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THREE SANDIA RESEARCHERS RECEIVE TOP HONORS

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Digging hydrocarbons

Sandia research investigates how organic reactions affect Earth’s atmosphere

By Michael Padilla

Volatile organic compounds can be found in the air — everywhere. A wide range of sources, including plants, cooking fuels and household cleaners, emit these compounds directly. They are also formed in the atmosphere through a complex network of photochemical reactions.

Sandia researchers and colleagues from other institutions investigated the reactions of hydroxyl and methylperoxy radicals to understand their impact on the atmosphere’s ability to process pollutants.

The work, which was published in Nature Communications, showed that the reactions can impact levels of a key chemical marker used to assess the understanding of the processing and abundances of pollutants. This ultimately improves the understanding of how both nature and human activity impact the chemical composition of the atmosphere.

Recent studies in this area had indicated that the reaction of methylperoxy with the hydroxyl radical occurs more rapidly than previously thought, and so this reaction could impact our current understanding of chemistry in low-temperature combustion and in the Earth’s atmosphere.

The hydroxyl radical, an important molecule in combustion and atmospheric chemistry, initiates the oxidation, or processing, of fuel and pollutant molecules. When this radical reacts with fuel molecules in the presence of oxygen, a new class known as peroxy radicals is formed. In the Earth’s atmosphere, when the hydroxyl radical reacts with methane — which is both a greenhouse gas and the most abundant hydrocarbon — methylperoxy is created.

Impacts to combustion

Rebecca Caravan, a Sandia postdoctoral appointee and lead researcher of the collaborative new effort, said investigating the subsequent reactions of peroxy radicals is critical to understanding low-temperature combustion because the peroxy radical’s fate determines to what extent fuel will undergo...

International Year of the Periodic Table

Mike Brock polishes the entry tiles that are laid out in the pattern of the periodic table of the elements at the National Museum of Nuclear Science & History. Proclaimed the “International Year of the Periodic Table” by the United Nations General Assembly and UNESCO, 2019 marks the 150th anniversary of Dimitri Mendeleev’s publication of a periodic table that arranged the elements by atomic mass.

National Periodic Table Day is observed annually on Feb. 7 to commemorate John Newlands’ 1863 publication of a table that grouped the 56 known elements following his Law of Octaves, which asserted that when the elements were arranged by increasing atomic weight, those with similar characteristics would occur after every seventh element.

Of the table’s 118 elements, 22 have been discovered by Department of Energy scientists.

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POWERED BY STATISTA
Can systems help us achieve our goals?

By Gabe Martinez

With the new year 2019 now in full swing, I have been thinking a lot about resolutions, and about my personal and professional goals, as I’m sure many others must be going through the same process. I decided to write something and I do hope that some may find it beneficial.

I have been reading a lot about the hows and whys of goal setting and such related topics as creating good habits, setting up systems for success and personal growth in general. Perhaps because it’s somewhat of a fad and I keep seeing articles on these topics, or perhaps because I have been immersed in the subject, I have decided to write about it.

I’ve followed various leads to many different sources. Whatever the reason, I have learned some things from my reading that have helped me gain traction on setting my own personal goals, but I’ve also learned from some recent experiences.

One important thing about goal setting is that it seems to be much of a skill that needs to be learned and developed than a simple task like writing a note on a to-do list. Goal setting skills aren’t taught in school, but there are many experts and books available on the subject.

Maybe you’ve heard of people like James Clear, Michael Hyatt or Brian Tracy, or have read some of their books or blog posts. These subject matter experts, among others, have written extensive articles on the proper way to set goals and build good habits. With all the material out there, I’ve learned that not all methods work for everyone, but it’s valuable to identify one that sounds right for you and give it a solid try.

Like most people, I used to set very vague and generic New Year’s resolutions: eating healthier, reading more, exercising consistently, being more patient with colleagues and friends. Probably not surprisingly, I failed to keep all of them. Now that February has rolled around, I imagine that a lot of people are facing the same problem keeping their resolutions.

