarbon fuel spontaneously igniting at temperature and pressure conditions typical of a modern diesel engine. This work was performed with her current postdoctoral appointees, Giulio Borghesi and Alex Krisman, who represent the latest of a long line of 23 postdocs who have worked with Jacqueline and gone on to impactful careers on their own. The simulation incorporated a chemical model for low- and high-temperature oxidation developed by professor Tianfeng Lu from the University of Connecticut. The simulation revealed how initial reaction waves rapidly move into fuel-rich mixtures, accelerating overall ignition. This result demonstrates that ignition timing, which affects fuel efficiency and emissions in a diesel engine, depends not only on complex low-temperature ignition chemistry, but also on its coupling with laminar and turbulent transport processes.

The simulation required restructuring the simulation code, S3D, to run effectively on the Oak Ridge Leadership Computing Facility's Titan, the largest supercomputer in the US, which combines a mix of central processing units (CPUs) and graphics processing units (GPUs). Working with Stanford University computer scientists who had developed a novel programming model for such heterogeneous supercomputers, the S3D code was able to run seven times faster than before, making it feasible to perform this ground-breaking simulation.

Looking ahead Jacqueline says she intends to expand her research in two opposite directions.

"On the one hand, I would like to extend the range of scales and geometric complexity for first principles simulation of reactive flows so that these simulations, which have historically been limited to small canonical configurations, can be more relevant to practical applications. This is ongoing multi-laboratory research supported by the Department of Energy's Exascale Computing Project," she says.

"Conversely, as computers and algorithms become



SANDIA RESEARCHERS Giulio Borghesi, left, Jackie Chen, center, and Alex Krisman recently identified novel behavior of a key, temperature-dependent feature of the ignition process called a cool flame in the fuel dimethyl ether.

(Photo by Dino Vournas)

more capable," Jacqueline says, "I envision the development of multiscale simulation methods that can drill down to extremely small scales, enabling us to simulate molecular interactions within flow-generated temperature and composition gradients."

Using molecular-level methods such as Direct Simulation Monte Carlo, Jacqueline believes that it may be possible to develop reaction-rate models for important chemical reactions in nonequilibrium flow. Such models can then be used in larger-scale simulations of complex reacting flows. The ability to capture nonequilibrium effects on gas composition has implications, for example, for predicting the reliability of pulsed plasma ignition to restart a jet engine at high altitudes following a flame-out condition.

Jacqueline's advice to young scientists and researchers is to "believe in yourself, embrace technology advances not only in your own field but in cross-cutting fields, and cultivate strong collaborations."

Jacqueline says many new scientific discoveries will be made at the intersection of multiple disciplines and will require creative thinking and a willingness to work outside of one's comfort zone as part of a team.

"I'd also like to encourage more women to consider education and careers in science and engineering," she says. "Unlike my generation, there are increasingly more role models across the entire research-and-development enterprise. It's a rewarding career and a good time to jump in."

Employee death

Just do it!

Jennifer Roth passes away, leaving a legacy of dedication, loyalty, and kindness

By Troy Rumler

Jennifer Roth was a friend and mentor to those who knew her in Talent Management and Development (TM&D). She died Feb. 8.

"Jennifer was like the human version of the Nike sports company tagline: Just do it!" says Michael Casady, her senior manager. "She was action-oriented, high-energy, and quite respected by those who were lucky enough to be around her."

As a course manager, Jennifer provided administrative, billing, database, and logistical support for TM&D courses, particularly within the nuclear weapons program. She had a love for the work, her colleagues, and the mission of Sandia, and was known for her willingness to lend a helping hand to students and her instructors. Above all, though, she is remembered for making time to strengthen and befriend others.

"She would often sit with me for a time just to catch up, which I found to be a refreshing attitude in our typical rush mode, and I will miss that time with her," colleague Tony Bryce recalls.

"Jennifer touched me personally and made me a stronger individual to believe in myself and never give up hope," another colleague, Christina Louise Chavez, says. "I used to visit her at the hospital during her illness, and she would always tell me not to worry about her, that she was going to fight her illness and win.



JENNIFER, A COURSE MANAGER, provided administrative, billing, database, and logistical support for TM&D.

Instead of me comforting her, she was comforting me."

Jennifer was a retired deputy in the Bernalillo County Sheriff's Department and started her career at Sandia as a contractor in 2012, accepting a permanent position in 2014. Her expertise and experience shone in her ability to exude cool-headedness in stressful moments, and reason in chaotic environments.

"She was always professional and very patient with people," Tony says.

