

TECHNOLOGY TODAY®

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DRUG-
ELUTING
IMPLANTS

ECOFRIENDLY ETHYLENE PRODUCTION

SwRI engineers and scientists develop and validate novel processes to upgrade and refine hydrocarbon products from conventional and alternative sources using our large-scale pilot plants and extensive laboratory facilities. SwRI recently helped a client successfully scale-up a new, lower environmental footprint process for producing a key petrochemical used as a raw material in a wide range of products. According to the client, the new process will reduce CO₂ emissions for ethylene production by over 80% compared to conventional steam cracking and will emit essentially no NOx emissions, another major environmental concern with conventional production. SwRI fabricated, built-up and currently operates the pilot unit.



TECHNOLOGY TODAY®

Executive Director of Communications

Tim Martin, Ph.D.

Editor

Deb Schmid

Assistant Editor

Rob Leibold

Contributors

Joanna Carver

Robert Crowe

Lisa Peña

Maria Stothoff

Tracey Whelan

Design

Jessica Vidal

Photography

Larry Walther

Ian McKinney

Circulation

Stephanie Paredes

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Address correspondence to the Editor,

Communications Department,

Southwest Research Institute,

P.O. Drawer 28510, San Antonio, Texas 78228-0510,

or e-mail dschmid@swri.org.

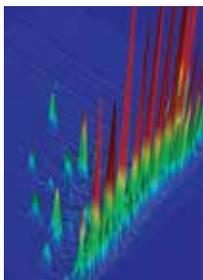
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ABOUT THE INSTITUTE

Southwest Research Institute is a premier independent, nonprofit research and development organization. With nine technical divisions, we offer multidisciplinary services leveraging advanced science and applied technologies. Since 1947, we have provided solutions for some of the world's most challenging scientific and engineering problems.

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D024357

ON THE COVER

SwRI developed Floodlight, a machine learning-based tool, to automate and speed up the signal quality review of gas chromatography time of flight mass spectrometry data, shown here. These chromatograms can be used to identify the chemical components found in consumer products, but the data must be processed to identify and eliminate spurious signals.

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EMPLOYMENT

Southwest Research Institute is an independent, nonprofit, applied research and development organization. The staff of more than 2,700 employees provide client services in the areas of communication systems, modeling and simulation, software development, electronic design, vehicle and engine systems, automotive fuels and lubricants, avionics, geosciences, polymer and materials engineering, mechanical design, chemical analyses, environmental sciences, space science, training systems, industrial engineering, and more.

SwRI is always looking for talented technical staff for its San Antonio facilities and for locations elsewhere in the United States. We welcome your referrals. Check our employment opportunities at swri.jobs.

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Affirmative Action Employer
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Gender Identity/National Origin/Disabled/Veteran
Committed to Diversity in the Workplace**

A yellow rubber duck is positioned on the left side of the image. The background is a deep blue with a heatmap overlay, showing various colors from yellow to red, indicating chemical concentrations. The duck is the central focus, and the heatmap is applied to the entire scene, including the duck and the background.

Everyday
objects like a
child's bath
toy contain
hundreds of
chemicals.

FLOODLIGHT:
EXPOSING COMPREHENSIVE
CHEMICAL CONTENT

By Keith Pickens, Ph.D., and Kristin Favela, Ph.D.

We live in a chemical world.

The water we drink (H_2O), the oxygen we breathe (O_2), the sugar on the table ($C_{12}H_{22}O_{11}$) and everything we touch, taste and use are made up of an array of chemicals. Traditionally, when a chemist analyzes medicine, cosmetics or environmental samples, the question asked is how much X, Y or Z is in the sample.

Recent advances in analytical technology have raised a different and more fundamental question: What is everything in this sample? The answer is frequently an astonishing array of chemicals, often hundreds or even thousands of different chemicals in a single sample. All these compounds — some known, some unidentified, some benign and some harmful — are part of the chemical world we live in.

Trying to understand the chemical cocktail we are exposed to has led to the emerging field of exposomics, which is the science of understanding why one person gets ill from a chemical exposure while another does not. Heredity plays a part, but it is not the complete story. The largest difference is associated with the variation of exposures to the array of chemicals that we just now are starting to recognize in our world.

