Cracking the code to soot formation

Scientists unlock mystery to help reduce hazardous emissions

By Michael Padilla

The longstanding mystery of soot formation, which combustion scientists have been trying to explain for decades, appears finally solved, thanks to research led by Sandia.

Soot is ubiquitous and has large, detrimental effects on human health, agriculture, energy-consumption efficiency, climate and air quality. Responsible for significantly increased rates of cardiovascular and pulmonary diseases, soot also contributes to millions of deaths worldwide annually, largely from indoor cooking and heating in developing nations. It leads to tens of thousands of deaths in the U.S. every year, predominantly from anthropogenic emissions to the atmosphere, referred to as black carbon.

By understanding soot formation, we have a better chance of being able to reduce its dangerous emissions from engines, forest fires and cook stoves and control its production and characteristics during industrial processes,” said Sandia researcher Hope Michelsen, adding that everyone knows what soot is, but nobody has been able to explain how gaseous fuel molecules become soot particles.

She said soot formation turns out to be very different from the typical process of gas molecules condensing into a particle, instead requiring fast chemical reactions rather than condensation.

The solution also can apply to other high-temperature conditions, such as interstellar space, where large quantities of carbon-dust particles are formed, she said.

This groundbreaking work was published in a Science magazine paper, “Resonance-stabilized hydrocarbon-chain reactions may explain soot inception and growth.” Authors include Hope, Olaf Johansson and Paul Schrader from Sandia, and Kevin Wilson and Martin Head-Gordon from Lawrence Berkeley National Laboratory. Head-Gordon is also a chemistry professor at the University of California, Berkeley.

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Q&A with 2019 Truman Fellows

By Troy Rummler

Sandia will welcome two new Truman Fellows in October. Pauli Kehayias and Thomas O’Connor will join the Labs for the next three years to apply breakthroughs they have made in their respective fields to Sandia applications. They join six other Truman Fellows now conducting research at the Labs.

Lab News spoke to both incoming fellows about how they plan to fold their innovations into Sandia’s R&D program.

Since 2004, Sandia’s Harry S. Truman Fellowship in National Security Science and Engineering has sponsored high-risk, potentially high-value R&D through the Laboratory Directed Research and Development program. Candidates propose bold, cutting-edge research with a strong tie to Sandia’s mission and must earn the endorsement of a selection committee of senior scientists, their future peers and Sandia’s Chief Research Officer.

“Those who stay at Sandia after their three-year fellowships end become leaders of the next generation of Sandians,” said Cindy Phillips, chair of the Truman Fellowship Selection Committee.

(Continued on page 4)

Mystery solved — Scientists have discovered a mechanism for soot formation, solving a longstanding scientific mystery. In this image of a candle flame, the colors are from hot soot luminescence. The mass spectrum at the bottom shows the peaks for the radicals that drive reaction. The incipient soot particle shown between the two arrows is the cluster that marks a transition to the condensed phase. Fast reactions grow the particle shown at the top of the flame.

(Image courtesy of Hope Michelsen)

Business partnerships, technology transfer earn Sandia four regional awards

By Manette Newbold Fisher

Sandia has won four regional awards from the Federal Laboratory Consortium for its work to develop and commercialize innovative technologies. The annual FLC awards program recognizes federal laboratories and their industry partners for outstanding technology transfer achievements.

“New technologies and partnerships continue to emerge from Sandia, showcasing the Labs’ talented workforce and our impact in national security, emergency response and scientific modeling,” said Jackie Kerby Moore, manager for Economic Development and the Labs’ FLC representative.

The consortium’s Mid-Continent and Far West regions recognized Sandia’s achievements in four areas.

(Continued on page 7)
Lab News Notes: How to do science in retirement

Detecting quark nuggets, a candidate for extreme ball lightning and dark matter

By Pace VanDevender, Sandia retiree

Thirteen years ago, I was retiring early from a wonderful job as Sandia chief technology officer and vice president of science and technology to become an 80th century “gentleman (that means self-funded) physicist.” I wanted to understand two mysteries before I died: puzzling electromagnetic signals observed on the Los Alamos-Sandia FORTE satellite and extreme ball lightning. The resulting adventure has had many twists and turns that led to dark matter and the first of five planned publications: Detection of Quark-nuggets—a candidate for dark matter.