"I appreciated her common sense in the face of confusion," adds co-worker Diane Miller.

"Jennifer was a very strong individual, and with her security background, she brought her expertise in helping the training division become a stronger organization because of her; she has mentored many staff members," Christina says.

Jennifer was born Dec. 6, 1957, in Dayton, Ohio, and



JENNIFER WAS A RETIRED DEPUTY in the Bernalillo County Sheriff's Department.

spent most of her life in New Mexico. She graduated from Socorro High School and graduated from the New Mexico State Law Enforcement Academy in 1985. She loved family, gardening, and reading — especially history — and eagerly shared what she learned with her co-workers.

She graduated cum laude from National American University in 2002 with a Bachelor of Science in applied management and had been pursuing a master's degree in security at the University of New Haven.

"Jennifer has left an indelible mark on this team," says her manager, Angie VanArsdale. "We will be forever grateful for having had the opportunity to share this space and time with the most beautiful of human spirits."

In lieu of flowers, donations may be made in her name to the Cancer Research Institute at www.cancerresearch.org

SANDIA CLASSIFIED ADS

Note: There will be no ads in the March 30 edition of the Lab News. The Classified Ad deadline for the March 16 edition will be Friday, March 9 at noon.

MISCELLANEOUS

DINING ROOM SET, large farm table, w/6 chairs, like new, photos available, \$700 OBO. Gallegos, 505-263-4456.

BUFFET & HUTCH, wood framed, glass doors, canister lighting, chestnut finish, hardwood solids/veneers, cherry finish, \$2,500 OBO. Reed, 575-640-0529.

QUEEN BED, American Home sleigh bed, w/Tempurpedic mattress & ergo base, \$1,000 OBO. Walter, 505-850-5171.

CAMERA SYSTEM CASE, Vanguard VPG-13, aluminum construction, 18" x 13" x 7", w/strap, new, \$60. Johnson, 292-0677.

SNOW/MUD TIRES, GT Radial Champiro IcePro, 205/55/R16, <1K miles, set of 4, \$200. Tarpley, 505-259-1497.

SPEAKERS, Bose 501, \$200/pair; Yamaha 7.1 receiver, 120-W per channel, \$120; Sony sub-woofer, 200-W, \$75. Endres, 505-263-1616.

BOOKCASE, dark wood color, 30" x 71" x 12", very good condition, \$10. Kelly, 505-306-4365.

BENCH GRINDER, 6-in., 2-wheels, \$125 OBO; 5-gal. gas can, \$9; 2 folding lounge chairs, \$45 ea. or \$80/both; 2 bicycle safety helmets, new, \$10-\$12. Garcia, 554-2690.

GE ELECTRIC STOVES, used, great condition: white, smooth top, \$200; traditional, \$100 OBO; photos on request. Martinez, 505-515-6159.

'LIVE IN CENTRAL PARK (REVISITED), SIMON & GARFUNKEL', 2, Popejoy, March 25, 3 p.m., orchestra, center, rG, \$130. Hosking, 505-823-9512.

GAS DRYER, LG Tromm, energy efficient, white, good condition, \$100 OBO. Elmazi, 505-856-2197.

UPRIGHT PIANO, antique, looks good, needs tuning, call for more details & photos, \$250. Stroud, 505-205-4051.

LED DLP TV, Samsung, 56-in., \$150; 2 wood entertainment centers, \$50-\$75; ~full propane tank, \$30. Mills, 217-621-2492.

RUSTIC MEXICAN TABLE, 84" X 40" X 30"H, \$250 OBO. Giering, 505-818-8195, ask for Lisa.

RECLINER COUCH, La-Z-Boy, gray leather, standard sofa width, pristine, 30 mos. new, \$975 OBO. Sanchez, 505-974-1655.

ELLIPTICAL TRAINER, Ironman, great condition, photos available, \$75; Schwinn double bike trailer, good condition, photos available, \$60. Vigil, 400-0629.

How to submit classified ads

DEADLINE: Friday noon before week of publication unless changed by holiday.
Submit by one of these methods:
 • EMAIL: Michelle Fleming (classads@sandia.gov)
 • FAX: 844-0645
 • MAIL: MS 1468 (Dept. 3651)
 • INTERNAL WEB: From Techweb search for 'NewsCenter', at the bottom of that page choose to submit an ad under, 'Submit an article'. If you have questions, call Michelle at 844-4902. Because of space constraints, ads will be printed on a first-come basis.