Today's modern analytical instruments have opened the door to answering the "what is in this sample" question through a procedure known as non-targeted analysis (NTA). The resulting thousands of possible chemicals in each sample represents a daunting challenge to chemists because even the most precise analytical equipment is not perfect. Each potential chemical signal requires a chemist to check whether it is a real indication of a detected chemical or a spurious data artifact. Data artifacts can occur as a result of preparative or investigative procedures and are invalid datapoints. Combing through the data to identify these signal artifacts is a difficult, time-consuming and expensive process that limits the resources available to characterize the unknowns and the assessment of suspect matches in a sample.

DETAIL

Exposomics is the study of the exposome, the measure of exposures an individual has over a lifetime and the subsequent effects on their health. Exposomics seeks to understand how exposures from our environment, diet, lifestyle, etc. interact with our unique characteristics — such as genetics and physiology — and affect our well-being.



Dr. Kristin Favela (background) led a team of chemists including Michelle Zuniga, developing rapid analytical methods to characterize chemicals in consumer products. SwRI has evaluated thousands of samples including millions of signals, data used as inputs for the Floodlight machine learning tool.

D019277_4820

To shine a light on this hidden chemical world, Southwest Research Institute has assembled the Artificial Intelligence for Mass Spectrometry (AIMS) team. AIMS includes chemists, data analysts and computer scientists with expertise in machine learning and mass spectrometry. SwRI has experience

DETAIL

Artificial intelligence (AI) mimics human cognitive processes on computer systems, allowing a machine to become increasingly capable of solving a problem.

developing autonomous solutions for many industries, including automated vehicles, robotics, space science and environmental chemistry. Drawing upon decades of experience, SwRI has developed Floodlight™, a novel software tool that efficiently discovers the vast numbers of chemical components — previously known and unknown —

present in the food, air, drugs and products we are exposed to every day. This cheminformatics machine-learning tool integrates algorithms with analytical chemistry software to provide deep analysis of data from gas chromatography mass spectrometry (GC/MS) and other instruments.