The FORTE signals were short-duration, narrow-band radio-frequency bursts captured in 1997, before FORTE’s fully optimized triggering system prevented the detection of the annoying anomalies. The anomalies were soon forgotten until I found them while looking for a way to detect extreme ball lightning from space.

In contrast to weather-related, sub-second-duration ball lightning, extreme ball lighting occurs even in clear weather and lasts for 10 seconds to 20 minutes without a power source. Therefore, it is self-energized, but the power source is a mystery. My son and I investigated an extreme-ball-lightning event in Ireland. The yield, strength and electrical conductivity of the peat and the size of the deformations were consistent with the core of the extreme ball lightning, weighing about 1,000 tons, being more than 10,000 times more dense than gold, being magnetically levitated and rotating more than a million times per second!

After eliminating black holes (no magnetic field), naked singularities (unstable), the gravitational equivalent of an atom or GEA (insufficient magnetic field), we found quark nuggets were consistent with the observations. Quark nuggets are theoretical aggregations of strange up and down quarks (the building blocks of protons, neutrons and similar particles) in essentially naked singularities (unstable), the gravitational equivalent of an atom or GEA (insufficient magnetic field), we found quark nuggets were consistent with the observations. Quark nuggets are theoretical aggregations of strange up and down quarks (the building blocks of protons, neutrons and similar particles) in essentially naked singularities (unstable), the gravitational equivalent of an atom or GEA (insufficient magnetic field), we found quark nuggets were consistent with the observations. Quark nuggets are theoretical aggregations of strange up and down quarks (the building blocks of protons, neutrons and similar particles) in essentially

That allowed me to calculate the energy deposition as a function of quark nugget mass so I could plan to detect them. Soon thereafter, I showed that the torque on the nuggets as they passed through the atmosphere would spin them to millions of revolutions per second. Their mass density, magnetic field and rotational velocity are just right for explaining the deformations from the ball lightning in Ireland and the FORTE signals. So quark nuggets became the sole hypothesis for both phenomena.

In 2015, I showed that quark nuggets would interact with matter through their immense magnetic field in the same way the earth interacts with the solar wind. That allowed me to calculate the energy deposition as a function of quark nugget mass so I could plan to detect them. Soon thereafter, I showed that the torque on the nuggets as they passed through the atmosphere would spin them to millions of revolutions per second. Their mass density, magnetic field and rotational velocity are just right for explaining the deformations from the ball lightning in Ireland and the FORTE signals. So quark nuggets became the sole hypothesis for both phenomena.

I just had to detect them in as many ways as I could afford.

Fortunately, mentoring Sandians in the centers for military systems, radiation science and pulsed power provided the joy of working, through them, on Sandia’s missions, as well as some supplementary income that funded the senior suite and paid students for data analysis while they experienced real research. In addition, the New Mexico Small Business Assistance program funded Bob Schmitt to do the hydrodynamic simulations of a quark nugget impact—a vital contribution to our paper.

As explained in the paper, the most promising way to detect quark nuggets is to look for their impact in a very large and very quiet lake. So we constructed and now operate three sophisticated sensors in the Great Salt Lake, Utah, looking for dark matter impacts. The lake is a very hostile place for electronics and metals. The first system lasted four days, and the first platform lasted three months. Continual improvements have increased the lifetime of the electronics to a year and the lifetime of the platforms to at least 30 years. We are now calibrating the system with explosions throughout the lake to simulate quark nugget impacts. Then we can observe.