The reason for my failure was that I lacked a system to help me achieve those goals. One solution that has helped me a great deal is to focus on building a single small, sustainable habit. Then, I find it easier to build upon that one, and then another, one at a time. Over time, the compounding of a small habit leads to lasting change.

I had lost my love of reading shortly after graduating college. I went into the workforce as a design engineer for a private firm, started a family and just plain got busy. “I’ll get around to it,” I told myself many times. Or, “I’m going all in and will read one hour a day, starting today!” I think that lasted one day. Then I started thinking about some advice I had read on Clear’s website: focus on systems rather than on generic goals. Start with a small habit, something simple and easy to do every day.

So I started reading five minutes a day. That’s all, just five minutes. I’m proud to say it worked. For 70 days, I read just five minutes every day. I was quite surprised at how many books I read just by committing to the short amount of time; but eventually I increased my reading time while reestablishing my love of reading. Still, there are days when I don’t have time to read even 30 minutes a day, but I always fall back on my initial habit: read five minutes a day. It’s a small task, easy to stick with and easy to fall back on.

I’ve started to apply this principle to other aspects of my life and have been seeing good results. I’m beginning to see the value in putting an easy-to-follow system in place and mastering that system, which helps me to do something consistently every day that gets me closer to achieving my goals. It applies to my current role as a mechanical systems engineer at Sandia. I’ve been able to break down long-term tasks, such as writing strategic plans, into manageable, short-term tasks and work on a little bit daily. It has saved me from rushing to complete large projects at the last minute.

Goal setting is a fascinating subject, one that has been studied by many people over the centuries. New data comes out all the time about the best way to set and achieve goals. But the simple fact is the key to success is using a system that works best for your goals, your situation and your life.

Here’s to a productive 2019!
EXERCISE:
Drone attack, pipe bomb put Sandia to the test

Story and Photos by Michael Padilla

A sunny winter day at Sandia/California turned into mayhem when seven employees were injured by a pipe bomb dropped from a small unmanned aircraft system — a drone.
The bomb created significant blast injuries, head trauma and lacerations. The drone malfunctioned and crashed into the fence line to the west.
The Alameda County Fire Department was unable to respond immediately due to multiple concurrent bombing attacks at Lawrence Livermore National Laboratory.

That was the exercise scenario presented to Sandia/California’s medical staff and Protective Force last month. The exercise also tested the emergency alert system used to notify members of the workforce.

Once on the scene, Dr. Dan Azar and Michelle Tamaru of the medical team acted quickly to determine the extent of the injuries and began immediate triage for transportation to local hospitals. Meanwhile, incident commander Lt. Jeremiah Johnston ordered a sitewide shelter-in-place order to ensure that workforce members weren’t in harm’s way.

Exercise planner Anthony Trimble said the Sandia/California Emergency Response Organization trains constantly to be self-sufficient in a disaster.

Anthony said the drone crashing into the fence line added a security threat to the scenario, which affected how quickly the Protective Force could respond to the medical staff and stressed the resources of the medical team.

“To accomplish our goal of being self-sufficient, we train and exercise our response capabilities as though help was not just across the street,” Anthony said. “In a large-scale regional disaster where county resources are unable to respond, the Emergency Response Organization needs to be able to protect members of the workforce and respond to those impacted.”

The exercise ended once all critically injured personnel were transported to hospitals in the region.

“The increased availability of drones makes it plausible that first responders could encounter them on site in numerous scenarios, whether malicious or not,” Anthony said.
Digesting hydrocarbons

CONTINUED FROM PAGE 1

autogation. The researchers wanted to understand how the reaction of hydroxyl and methylperoxy radicals could impact this — for example, whether autognation could be inhibited due to the removal of reactive radicals and the production of relatively unreactive compounds.