Ad rules

1. Limit 18 words, including last name and home phone (If you include a web or e-mail address, it will count as two or three words, depending on length of the address.)
2. Include organization and full name with the ad submission.
3. Submit ad in writing. No phone-ins.
4. Type or print ad legibly; use accepted abbreviations.
5. One ad per issue.
6. We will not run the same ad more than twice.
7. No "for rent" ads except for employees on temporary assignment.
8. No commercial ads.
9. For active Sandia members of the workforce, retired Sandians, and DOE employees.
10. Housing listed for sale is available without regard to race, creed, color, or national origin.
11. Work Wanted ads limited to student-aged children of employees.
12. We reserve the right not to publish any ad that may be considered offensive or in bad taste.

PARAKEETS, 2, male, w/cages, toys & food, 1 green-yellow, 1 ice blue, photos available, \$50. Willis, 286-1937.

INK CARTRIDGE, HP60XL, bought wrong one, cost \$50, asking \$10. Vrooman, 505-249-8414.

TRANSPORTATION

'10 CHEVROLET SILVERADO LTZ Z71, 4x4, loaded, original owner, dealer serviced, 107K miles, \$19,500 OBO. Richard, 238-6760.

'91 HONDA ACCORD, 4-dr., white, blue interior, dealer serviced, Michelin tires, gas-saver, perfect condition, \$5,000. Behar, 821-9299.

'15 JEEP RENEGADE LATITUDE, FWD, Sierra blue, black interior, 5-yr./100K mile warranty, call for details. Ramos, 972-951-0290.

'09 INFINITI G37, new windshield, tires, 126K miles, \$8,500 OBO. Parker, 505-944-6929, call or text.

'11 TOYOTA PRIUS, 4-dr., silver, tinted windows, multi-disc player, runs great, very fuel efficient, 52K miles, \$11,000 OBO. Sandoval, 505-980-5329.

RECREATION

'99 BMW K1200 LTE ABS, garage-kept, 38K miles, steel brake lines, needs battery, \$2,700. London, 505-720-6979.

'14 5TH WHEEL TOY HAULER, 4 Seasons, 6-KW generator, gas tank for toys, 3 AC, 4 TVs, \$62,500/offer. Babb, 228-5225.

REAL ESTATE

4-BDR. HOME, 3 baths, 3,939-sq. ft., modern architecture, 2 suites, Four Hills neighborhood, \$545,000. Mohagheghi, 505-321-3399.

5-BDR. HOME, 3 baths, 4,046-sq. ft., 4-car garage, large corner lot, views, 10 mins. to Sandia, MLS#907862. Esch, 505-298-8914.

1/2-ACRE LOT, Angel Fire, near cc/golf course, buildable, part of Angel Fire Resort, beautiful, \$30,000. Segura, 505-490-2756.

2-BDR. HOME, 1 bath, remodeled, 926-sq. ft., granite, new plumbing/sewer, mechanical, electrical, wood floors, xeriscape, popular Ridgecrest Dr., \$205,000. Dussart, 505-450-8535.

WANTED

VINTAGE TOOLS, fishing, hunting items; also buying old metal toys, watches & jewelry. Shaffer, 505-573-8282.

VOLUNTEERS, Fabulous Felines, help with the kitties, http://fabulousfelines.org. Stubblefield, 263-3468, fabulousfelines@comcast.net.