For future Gentleman Scientists or Engineers, some of the lessons I learned might be useful: 1) Build a team with the diverse expertise needed. Fortunately, the internet connects everyone, and finding interested people is not so hard. Our team members resided all over the U.S., the United Kingdom and the Republic of Ireland. 2) Include someone specifically tasked to be super critical and keep the team from believing its own constructs. Be thankful for them. In addition to my son, Aaron, my friend and former boss Bill Brinkman (former Sandia and Bell Labs vice president and director of the DOE Office of Science) fulfilled that role wonderfully. I recall that they independently asked, “where is the physics in this draft paper?”

Contact me at pacevandevender.com for more lessons learned, to get students to assist you, or to mentor students through the Student Research Institute, which is being formed by Ian Shoemaker, former Sandia intern and assistant professor of physics at the University of South Dakota.

Lab News Notes

Editor’s Note: Lab News seeks guest columnists with observations on life at the Labs or on science and technology in the news and in contemporary life. If you have a column (500-750 words) or an idea to submit, please contact Jim Danneskiold, the acting editor.
Society of Women Engineers recognizes Jackie Chen with its highest honor

By Michael Padilla

Jackie Chen has been recognized with an Achievement Award from the Society of Women Engineers for her impact on the society and the engineering community. The award is the highest honor given by the society and recognizes outstanding technical contributions of at least 20 years in engineering.

The award also recognizes Jackie’s continuing dedication to the society’s mission. SWE highlights the impact and importance of women in engineering across the globe, leading by example and demonstrating that a career in engineering can be a fulfilling, rewarding pursuit for women of any background.

Jackie will accept the award at the society’s annual conference, WEB18, in Minneapolis, Minnesota, on Oct. 19, during the formal awards banquet.

“I am honored to be recognized by the Society of Women Engineers for my research on computational simulation of turbulent reacting flows with complex chemistry,” said Jackie, who has spent her entire career working at Sandia’s world-renowned Combustion Research Facility. “I appreciate the work that SWE continues to do to highlight the importance of STEM and the impact the society has on the future generation of women engineers.”

Chris Shaddix, Jackie’s manager, submitted the nomination for the award. Chris said Jackie has truly outstanding technical achievements, a prodigious technical publication record and extensive professional leadership activities in the engineering profession.

Jackie’s research has led to a deep understanding of the complex interactions of fluid flow and chemistry in flames, as revealed by some of the largest computational simulations ever performed, using some of the world’s largest supercomputers. She has been elected to the most prominent advisory panels in the nation associated with both combustion research and scientific computing research and will be inducted to the National Academy of Engineering in September. Jackie regularly gives plenary and keynote talks and has been interviewed many times by the news media and other public communications associated with those fields.

According to the Web of Science, Jackie has published more than 135 papers — mostly in top research journals. Her papers received more than 580 citations in 2017 alone.

Jackie’s research has focused on elucidating the combined influence of chemical reactions and fluid flow on combustion processes. She has developed a unique computer code to calculate the properties of turbulent fluid flow and flames. The code scales efficiently across the hundreds of thousands of processors present in modern supercomputers. Jackie has devoted her career to a type of calculation called direct numerical simulation, which is the most accurate approach possible for modeling flames and turbulent flows because it fully resolves all relevant spatial and temporal scales of the flow and its associated chemical reactions.

“The men and women recognized have broken boundaries in their careers and personal lives,” said Penny Wirsing, president of SWE. “They are leaders paving the way to empower and inspire future women engineers across the globe.”

Animal planet

Sandia/California is home to snakes and bunnies and birds, oh my!

By Michael Padilla

Photos courtesy of Robert Holland

Robert Holland and his team are outside Building 915 on Sandia’s California campus looking for a swarm of bees that were reported circling the plans and alarming passersby. Their mission: find the busy bees, figure out how to contain them and restore order to the campus.

The reported bees were never found. However, Robert said beekeepers had removed a previous swarm from the site. He added that the most important protection for bees is minimizing pesticide use.

Robert, known to some as Sandia/California’s “animal wrangler,” receives calls on a regular basis about the many animals on site. From snakes to squirrels to foxes, Robert is knowledgeable about and keen on the animals that reside on campus.

“The site is a habitat for a range of wildlife species, many of which nest, den or forage around various areas of the campus.”