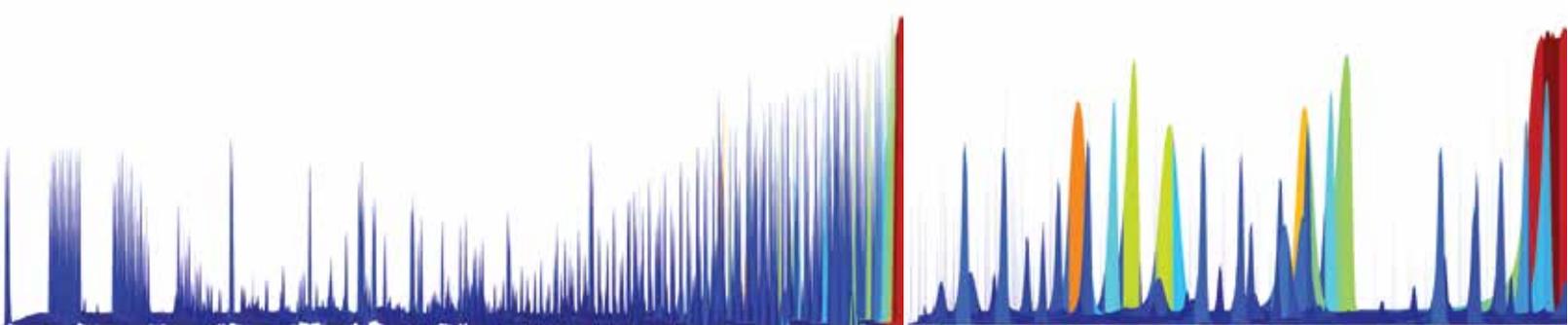
CHEMICAL SPECTRA

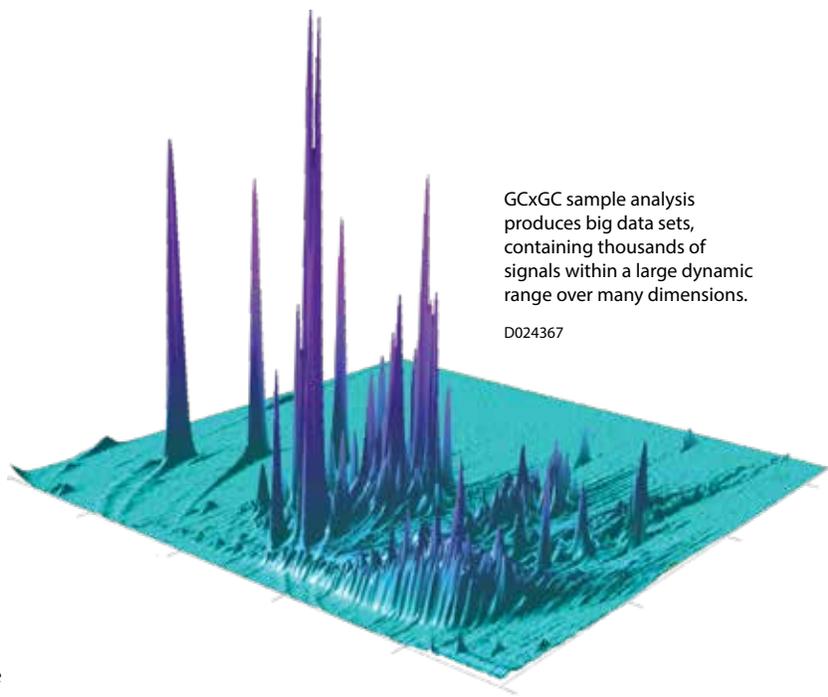
Mass spectrometry measures the mass of different molecules within a sample. Because everything from individual elements to

large biomolecules such as proteins is identifiable by mass, scientists can use mass spectrometry to identify molecules and detect impurities in a sample. The resulting data are shown as a series of graphical peaks and/or colorful spectra that indicate the identity and volume of chemicals present.

Traditionally, targeted analysis (TA) matched identified components against a library of chemicals, providing a list of all chemical matches. Components not associated with library matches were typically ignored. NTA, by contrast, examines every resolved peak without using a pre-defined list of targeted chemicals. NTA methods applied to complex mixtures could identify thousands of unknown compounds that are not yet in databases and have never before been described or studied.

High-resolution chromatographic and mass spectrometric systems are the primary tools of NTA. The chromatograph separates components in a mixture so that, ideally, only one compound at a time is processed by the mass spectrometer, which measures the mass of the intact ionized chemicals and/or their fragmented ions. This chemical fingerprint is a powerful identification tool. The state-of-the-art comprehensive gas chromatography time of flight mass spectrometry (GCxGC-TOF MS) instruments use two integrated GC columns that separate





GCxGC sample analysis produces big data sets, containing thousands of signals within a large dynamic range over many dimensions.

D024367

components by boiling point and polarity or charge. This combination segregates the different data peaks more distinctly and arranges the images in patterns according to compound structure, useful when studying complex samples.

Using GCxGC-TOF MS, SwRI recently conducted an NTA study to characterize the chemicals in 100 consumer products. Initial analyses detected 4,270 unique chemical signatures across the products; 1,602 could be identified tentatively and 199 could be confirmed using chemical standards. Of those signatures that could be seen in the samples, approximately 80% of the chemicals were not listed on consumer product data sheets.¹

This study highlighted not only the ability of NTA to comprehensively investigate the chemical compositions of complex matrices but

