In most situations, breaking things apart isn’t the best way to solve a problem. However, sometimes the opposite is true if you’re trying to characterize complex chemical compounds. That’s what Sandia scientists Nils Hansen and Scott Skeen did to definitively identify soot precursor species in a flame.

The researchers discovered aliphatically bridged polycyclic aromatic hydrocarbons and PAHs with aliphatic side chains, which have been hypothesized to serve as “seeds” for soot particles in engine emissions. These are different variations of normal PAHs.

The newly recognized compounds can be used to create more detailed, up-to-date models of combustion that, in turn, can help in the design of cleaner, more efficient engines that emit less soot and fewer harmful hydrocarbons into the atmosphere.

“The role of these molecules as soot precursors has been hypothesized and there is indirect experimental evidence of their presence on the surface of soot extracted from flames” Scott said. “Until now, however, no one had definitive experimental proof of their existence in the flame’s gas phase.”

Working with former Sandia post-doctoral researcher Brian Adamson and Musa Ahmed of Lawrence Berkeley National Laboratory, Nils and Scott recently published their discovery in the Journal of Physical Chemistry A. Funding for the research came from Sandia’s Laboratory Directed Research and Development Center.

‘Talking Soot’ — Scott Skeen, Nils Hansen and Brian Adamson (left to right) discuss the tandem mass spectrometry technique they used to detect aliphatically linked polyaromatic hydrocarbons in a sooting flame. Photo by Michael Padilla

— CONTINUED ON PAGE 3

Creating the Future

By Jennifer Awe

What might the global security environment look like in 20 years?
What are the most significant national security challenges in this environment?
What role should Sandia play in addressing these challenges?
Answers to these questions, examined over a 15-month period by more than 1,000 experts inside and outside the Labs, led to Sandia’s new Creating the Future strategic direction document, and Labs-level strategic priorities.

“Given the pace of global events, we believe such a long-range view is essential to avoid technology surprises and ensure that the U.S. is prepared to meet future threats,” Labs Director Steve Younger said. “Rather than let things happen and respond to them, we have an opportunity to create the future.”

But, just how do you Create the Future?

— CONTINUED ON PAGE 4

Deconstructing deleterious soot

Sandia discovers compounds in soot formation, findings could lead to cleaner engines

By Sarah Sewell

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Lunar eclipse rises over Sandia Labs

By Jennifer Awe

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— CONTINUED ON PAGE 4
Why Doesn't It Hurt?  — Dawn Acevedo of Vitalant (left) helps Courtney Chavez prepare for some nourishing cookies, while Courtney provides blood that potentially could save up to three lives.

Photo by Amy Tapia

T he Vitalant bloodmobile collects donations at Sandia National Laboratories on alternate Fridays by Internal, Digital Advertising Inc., for the U.S. Department of Energy’s National Nuclear Security Administration.

The next donation day is Monday, Feb. 5, 9 a.m.-3 p.m., at the KAFB Outdoor Recreation Center. Walk in or make an appointment. Watch the Sandia Daily News for future donation events. Always bring an ID to a donation appointment, wearing a Sandia badge cannot be used for identification. Events. Always bring an ID to a donation appointment, scheduled an appointment at Vitalant.org.
Deconstructing soot

Research and Development program, while Ahmed is supported by the DOE’s Office of Basic Energy Sciences.

The team used an analytical technique called tandem mass spectrometry — using an instrument provided by Lawrence Berkeley Lab and cleverly customized by Adamson — to identify polyaromatic hydrocarbons in flames that produce soot, something never done previously.

The device removes an electron to positively charge, or ionize, large molecules sampled from the flame, measures the molecule’s masses then further identifies the chemical structure by the way the ionized molecules crack apart.

**Discovery builds on recent Sandia research**

Recent work by Sandia scientist Hope Michelsen, technologist Paul Schrader and former postdoctoral researcher Olaf Johansson broke ground by demonstrating chemical chain reaction processes in which hydrocarbons could form in soot. That work highlighted the challenge of detecting and characterizing the compounds that participate in these processes.

One area of debate is whether the chemical byproducts in soot are purely polyaromatic hydrocarbons, made up of ring-shaped groups of atoms, or contain extra, non-cyclic structures called alkyl, or aliphatic, chains. These long hydrocarbon chains can make the links among polycyclic aromatic hydrocarbons more stable at the high temperatures of combustion, greater than 2,000 degrees Celsius.