For most of Robert’s 27-year career at Sandia, he has been associated with the California site’s ecology program. His long-held interest in ecology was strengthened by several field ecology classes that he took while pursuing a bachelor’s degree in biology.

Robert’s primary advice to the workforce is never to attempt to touch or capture wildlife because they can carry dangerous diseases. He also warns never to feed wildlife, including birds, ground squirrels and foxes. Finally, he asks that workforce members close unattended storage spaces and equipment rooms and dispose of trash and food refuse in wildlife-proof bins.

Many of the animals are federally protected species, and Sandia corporate policy ESH100.2.ENV.2 prohibits trying to capture, touch, feed or approach wildlife.

Anyone who has wildlife problems (snakes, squirrels, turkeys, etc.) at the California site should call Robert at 925-294-3755 or the ES&H hotline at 925-294-ESAH. For pest issues (mice, ants, etc.), contact Maintenance at 925-294-6400.
The work was funded by DOE’s Office of Science. “This award represents years of scientific success as a result of years of support for focused, systematic work on developing a fundamental understanding of high-temperature phenomena at Sandia,” Hope said.

Soot formation examined

Soot is formed during the combustion of hydrocarbon fuels, such as oil, natural gas and wood. Although it has detrimental health and environmental effects, soot is extremely important to many of the technologies we rely on, such as boiler performance, glass production and carbon-black generation for rubber-product reinforcement and flame retardants.

Despite the ubiquity and importance of soot, the basic chemistry explaining why the molecules in a flame stick together to form soot particles remains a scientific puzzle until now, Hope said. In its final form, soot is a solid very similar to graphite, but it is initially formed from gaseous hydrocarbons. Experimental evidence indicates that it transitions from a gas to a liquid before it becomes a solid.

Scientists have been trying for decades to explain that transition.

“Most people are familiar with how the gas phase of water — water vapor — condenses into droplets when it cools. Cooling it further will turn it into ice, the solid phase of water. Soot is different,” Hope said.

Soot particles are formed when gaseous molecules are heated to high temperatures, and they don’t easily turn back to gaseous molecules the way water droplets do when they are heated up.

Strong chemical bonds hold soot particles together. “Making soot is more like baking a cake than it is like condensing water. Heating liquid cake batter to high temperatures turns it into a stable solid form,” Hope said.

Scientists have long suspected that chemical bonds must be formed to make soot. However, soot formation is fast, and researchers did not understand how the required chemical bonds could form so quickly. To make the problem even more difficult, researchers were not sure which gas-phase molecules were involved in producing soot.

“It’s very difficult to make measurements in a flame,” Hope said, “and without measurements of the participating molecular species, it’s like trying to figure out how a cake is made without knowing the ingredients.”

Radical species of flames studied

The key to soot formation, it turns out, is resonance-stabilized radicals, Olaf said. In general, molecules that are radicals have unpaired electrons they want to share, which makes them reactive. But, unlike most radicals, resonance-stabilized radicals have unpaired electrons that participate in other molecules in the molecule.

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Sandia hosts Albuquerque’s first CyberPatriot Advanced CyberCamp

By Troy Rummel
Photos by Amy Tapia

A bout 20 high school and middle school students came to Sandia recently for Albuquerque’s first CyberPatriot Advanced CyberCamp, a weeklong cybersecurity workshop supporting the Air Force Association’s CyberPatriot program. The workshop taught students advanced security concepts and prepared them for an upcoming competition season this fall.

Twelve Sandia volunteers from Albuquerque and Livermore pitched in as coordinators, teachers and support staff. Some also mentor CyberPatriot teams throughout the school year. Most students came from Albuquerque schools, though a few came from Los Lunas and Moriarty.

Co-coordinators Ted Lapina and Troy Stevens, both high school mentors, say they enjoy demonstrating general cybersecurity principles for students, but Sandia specialists served an indispensable role teaching niche topics.