"Determining the impact of any specific reaction within any given environment requires knowing both how fast the reaction occurs and the proportion of reaction products," Rebecca said. "Carefully quantifying the products is often the more difficult task. A relatively small change in these reactions can significantly change the magnitude and even the direction of the impact a reaction has in a given environment."

Recent theoretical work indicated that possible products of the hydroxyl radical and methylperoxy reaction could be methanol and oxygen. These products would have significant impact on our understanding of the chemistry in Earth's troposphere, or the atmosphere up to about six miles, which contains around 75 percent of the atmosphere's mass.

Rebecca said that methanol has long been significantly underpredicted in the troposphere by atmospheric models. Because methanol can be formed from multiple sequences of oxidation reactions in the troposphere, understanding how chemical reactions contribute to the levels of methanol in the atmosphere sheds light on how the atmosphere processes hydrocarbons emitted by both nature and human activity, therefore helping us understand the influence of both on the chemical composition of the atmosphere.

Sandia combustion chemist Craig Taatjes, the principal investigator of this research effort, said, "We recognized that our fundamental measurements of methanol yield from the hydroxyl radical and methylperoxy reaction could have an impact on modeled atmospheric methanol abundance, so we brought in modeler colleagues who could focus on those consequences of our investigations."

International collaboration

The discrepancy between modeled and measured methanol is particularly significant in the remote troposphere, regions with relatively limited influence from human activity.

Dwayne Heard, professor of atmospheric chemistry at the University of Leeds in the U.K., said an understanding of the chemistry of these regions is needed before human impacts can be understood.

"We know that changes in man-made emissions are leading to a warming of the atmosphere and a change in the quality of the air that we breathe," Heard said. "However, set against this is the role of natural processes that occur everyewhere — for example, the oceans where there is relatively little influence from humans."

Studies of radical-radical chemistry are complicated; the multiple side reactions need to be understood along with the reaction of interest. To tackle this, researchers from Sandia and NASA's Jet Propulsion Laboratory used Sandia's Combustion Research Facility and the Advanced Light Source to observe and characterize the chemistry and reaction products.

The researchers then worked to interpret their experimental observations via models and calculations. They examined the role of longer-timescale chemistry on the reaction products by collaborating with partners at the University of Cambridge, who used their atmospheric simulation chamber. Additional team members at Sandia's Combustion Research Center and the University of Bristol in the United Kingdom used a global chemical model to assess the impact of the experimental results on the troposphere.

"It was a highly collaborative, international project with each party bringing their own world-class capabilities," Rebecca said.

The Sandia team was funded by the Department of Energy's Basic Energy Sciences Office. The co-authors of the paper were supported by NASA and British and French agencies.

Impact on the atmosphere

Because of this collaborative effort, it is now understood that around 25 percent of methylperoxy radicals in the troposphere are removed by the fast reaction with the hydroxyl radical, meaning that fewer peroxy radicals undergo other reactions known to lead to methanol. To counterbalance that, the methanol yield from the reaction of hydroxyl radicals with methanol would need to be about 15 percent, but the authors measured yields of 6-9 percent.

The implications of this result on the understanding of tropospheric methanol are significant. The hydroxyl radical and methylperoxy reaction fails to resolve the discrepancy between higher measured yields and lower modeled methanol abundances; in fact, the findings exacerbate the discrepancy. Methanol in remote regions is now underpredicted by around 12 percent in 3.5 global models of the atmosphere.

"This work highlights our incomplete understanding of key tropospheric chemical reactivity. We are missing significant reactions, opening the door to further investigation," Rebecca said.

Cambridge University professor Alexander Archibald, an expert in the field, said the experiments that Rebecca led demonstrate that methanol has additional secrets to reveal.

"While the reaction between methylperoxy radicals and hydroxyl radicals may not be a major source of methanol, models still underestimate the amount of methanol," said Archibald. "The exciting work that Caravan and co-workers have performed closes one chapter in the story, but the book remains unfinished. Further work is required to help complete our understanding of this important compound in the atmosphere."