“Without the tandem component of this new mass spectrometer, each molecule’s mass is obtained but no information about its structure is revealed. You see something at mass 78, at mass 128, etc., but you don’t know what it is. You just use your chemical intuition,” Nils said. “To overcome this problem, we generated a flame in which the air is in the center of the flame with the fuel on the outside,” he said. “This is perhaps the first time that such a flame has been attached to a tandem mass spectrometer.”

**Engines creating solid soot from gas**

In an engine, soot particles form when gaseous, carbon-containing molecules that originate from the fuel escape oxidation and combine to create larger molecules that eventually turn into a solid material.

Soot is harmful to the environment and a significant contributor to global climate change. Moreover, it impacts public health by damaging the lungs. Substantial evidence links polycyclic aromatic hydrocarbons and soot formation, although the evidence isn’t completely conclusive.

The chemical components leading to soot are difficult to decipher. What is known is that when the chemicals in hydrocarbon fuels are broken down during combustion, new molecules form rapidly.

The search for soot precursors is motivated by the need for cleaner engines that still run efficiently. Under certain driving conditions, diesel emissions exceed government regulations. This has led to the use of particulate filters that effectively capture soot particles from diesel exhaust, but they make the vehicles significantly more expensive and less efficient. Engines that produce less soot would need smaller particulate filters, reducing costs and increasing fuel economy.

Engine manufacturers typically use computer simulations to improve engine designs. They model the fuel injection, combustion and pollutant formation processes. Scott said that better understanding of the chemical reactions involved in soot formation — should lead to models that more accurately describe the effects of engine design parameters on emissions and efficiency.

“If we can understand the chemistry, we can develop a model that will allow engine designers to model fuel injection, air flow and design of internal engine surfaces, among other things, that will keep these compounds out of the atmosphere,” Scott said.

**Future steps**

This discovery of alkyl-substituted and aliphatically-bridged PAHs in soot opens up a new starting point for using tandem mass spectrometry to decipher the complex chemistry of pollutng emissions, the team said.

In the published paper, the team analyzed compounds at two different masses. However, the technique potentially could lead to identification of thousands of different types of compounds. Even for the most basic polyaromatic aromatic hydrocarbons, there are about a hundred different ways the atoms can come together. Seeing all the different arrangements presents a formidable challenge. Musa will continue his work with Sandia scientists and plans to use complementary methods such as infrared spectroscopy for less ambiguous identification of alkyl-substituted and aliphatically-bridged PAHs in soot.

The Sandia scientists hope to collaborate with data scientists to develop more efficient, realistic models of engine soot formation, ultimately leading to designs for cleaner, more efficient engines.
Creating the future

CONTINUED FROM PAGE 1

environmental scans, workshops, Labs-wide crowdsourcing, surveys and leadership meetings and engagement.

The imagined futures reflected a complex global security environment driven by several key dynamics: technical convergence and individual empowerment; a polycentric world with new actors challenging institutions; climate change and constrained resources; continuing superpower dynamic with emerging frontiers of engagement; and accelerated information diffusion.

Discussions about how to prepare for these dynamics focused on five broad roles for Sandia to play in addressing these challenges: anticipator, technical advisor, technology developer, systems integrator and rapid responder. Variations on the roles can be found within the Labs’ strategic priorities.

Labs-wide teams composed of experts in technical fields, mission support and strategy studied national security topics and presented their findings to executive leadership. Sandia’s leadership team then finalized the topics and language, and developed a set of Labs-level strategic priorities:

1. Deliver on today’s commitments.
2. Maintain an agile and effective nuclear deterrent.
3. Anticipate threats to national security through intelligence science.
4. Develop transformational technical solutions to detect threats to national security.
5. Invent and demonstrate pathfinder systems to address threats.
6. Deploy outstanding engineering, science and technology to our missions.
7. Unleash the power of Sandia.

Avoiding another ‘Sputnik moment’

The Labs’ strategic direction document hopes to serve as Sandia’s “North Star.” It’s a living document that provides a framework for decisions needed to bring the purpose statement to life over the next two to three decades.

Steve recently met with each priority team and challenged them to take up this charge. “Team members have served in addition to their responsibilities and on to the next big idea. Variations on the roles can be found within the Labs’ strategic priorities, but the recognition that other nations are spending a lot of time and money on discovery is part of what fueled leadership discussions about risk acceptance, and how Sandia might work within its governing parameters to think big. Innovative, forward-leaning people throughout Sandia have taken up this charge.

“Team members have served in addition to their ‘day jobs’ for over a year,” said Elizabeth Roll, senior strategist. “They’ve become subject matter experts on their priority and have helped the rest of us better understand the threat space and opportunities for impact.”

Now what?