First place — Tiffany Tafoya took first place in her division at the strongman competition that was part of the 2018 Rio Grande Celtic Strongman Games and placed third in the 2018 U.S. Strongman Nationals this summer.

Tiffany Tafoya, a Sandia missile defense technologist, deadlifts cars and carries around giant heavy stones in her free time. She’s also really good at it.

Tiffany trains in strongman, a weightlifting-based sport that involves physical and mental strength, speed and endurance. Her passion for the sport has led her to compete in the U.S. Strongman Pro-Women’s World Championship, the U.S. Strongman Pro-Athlete division, the U.S. Strongman Pro-Women’s World Championship, and with God, and the heart that I had to get back into it. I was able to push through and recover my strength."

After about six months of training, Tiffany went on to win the 2018 Rio Grande Celtic Strongman Games and qualify for nationals. Each strongman competition can have a different mix of events, which provides fresh challenges for the competitors. The Celtic games included a log clean and press, an 18-inch deadlift, a kettlebell toss, a farmer’s carry and a sandbag carry. There weren’t enough lightweight women registered, so they ended up combining our classes," Tiffany said. "So I was competing with girls weighing 165 pounds, while I weighed about 131. It was pretty intense, but it was fun."

At Nationals, Tiffany had to do 80-pound circus dumbbell repetitions, a car deadlift (a Chevy Cruze), an arm-over-arm car pull, 440-pound tire flips followed by a 500-plus-pound sled pull and a lift of series of atlas stones (170, 190, 210 and 225 pounds) into a 10-inch tow truck bed. Her third-place finish qualified her to compete in the U.S. Strongman Pro-Women’s World competition in October in Memphis, Tennessee. "The stuff we do is insane, but my body has really been taking to it," Tiffany said. "I’m stronger now than I was before getting smart, and I train smart." Tiffany says her ultimate goals are to earn her professional strongman card, which is something she can achieve by placing in the top three at the upcoming world competition, and to someday compete in a strongman Arnold competition. "It’s a way of saying that you are a professional athlete, that you’ve worked hard and earned that card," Tiffany said.

Tiffany hopes she can also encourage other women to try strength training. "You never know how strong you are until you try. You’ll be amazed at how strong you really are."
tours early in the design cycle. Another active project involves modeling tire materials for the best combination of material properties. Sandia also advanced simulating the flow of turbulent air around tires, enabling noise modeling of tires in use.

Ted Blacker, Sandia’s program manager for the Goodyear CRADA, explained why the partnership has been successful. “We focus on strategic technical challenges where advanced technology from both sides can change the future,” he said. “Almost without fail, the new capabilities they brought to us and the improvements they made to our tires — help us with simulations in our national security work.”

The FLC Awards provide feedback to Sandia about the value of our technology partnerships,” Blacker said. “What Sandia has achieved with Goodyear has been the best combination of material properties. Sandia also advanced simulating the flow of turbulent air around tires, enabling noise modeling of tires in use.”

New capabilities emerge for emergency planning

To improve emergency planning, exercises and protocols, Sandia, the California Fire and Rescue Training Authority (CFTRA), and the Sacramento Metropolitan Fire District collaborated to deploy SUMMIT, or the Standard Unified Modeling, Mapping and Integration Toolkit. The software, initially developed through funding from the Department of Homeland Security, helps users create and share models for emergency planning.

This collaboration won a Far West Region Outstanding Partnership Award. "Sandia and the CRADA’s strong relationship over the past four years has yielded many benefits," said Sandia manager Nareyo Tedencieman. "CFTRA has gained early access to emerging technologies that can enhance preparedness across the state, and Sandia has gained operational partners that help guide research and development with their real-world experiences.”

Emergency planners need to understand consequences of disasters and the impacts of response options for natural risks such as earthquakes and wildfires, and man-made risks such as improvised explosive devices. Emergency responders also need real-time and projected event details such as infrastructure damage, possible numbers of casualties or evacuees, and displaced citizens.

Other technologies used by the California authority track resources and maintain situational awareness of current activities such as current weather or location and size of a fire. The models within SUMMIT provides forecast for growth of fires. The growth of natural and unnatural disasters could spread, and what critical infrastructure might be affected.