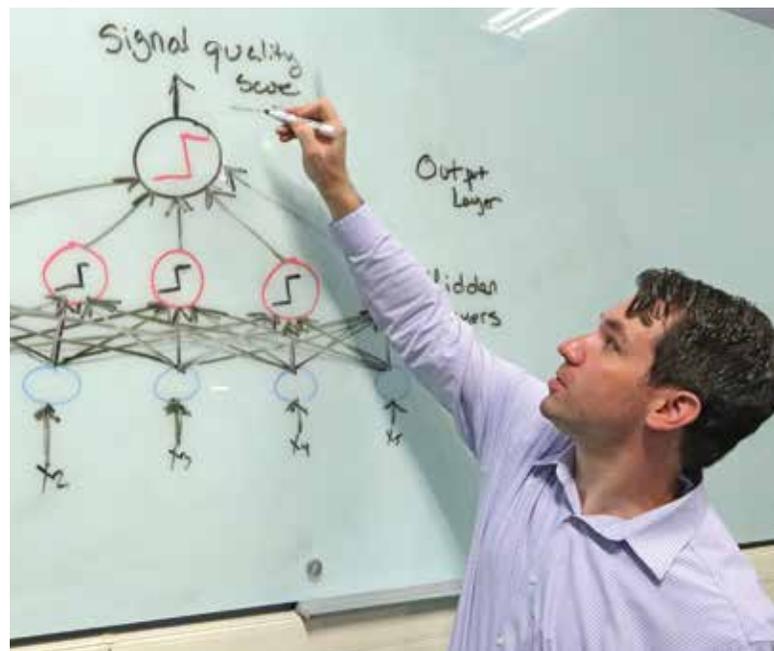
DETAIL

A matrix refers to overall composition of a sample to be analyzed. Matrices can have considerable effects on analyses and the quality of the results.

also how the tremendous amount of data generated limited throughput. GCxGC experiments result in chromatograms, complex data files and peak lists. Chemists must painstakingly analyze the quality of the peaks in the complex data sets because 20% to 50% are artifacts, which creates a major bottleneck in the process. The time needed to remove the low-quality signal artifacts limits the number of full investigations that are feasible. Reducing the manual review time for GCxGC data would allow more samples to be processed using NTA workflows.

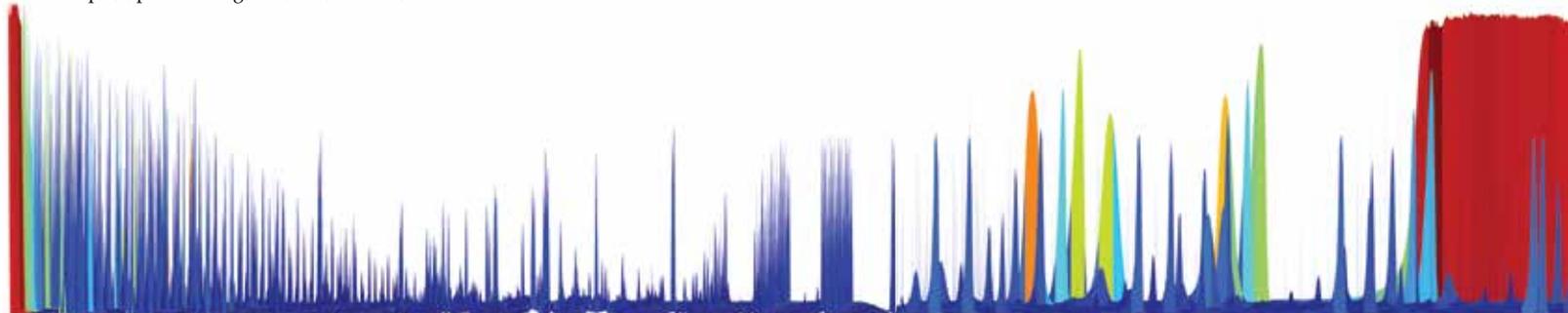
To address this limitation of gas chromatography-based studies, SwRI's Floodlight artificial intelligence, machine-learning-driven tool automates the signal quality review of GCxGC-MS data in a high-throughput manner. The "secret sauce" in this neural-network-based solution is the copious amounts of processed NTA data SwRI had available to teach the tool.

D024329_5554



Dr. Andrew Schaub illustrates how an artificial neural network can predict a single output value or signal quality score using a list of inputs from a given set of features analyzed across multiple layers of processors.

¹ <https://pubs.acs.org/doi/abs/10.1021/acs.est.7b04781>



D024372 / D024373

Michael Hartnett demonstrates how users access Floodlight data through a modern, intuitive web-based interface.



D024329_5672

DATA DEEP DIVE

SwRI enlisted its computer specialists to evaluate artificial intelligence techniques to automate the review process, specifically using machine learning. The team identified deep learning techniques, also known as neural networks, to develop algorithms that would learn from datasets where chemists had already combed through and identified data artifacts. This allowed the algorithms to learn to do this tedious process autonomously.