Sandia named one of America's Best Employers for Diversity

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The honor is based on an independent survey of employees at companies with more than 1,000 employees across all industry sectors.

"As much as I like this only happens if we're all working to understand diversity and inclusion, as well advance the initiatives in our own spaces," said Esther Hernandez, chief diversity officer. "This accomplishment belongs to every Sandian who is championing inclusion and diversity in our day-to-day work."

Diversity and inclusion is a strategic objective for the Labs, she said, which keeps the topic at the forefront of daily operations. With a strong commitment from the laboratory leadership, inclusion and diversity are part of weekly tier meetings, she said.

Esther also pointed to the Labwide focus on understanding unconscious bias and its potential impact on diversity in recruiting, interviewing, hiring, developing talent and many other areas as moving us in the right direction," she said. "Executive decisions such as scanning all job postings for language that might discourage women and minorities from applying are also playing a key role in advancing our efforts."

"Our leadership understands that inclusion and diversity are business imperatives that give Sandia a competitive advantage. Additionally, we all agree that it's just the right thing to do."

Sharon Black, chief diversity officer at the Los Alamos National Laboratory, said that the recognition is “a great honor and is a result of the hard work of our employees.”

In her nomination letter, Black said that the Labs’ employee resource groups (ERGs) are key to the Labs’ success in diversity and inclusion.

"The ERGs are comprised of members from all levels of the organization across all industry sectors, communities, and countries. The ERGs are also working to support the Labs’ mission through diversity and inclusion initiatives."
By Julie Hall  

Photos by Randy Montoya

**'Agile Manifesto' co-author launches clean code training at Sandia**

By Robert C. Martin

Martin, known as Uncle Bob, is co-author of ground-breaking books about creating better software. Martin recently gave nine talks over two days at Sandia.

In his opening talk, "Demanding Technical Excellence and Professionalism," Martin made the case that software developers have tremendous responsibility because of how pervasive and critical software is in our daily lives. He recounted several examples where problems with software had catastrophic consequences.

In the recent Volkswagen emissions scandal, the company developed and installed software in millions of so-called “clean diesel” cars that was designed to cheat U.S. emissions tests. The exhaust control equipment had been programmed to shut off once the cars left regulators’ test beds, releasing pollutants into the atmosphere that exceeded legal limits. Some former employees are now in prison, and Volkswagen has agreed to pay back more than $20 billion to states, dealers, regulators and car owners.

In another example, a software glitch in trading firm Knight Capital’s computers caused it to rapidly buy and sell millions of shares in minutes rather than over what was supposed to be a period of days. The company lost about $440 million in less than an hour.

"When developers write clean code, they’re helping their future selves and co-workers," John said.

**Clean code also reduces the cost of maintenance**

At Sandia, some software teams spend half of their time on maintenance, said manager Manoj Bhardwaj. By applying Martin’s principles, one team, using clean code principles over the past few years, has reduced maintenance costs to less than 10 percent, which translates to savings of millions of dollars over many years just for one team.

"As more and more teams apply these principles and deliver sustainable code, the potential savings Labwide could be in the tens of millions," Manoj said.

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**Software exists to control hardware**

The purpose of software is so the behavior of machines (hardware) can be easily changed, he said. “If your software makes the behavior hard to change, your software thwarts the very reason that machines that govern everything.”

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**Importance of clean code to Sandia**

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Three earn national honors CONTINUED FROM PAGE B

TRAILBLAZER — Olivia Underwood, who oversees the production of long-living, specialized electrical connectors at Sandia Labs, has been selected to receive a 2019 Science Spectrum Trailblazer Award for “actively creating new paths for others in science, research, technology and development,” according to the award citation. Photo by Stephanie Blackwell

This trailblazer inspires African American youth to pursue STEM careers

In 2015, Olivia was one of 312 black women in the United States who earned doctoral degrees in science, technology, engineering or mathematics. Together, they represented a mere 1.1 percent of all such degrees. Now, Olivia leads a team of engineers and is creating pathways for others to follow.