SUMMIT was used in an exercise called Decisions Matter that simulated a terrorist attack involving an improvised explosive device planted next to a chlorine tanker. The explosion caused a hazmat emergency response, and SUMMIT helped emergency responders determine current and future threats — including hazardous materials first responders and public health officials — calculate population health impacts and medical surge requirements, as well as analyze evacuation routes and warning issues.

"It’s been a positive, mutually beneficial experience to have a national lab deploy technologies with local responders,” said Sandia researcher Lynn Yang. "First responders are very well trained in day-to-day events; we try to help plan for the catastrophic incidents that are rarely encountered but that potentially have very large consequences.”

Organic glass nuclear detectors on the horizon

It could soon be more difficult to smuggle nuclear materials through U.S. ports and borders using organic glass scintillators. The small, handheld detectors engineered by a Sandia team and Carnegie Mellon University were recognized as the Outstanding Technology Development Award.

Sandia’s organic glass scintillator has been engineered for high detection efficiency of radioactive material without high production costs. Organic scintillators produce light in response to the presence of nuclear materials. Depending on the amount of light produced and the speed with which the source can be identified.

The simplicity and low cost of manufacturing could allow for widespread use. Currently, threat detection scintillators are either made from expensive materials or plastics that have limited ability and cause frequent false alarms.

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Organic glass nuclear detectors on the horizon
Students from more than 40 New Mexico schools benefitted from Sandia’s annual K-12 Computer Donation Event, where more than 1,100 computers and related accessories were distributed.

Representatives from schools around the state gathered at Reapplication last month, some driving trucks and trailers for up to four hours to pick up the donations. They collected desktop computers, laptops and iPads for students, along with printers, power cords, keyboards, mice, headphones, monitors and speakers. This year, Sandia distributed 842 desktops, 327 laptops, 46 iPads and nearly $100,000 in peripherals and accessories.

Michael Somuk, who leads the supply chain team that put together the project, said all equipment was in good condition following use by employees for day-to-day work and special projects. Once the equipment reaches the end of its useful life at Sandia and is no longer needed, it’s donated to schools.

Ben Potts, director of technology for Silver Consolidated Schools, said the annual donations benefit nine schools in his district. Before the Silver City district started participating five years ago, students used outdated equipment, and the district was behind in preparing for the statewide digital rollover for standardized testing. Potts said every computer lab in the district now uses equipment from Sandia, including a new technology lab at the high school.

“We’ve been able to add labs, and for the most part, teachers are able to obtain as many computers, laptops and iPads as they need,” Potts said, adding that as older equipment is rotated out, teachers continue to use it to teach students about the insides of computers or use parts to teach robotics, further extending the useful life of the computers.

“It’s a win-win for everybody because the schools get computers and equipment in good shape,” said Michael. “In New Mexico, that is extremely valuable because some school districts have extremely tight budgets. We’ve had schools come to us and say, if it wasn’t for this program they wouldn’t have any information technology resources.”

By Manette Newbold Fisher
Photos by Randy Montoya

PC PREP — Supply Chain team lead Michael Somuk prepares for Sandia’s annual K-12 Computer Donation Event. More than 40 New Mexico schools participated this year.

COMPUTERS FOR KIDS — A school representative checks out a pallet of monitors. In addition to computers, monitors and printers, schools were able to choose what they needed from a selection of keyboards, cords, mice and other related accessories.

SCREEN TIME — Keith Leguiz of El Camino Real Academy in Albuquerque was one of more than 40 school representatives who collected monitors and printers during the K-12 Computer Donation Event held at Reapplication. Sandia’s supply chain team works with schools to determine their needs ahead of the event.

TECHNOLOGY TRANSFER — Reapplication team employee Marcus Barela (left) records property information prior to its release from Sandia. Bernadette Bazen (center) and Semiramis Novak, also on the Reapplication team, help load desktop computers into a vehicle for one of the schools.