DETAIL

An algorithm is a set of steps for a computer program to accomplish a task.

Machine learning algorithms automate the processing and interpretation of large amounts of complex data by extracting and learning patterns from raw data using supervised and unsupervised learning. Supervised learning maps an input to an output based on an example input-output pair. It infers a function from labeled training data, in this case data that have spurious signals labeled, so the computer learns which data signatures are relevant as well as those that are not.

The team used an artificial neural network (ANN) as a predictive model, trained using supervised learning, to classify data. Known inputs are fed into the top layer of an ANN, which

passes those values through one or more hidden layers. The supervised learning algorithm analyzes the training data and produces an inferred function, which can be used for mapping new examples. An optimal scenario will allow for the algorithm to correctly determine the class labels for new, unlabeled datasets. This requires the learning algorithm to generalize from the training data in a “reasonable” way. ANNs have a high tolerance for noisy data and excel at classifying patterns.

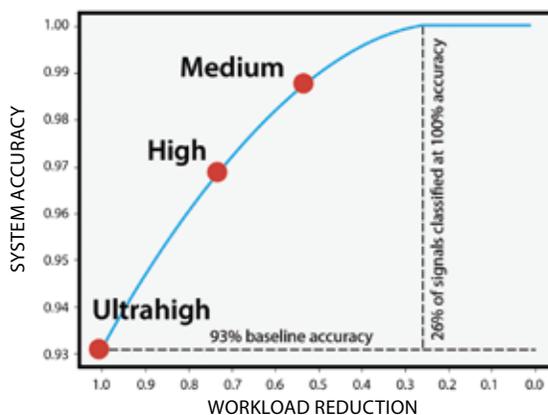
To use deep learning to identify the irrelevant peaks in the spectroscopic data, an image recognition neural network breaks down and examines different features. The algorithm is optimized through trial and error and computational back propagation through the various layers of the neural network, eventually narrowing down its predictions to something that is accurate. The learning process takes the inputs and the desired outputs and updates its internal state accordingly, so the calculated output is as close as possible to the desired output.

FLIPPING ON FLOODLIGHT

To automate the sample chemical profile review process, the AIMS team developed an ANN capable of assessing the signal quality of

Floodlight’s automated review process offers accuracies equivalent to those of a human expert. Even set for ultrahigh throughput, the tool provided accuracies of 93% or higher while reducing human workloads by 100%.

D024361



chemical peaks in the spectroscopic data. The team trained the Floodlight™ algorithm with an initial set of 128,044 curated spectra tagged with chemical metadata.

DETAIL

Metadata is a set of data that gives information about other data.

Chemists manually reviewed and labeled the spectroscopic data peaks from processed GCxGC-TOF samples. Datasets included a significant representation of both poor- and high-quality signals, diverse sample types and a range of ion intensity values within the representative samples. The model evaluated diluted and concentrated samples to assess the ion intensity values within peaks, which can span several orders of magnitude. Tuning the ANN and feature engineering techniques strengthened the model, resulting in improved predictions of signal quality.

Floodlight displays results using an intuitive web interface that can be accessed using most modern web browsers. It is scalable to institution-level with a server-client architecture or can be hosted on a single machine. The peak quality output score provided by the model can be set to determine which peaks are artifacts (low quality), ambiguous (medium quality) or reportable (high quality) because different projects have different demands with regard to the throughput and accuracy desired.

SwRI used threshold benchmarks to assess model performance. For rapid results, an ultrahigh-throughput threshold benchmark classified every evaluated signal as either low quality or high quality while maintaining 93% accuracy and reducing the workload by 100%. This accuracy is comparable to a human expert. A high-throughput threshold resulted in an 80% workload reduction, labeling 20% of peaks as ambiguous. The high-throughput threshold benchmark was 97% accurate at labeling peaks. The medium-throughput threshold benchmark labeled 60% of the peaks with 99% accuracy and left the remaining 40% peaks for manual review. The medium-throughput threshold

mimicked requirements typically seen for forensics or other applications requiring a low rate of misclassifications. Floodlight supports manual relabeling of peaks, which provides the machine learning algorithm with continual feedback, improving performance across diverse sample matrices over time. The ANN, with frequent input from the subject matter experts, continues to evolve and improve.