The strategic direction document outlines the why and what, intentionally leaving the how to be determined by the priority teams, and any area of Sandia that sees its work aligning with the intent of the priorities. Currently, teams are busy working on priority development and deployment, which will take the planning project well into 2019.

“This is really hard, and it takes time,” Steve said. “I’m asking folks to not focus only on what Sandia does today, but what we need to do in the future in order to tackle a big idea that changes the world. With a 20-year horizon, we can spend a percentage of that time thinking.”

Each priority has an associate labs director as champion, a director lead and a supporting team (in some cases multiple teams, or variations) tasked with overseeing the big ideas that will give the priorities substance and attention over the years, and tracking their progress through familiar methods – management reviews, milestones, etc.

“Implementation is spread throughout Sandia, with no priority existing in a vacuum,” Elizabeth said. “We’ve worked with these groups from the beginning – everyone from ALDs, directors, managers, and staff from every division. We did this with intention, so that the deployment phase would not be a surprise to those charged with making it happen.”

With or without a strategy, Sandia would continue to play its part in the global security environment, delivering exceptional service in the national interest. However, a strategy may help Sandia do more than that, allowing the Labs the freedom, and permission, to think beyond current responsibilities and on to the next big idea.

“There is something out there as important to national security as the Manhattan Project,” Steve said. “We’re the ones to find it.”

Photo by Norm Johnson

LONG-RANGE PLANNING — Sandia managers gathered more than a year ago to brainstorm about the Labs’ future directions and priorities. Many of their ideas went into the recently published Strategic Direction document.

Photo by Amber Harwell
Middle school teams design cities of the future

by Valerie Alba
Photos by Cliff Ho

Students from 18 rural and urban middle schools took part in the sixth annual New Mexico Future City Competition regional finals at the UNM School of Architecture and Planning. Each of the 37 teams worked with an educator and mentor skilled in the fields of Science, Technology, Engineering and Math to design their vision of a resilient city that could withstand and quickly recover from natural disasters. The students also prepared essays and scale models of their cities and then presented their ideas to a panel of STEM professionals. The students vied for the chance to represent New Mexico at the national Future City Competition in Washington, D.C., in February. The winner, Citta Forte designed by Annunciation Catholic School students (bottom photo), featured smart grid technologies, autonomous vehicles and shock-absorbing buildings. Eighty-six volunteers supported the event, including 21 Sandia employees. “Taking a relevant infrastructure challenge and inspiring kids to come up with engineering solutions is just one of many avenues to sustain their interests in science and technology. Middle school students attending this event get new ideas by witnessing other models as well. The New Mexico Future City Competition is very fortunate to have strong community support from two national laboratories, New Mexico professional societies and local businesses,” said Amy Sun, Sandia engineer and regional coordinator for the New Mexico Future City Competition.
VICE ADMIRAL JOHNNY WOLFE VISITS SANDIA

NAVY VISIT — Vice Admiral Johnny Wolfe, director of Strategic Systems Programs for the Navy, visited Sandia last week and formally recognized Sandia and its staff for their key role in the development and production of the W76-1/M64A Life Extension Program. During his tour, he presented an award to W76-1 leadership. Pictured (left to right) are Chris O’Gorman, senior manager; Vice Adm. Wolfe; Mark Meyer of Military Liaison. Photos by Randy Montoya

SANDIA CLASSIFIED ADS

AD SUBMISSION DEADLINE: Friday noon before the week of publication unless changed by holiday.
Questions to Michelle Fleming at 505-844-3942.

Submit by one of the following methods:
• EMAIL: Michelle Fleming (classads@sandia.gov)
• FAX: 505-844-0645
• MAIL: MS MD42 (c/o mp)
• INTERNAL WEB: Click on the News Tab at the top of the Techweb homepage. At the bottom of the NewsCenter page, click the “Submit a Classified Ad” button and complete the form.

SANDIA LAB NEWS
February 1, 2019

AD SUBMISSION GUIDELINES

AD RULES
1. Limit 18 words, including no phone number or email address.
2. Include organization and full name with ad submission.
3. Submit ad in writing.
4. No phone number.
5. No “for rent” ads except for employees on temporary assignment.
6. No commercial ads.
7. For active Sandian members of the workforce and retired Sandians only.
8. No housing listed for sale is available without regard to race, creed, color or national origin.
9. No commercial ads.
10. No “for rent” ads except for employees on temporary assignment.
11. No “for rent” ads except for employees on temporary assignment.
12. We reserve the right not to publish any ad that may be considered offensive or in poor taste.
13. All ads may not run more than twice.
14. The same ad may not run more than twice.
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Mileposts