Her motivation in part is to change the picture she has seen throughout her groundbreaking career.

“There are very few minority women in STEM fields,” said Olivia, the first African American to receive a doctoral degree in materials science at The University of Alabama in Huntsville.

Prior to joining Sandia, Olivia voraciously sought out opportunities to work on a vast range of mechanical systems, reporting back to her school which opportunities were best for students in her metallurgical and materials engineering program.

She performed analyses on minivan components for a subsidiary of Honda Motor Co. Ltd. and on military helicopters for a subsidiary of CGI Group at Redstone Arsenal, home to the U.S. Army’s Aviation and Missile Research Development Center. She also worked with three national laboratories, including Sandia, where she continuously serves her community.

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After joining Sandia, Olivia moved from her postdoctoral role to a principal member of technical staff. She began her career in the Advanced Science and Technology Division and has successfully transitioned to support Sandia’s core mission of nuclear deterrence.

Now Olivia oversees the development of specialized components. Her experience in metallurgy gives her team an advantage diagnosing defects in materials, so products work reliably for decades.

Her work has been recognized internationally. In 2017, Olivia was selected as one of the two USA Early Career Scholars to attend the European Microbeam Analysis Society 2017 conference in Konstanz, Germany, where she presented her research on abnormal grain growth in a nickel alloy.

Her focus on professional growth has been matched by a determination to create pipelines of talent for the future. She teaches “What is Materials Science?” — a Sandia-sponsored summer class for middle school and high school students. “I wasn’t exposed to the field of materials science until I went off to college. I want students to be aware of this amazing field early on in life,” she said.

In 2018, she established the Dr. Olivia D. Underwood Scholarship at her alma mater, Bibb County High School, and presented it to a female, African American graduating senior. Through her outreach co-chair role in SWAN, the Sandia Women’s Action Network, she advances the organization’s stated purpose to “engage members of the workforce and the local community to support activities for local youth in math, science and engineering” and “promote opportunities to improve visibility of women in science and act as a force for good in Sandia’s local community.” She is also a member of Delta Sigma Theta Sorority where she continuously serves her community.

Olivia was honored with a Science Spectrum Trailblazer Award, given to “men and women actively creating new paths for others in science, research, technology, and development,” according to the award citation.

She’s going to need to expand her trophy case, as Olivia also will receive the 2019 Frank Crossley Diversity Award from The Minerals, Metals & Materials Society, which will be presented March 13 at the group’s annual meeting in San Antonio, Texas.

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Droves of deals now at SERP

By Stephanie Holinka

The Jewish Community Center of Albuquerque is now operating the Sandia Employee Recreation Program offices. All members of the workforce can get access to SERP discounts from their desktop, by phone or by visiting SERP.

SERP office manager Karen Susztar said SERP has expanded its partnerships to include more than 80 vendors, including 23 fitness facilities, eight ski resorts and the Sandia Peak Tramway. The partnership also includes six sports leagues, however these are only open to employees and eligible dependents.

SANDIA LAB NEWS | February 15, 2019

Mileposts

New Mexico photos by Michelle Fleming
California photos by Randy Wong

MARY LOU GARCIA
February 15, 2019

Recent Retirees

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CA photos by Randy Wong

Mary Lou Garcia 25
Karen Haskell 20
Kathy Pierson 20
Torry Spraggins 17
Caren Holinka 15
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Recent Retirees

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CA photos by Randy Wong

Mary Lou Garcia 25
Karen Haskell 20
Kathy Pierson 20
Torry Spraggins 17
Caren Holinka 15
Bruce Hamilton 15

By Stephanie Holinka

The Jewish Community Center of Albuquerque is now operating the Sandia Employee Recreation Program offices. All members of the workforce can get access to SERP discounts from their desktop, by phone or by visiting SERP.