CONCLUSION

Floodlight — an artificial intelligence machine learning-based tool that puts big data to work, screening the prodigious data collected by today's analytical chemistry instruments — is available for license. It automates GCxGC-TOF sample workflows to support deep analysis of large data sets. Using this high-throughput screening method, analytical chemists spend less time on spectral quality review while maintaining accuracies comparable to human experts. This frees chemists to focus on the most important tasks at hand: characterizing unknown compounds and assessing suspect screening matches in a given sample. Furthermore, Floodlight can potentially be adapted for other analytical chemistry techniques, such as liquid chromatography. The AIMS team is currently developing chemical data correlation and visualization tools, to shine a more powerful light on the chemicals that we interact with in our daily lives.

Questions about this article? Contact Pickens at keith.pickens@swri.org or 210.522.3910 or Favela at kristin.favela@swri.org or 210.522.4209.

SwRI's multidisciplinary Artificial Intelligence for Mass Spectrometry (AIMS) team:



Kristin Favela, Ph.D.	Jake Janssen
Austin Feydt	Keith Pickens, Ph.D.
John Gomez	Andrew Schaub, Ph.D.
Chris Gourley	Heath Spidle
Michael Hartnett	Adam Van Horn
Ken Holladay, Ph.D.	David Vickers, P.E.

ABOUT THE AUTHORS

Principal Scientist **Dr. Kristin Favela** leads efforts to comprehensively identify the chemical composition of complex samples in SwRI's Chemistry and Chemical Engineering Division. She is an expert in mass spectrometry who has developed and validated numerous methods now routinely used in industry. Institute Scientist **Dr. Keith Pickens** specializes in mixed software/hardware development in the Space Science and Engineering Division. His diverse interests include Jovian radiation effects, planetary protection, supercomputer modeling techniques to evaluate spaceflight hardware and now software tools for chemical analyses.



A STABILIZING FORCE

FOR MORE THAN 60 YEARS

SwRI models propellants to mitigate
the motion of sloshing fuel

by Grant Musgrove



Fundamental slosh experiments generated the data and know-how that allow today's engineers to accurately model the dynamics of liquid fuels to ensure the safe operation of tomorrow's launch vehicles and spinning spacecraft.

D014235

For 30 years, NASA flew a fleet of five space shuttles on 135 missions. From 1981–2011, these partially reusable low Earth orbital spacecraft systems launched from the Kennedy Space Center (KSC) in Florida. Prior to launch, each shuttle was strapped to two solid rocket boosters and an orange fuel tank towering over the boosters and the shuttle itself on the launchpad. This massive fuel tank housed the cryogenic fuel and oxidizer the shuttle engines used during launch. All launch vehicles, including the shuttle, require a tremendous amount of fuel to break free of gravity and enter Earth orbit. As payload mass increases, more fuel is required to launch. This presents a cyclic dilemma. The more fuel needed to lift a heavier payload, the more fuel needed to compensate for the fuel's added mass.

Rockets are the only vehicles where the fuel tank dwarfs the payload itself. The fuel, also called propellant, usually makes up more than 80% of the total launch vehicle mass. With so much of the mass dictated by a liquid, it is easy to imagine that any movement of the propellant can have drastic effects on vehicle trajectory. Inside the fuel tank, propellant can slosh back and forth much like a cup of coffee as you drive down the road. When most of a vehicle's mass is subject to this sloshing, the guidance, navigation and control (GNC) rocket systems must accommodate these effects while maintaining vehicle trajectory.

In the first few decades of the space program, Southwest Research Institute established itself as a world leader in the experimental investigation and analysis of propellant dynamics effects in spacecraft tanks. The Institute had its first program in this area in the 1950s before the National Aeronautics and Space Administration (NASA) was even established. This project studied the motion of liquid fuel when rocket thrust terminated. Since then, hundreds of millions of dollars in research and development activities have continued, with hundreds of programs applied to dozens of individual spacecraft and rockets. The research addressed two related but distinct propellant dynamics problems associated with launch vehicles blasting off from Earth's surface and spinning spacecraft in orbit or traveling through space. The Institute continues its strong program in propellant dynamics to support the emerging commercial space industry as well as new government initiatives.