New Mexico photos by Michelle Fleming
California photos by Randy Wong

Recent Retirees

New Mexico photos by Michelle Fleming
California photos by Randy Wong

Retiree Deaths

Stanley Zehr (77) June 6
Walter Morris (92) June 10
Howard Hugh Cole (95) June 13
Daniel Koloske (96) June 29
Robert Galloway (94) July 2
Margaret Howard (66) July 22
Joann Painter (86) July 31
Ronald Badu (79) August 16
Dwight Orr (87) August 17
Roger Boucill (79) August 29
Brandy Forrister (59) September 3
James Landaram (73) September 4
Deborah Eaton (82) September 18
Kenneth Flynn (85) September 19
William Wall (87) October 9
Kenneth Finders (94) October 9
Wiili Urbanoski (99) October 12

Green Serrano (82) October 23
W. Hugh Walker (79) October 27
Sharon Downey (64) October 28
Robert Fisher (79) November 1
David Yance (72) November 3
Richard DePima (77) November 7
Norman Elliott (95) November 8
Fred Johnson (98) November 8
William Arntzen (78) November 9
Julie Padres (99) November 9
Joe Castile (87) November 10
Helen Thompson (96) November 11
Lori Moore (94) November 16
Donald Robbins (94) November 17
Levi Hanchey (85) November 19
Charlene Brown (105) November 24
William Zagar (96) November 28

Wayne Tramp (89) December 1
John Remora (91) December 1
Rose Brightman (94) December 2
Raymond Klein (77) December 3
Robert Pasco (62) December 5
E. Archie Lackey (80) December 12
Richard Carlson (85) December 15
Alan Bello (94) December 17
Norman Blais (95) December 18
Norman Blais (95) December 18
Robert Carr (69) December 25
Emiliano Sanchez (62) December 25
Barbara Champion (89) December 28
Karl Smason (36) December 29
Allie Vinall (95) December 29
Lee Rieger (64) January 6, 2019
William Harman (96) January 6

Paul Selzweald (76) January 2, 2018
Robert Bono (52) January 10
Lola Loez (95) January 25
John Aragon (70) February 9
Joan Burnison (70) February 13
H. Parks Davis (71) March 8
Kari McBrat (97) March 8
Phinomena Harrie (91) March 16
Hattie Diez (64) March 27
Barbara McKinney (85) March 29
Joe Abeyta (79) April 26
Andrew Siller (66) April 27
Judy Ewing (79) May 17

Michael Mauser 30
Lynn Schnitor 30
Dwight Stockham 27
Tamera Ortega 24
Jeff Figiel 21
Tina Neiwander 20

Jeff Brinker 39
Bob Cutler 37
Debbie Duran 37
Bob Bonner 35

Mark Sposanover 25
David Clifford 20
John Dehaasje 20
Erin Varley 20
Ryan Kristenon 15
Victor LeJenawon 15

Cindy Serna 20
Barb Wampler 20
Dennis Anderson 25
Mike Da Mondo 25
Michael Lopez 25
Chris O’Gorman 25

Nick Vargas 15
Jason Min 15
Beverly Polyard 15
Talbot Smith 15
Mark Taylor 15

Mark Vargas 15
Nick Taylor 15
Joe Abeyta 30
Jeff Figiel 30
Lola Lenz 25
Tina Neiwander 25

More than 500 fourth-graders visited the Sandia/UNM Advanced Materials Laboratory at the University of New Mexico recently for a chemistry magic show, but instead were accused of dognapping the chemistry dogs, GreyShoes and Sister. For the rest of the week, the students applied their minds to the “Whodunit” and examined physical evidence, data and clues based on chemistry, biology and basic science. They analyzed purple water in the dogs’ drinking bowl and other liquids found at the scene of the dognapping, examined various fibers, powders, gases and other items, and gained hands-on experience in the disciplines that comprise Science, Technology, Engineering and Math.

All the activities were part of the 15th CSI Dognapping program, organized by LaRico Treadwell with help from Tinae Quintana of Community Involvement and numerous volunteers from Sandia, UNM and the Albuquerque Public Schools. This year, students came from Chelwood, Eugene Field, Emerson, Mission Avenue, Tomasita and Lowell elementaries. “The workshop promotes and challenges youth in scientific methods and encourages self-confidence and teamwork,” LaRico said. “They learn lab safety, how scientists must use all five of their senses and, most importantly, that it’s OK to ask questions and have fun.” The program — founded by Sandians Timothy Boyle and Bernadette Hernandez-Sanchez — won the ChemLuminary Award for Outstanding Kids and Chemistry from the American Chemical society, making Sandia the first national laboratory to do so.