Recent Retirees



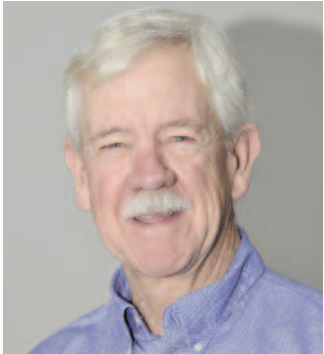
New Mexico photos by Michelle Fleming



Randy Summers 36



Allen Sault 29



Danny Donald 25



David Betsill 24



Emily Mitchell 23



Terry Owen 16



Mario Pino 15

Mileposts



New Mexico photos by Michelle Fleming



Mark Baumann 35



Denise Taylor 25



Elizabeth Taylor 25



Michael Rimbart 20



Doug Wall 20



Mark Cranfill 15



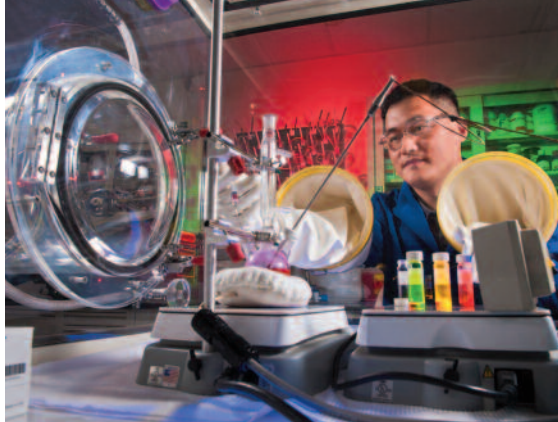
Diana Goold 15



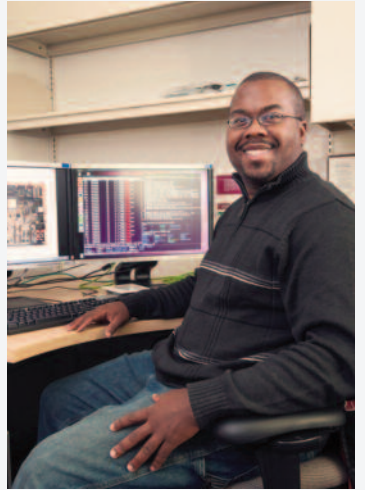
Evan Johnson 15



Anthony Leyba 15



Enabling the workforce to accomplish the mission



By Amy Treece

It's often said that "It takes a village," but at Sandia, it takes 12,000 people to accomplish the mission. To help those villagers do their jobs more easily and efficiently, Mission Services has come up with new tools and processes that do just that.

New apps for Logistics, Procurement, and project reporting

A new application, Move-It, lets people request Logistics services to move, store, and dispose of hazardous and nonhazardous materials. Developed by Supply Chain Management and Advanced Enterprise Software Engineering, the app gives customers a single, intuitive, and straightforward request system for Logistics services.

Every day, Sandia staff order goods and services. My Procurement lets internal customers easily view all aspects of orders in process, including who the buyer is as well as any expiring purchase orders.

Data drives informed decisions, and two corporate-supported reporting and analysis apps released in October give Sandia managers and business personnel needed data in user friendly, easily visualized form. Financial Analytics provides financial project reporting, from the programmatic level down to the lowest task level. It breaks out expenditure types and details, projects trends, and links directly to other financial systems. Org on a Page shows projects at the organization level for divisions, centers, groups, and departments. Users can drill down into project totals, identify the top five charged and managed projects, and obtain high-level non-base financial information, as well as data from Human Resources. The Enterprise Business Intelligence Portal replaces two other programs and significantly reduces the time and effort needed to gather, interpret, and share the HR and financial data used by managers in decision making and regulatory compliance.

For professional project managers, reliable information is key. The new Corporate Earned Value Management System brings to Sandia effective and efficient project planning and controls, and auditable, traceable, and reliable performance reporting. The EVMS processes aid in delivering projects within scope, schedule, and budget, and improve consistency for new project startups.

New tools for traveling, connecting and collaborating

Travel can be tiring, but enhancements to the Expense Report Plus system makes it a bit easier for the workforce on the go. ER Plus allows automated manager approval for low-risk travel expense reports, and verification of lodging costs based on Federal Travel Regulation. In addition, paperless receipts now can be used for travel and non-travel expense reporting, and travelers know exactly how much they have for their destination, thanks to last year's switch to per diem for meals and incidentals.

For those who use Sandia-owned iPhones and iPads, a new mobile credential simplifies remote access to internal web resources such as timesheets and expense reports. About 1,450 devices already use the credential, and more than 5,500 users received installation instructions.

Members of Sandia's workforce team up all the time, so Enterprise Collaboration Services (ECS) and partners worked with multiple organizations to increase Skype-based collaboration on the Sandia classified network by more than 50 percent. ECS provided cameras, headsets, and microphones to more than 200 people and worked with Nuclear Weapons Planning, Operations, Assurance, and the Classified Computing Continual Service Improvement team on personalized training so users could be comfortable using Skype on the classified network.

More collaboration also was encouraged through the Tiered Accountability (TA) boards, one of the six Laboratory Operating System enablers helping Sandia's workforce share information. Standard templates for the boards were updated, put into use by the Senior Leadership Team at Tier 5, and are now available for all boards. After pilot projects explored options for virtual tier boards, a platform based on Confluence Wiki will allow members of the workforce who can't attend TA meetings to fully engage with their teams to discuss priorities, identify problems, reinforce accountability, and track metrics. More than 180 tier boards are active at all levels of the organization, but the goal is for every team at the Labs to use its own tier board before the end of FY18.

Innovation at Sandia comes standard, whether providing support to the front lines or providing support for those behind the scenes, and the new tools aim squarely at increasing innovation.