SERP office manager Karen Susztar said SERP has expanded its partnerships to include more than 80 vendors, including 23 fitness facilities, eight ski resorts and the Sandia Peak Tramway. The partnership also includes six sports leagues, however these are only open to employees and eligible dependents.

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Three Sandia Labs researchers earn national honors in leadership and technology

By Troy Rummler

Three Sandia researchers were honored for their leadership and technical achievements at the Black Engineer of the Year STEM Global Competitiveness Conference this week.

Warren Davis, Quincy Johnson and Olivia Underwood received their awards during the conference in Washington, D.C. The annual meeting recognizes black scientists and engineers and is a program of the national Career Communications Group, which advocates for corporate diversity.

Lab News profiled the trio, their careers and achievements.

This scientist wants to help you see like a computer

“If you saw all the aquariums that fill Warren’s home, you might think he was a pet lover. But you’d be wrong.”

Warren just has a passion for recreating things. “I’ve got a sand bed that does denitrification in a certain layer,” mimicking a natural aquatic ecosystem, Warren said. “I’ve got animals that sift the sand bed so it doesn’t become anoxic. I have things that eat uneaten food particles that get trapped under the rocks.” It’s not a perfect model, he said, but it’s close.

Warren is also adept at recreating natural, mechanical processes to solve problems in engineering. In these cases, he takes natural phenomena — such as air flowing over a surface or a person taking a step — and uses machine learning to explain them mathematically by way of an equation, also called a function.

Machine learning can approximate complex processes much faster than they can be solved numerically, which saves companies time and resources, for example, if the goal is to predict how well a proposed aircraft design would hold up in flight. The savings compound when designers use machine learning to simulate multiple iterations.

“That’s what I do. I try to learn the functions that we care about,” Warren said.

He also has taken a leadership role helping Sandia and its business partners incorporate machine learning into their own research and development programs. On multiple occasions, he said, the addition of machine learning has transformed the way they work, making their research more efficient and agile long after his project with them has ended.

The technique sometimes delivers unexpected solutions.

“When I’m able to take a data set and come up with something people haven’t seen before or some underlying function it is truly an amazing, almost magical feeling,” he said.

Warren’s work earned him a Research Leadership award.

This leader lifts from both ends of Sandia’s supplier partnerships

As a product engineer, Quincy is a master of bringing together the worlds of design and manufacturing. He serves as the liaison for several companies that produce components for Sandia, leading from both sides of these partnerships and by so doing enabling Sandia to deliver on its national security mission.

Quincy entrenches himself into the supply chain to ensure partner companies succeed. He engages in planning, manufacturing, troubleshooting, quality control and documentation to improve and increase production. He has helped companies that have never made components for Sandia become qualified suppliers. He also investigates production issues and observes and evaluates supplier processes to make sure output is consistent.

“When I’m able to take a data set and come up with something people haven’t seen before or some underlying function it is truly an amazing, almost magical feeling.”

— Warren Davis

“Sometimes you need to understand the little nuances in the way one person performs a task,” he said. “You need to make sure that’s documented in the work instructions and written in a way anyone can understand in case that person ever changes.”

For example, something seemingly as minor as the way a worker cleans out equipment could ultimately have an impact on product performance, he said.

Quincy doesn’t spend all his time with suppliers, though.

At Sandia, he provides leadership as the voice of production from the beginning of a product’s development through the end of its life. Quincy supported multiple teams simultaneously as their components went through the transition into production to ensure their designs implemented the proper production standards so they ultimately would be manufacturable. In this role, Quincy took the initiative to guide certain teams that were lacking considerable production experience, effectively filling the void.

Called "an experienced product engineer with unquestioned judgment" by his manager, Tom Pfeifle, Quincy received a Modern-Day Technology Leader award.

Photo by Randy Montoya

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