SLOSH AND SPIN TESTING

Using scale models of tanks and novel spin test facilities, SwRI played a critical role running experiments to create some of the copious amounts of data initially needed to develop

DETAIL

Cryogenic fuels are typically liquefied gases stored at extremely low temperatures to maintain a liquid state. Space applications require both fuel and oxidizer propellants because the oxygen needed for combustion of ordinary fuels is virtually nonexistent in the vacuum of space. Liquid fuels combusted with oxygen offer high propulsion performance at relatively low cost compared to other fuel options.



D015387_8531

Fluid spin-up in large spacecraft fuel tanks can significantly affect vehicle stability. SwRI evaluated the DAWN spacecraft's fuel tank to measure transient effects using a surrogate fluid to simulate the actual propellant. The test results enhanced the launch vehicle stability control system and contributed to slosh modeling efforts.

simple models for the wide range of tank designs under investigation. Early in the space program, slosh motion had to be predictable without the benefit of computer simulations.

Engineers then developed models using a mechanical system — approximated as either a swinging pendulum or an oscillating mass-spring system — to represent the liquid sloshing motion. Compensating for differences in tank shape, internal features and fill levels required extensive test data to calibrate the models. Guidance, navigation and control (GNC) specialists still use these simple models today for system development for quick turnaround vehicle trajectory calculations.

In addition to fuel sloshing back-and-forth in tanks, a vehicle propellant system presents additional challenges and concerns, such as tank pressurization, propellant distribution and “pogo.” Pogo is described as the self-excited longitudinal oscillations in space launch vehicles — so named because the phenomenon vibrates the rocket up and down in a manner similar to bouncing on a pogo stick. While pogo events are usually short-lived, they can still damage the payload or the vehicle depending on acceleration levels achieved during the unstable interaction. For example, pogo was responsible for the center engine cutoff during liftoff of Apollo 13.

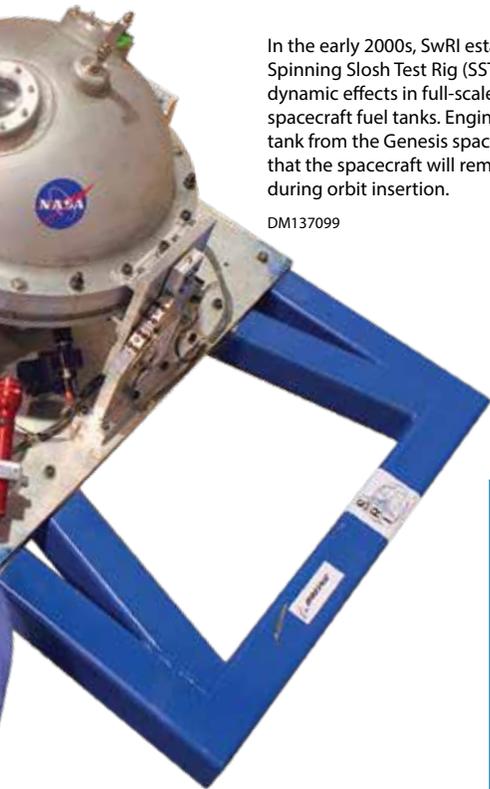


Propellant distribution in the storage tank is critical to operations. The tank sump feeds the engine fuel during operations. At liftoff, gravity keeps the propellant in contact with the sump. For space maneuvers and landing, though, zero gravity allows the liquid in a fuel tank to form a blob in a random location, requiring precautions be made to ensure the fuel pump can draw fuel.

Engineers continue to develop reduced order models (ROMs) — simplifications of high-fidelity, complex models — to understand propellant behavior and its effects in GNC simulations to quickly study a system’s dominant effects using minimal computational resources. More recently, SwRI has been applying modern analysis methods to this old problem as well as other propellant system considerations.

SwRI evaluates the effects of fluid motion in spacecraft propellant tanks, such as this full-scale model of a tank with a damping internal diaphragm used on the New Horizons and Deep Impact spacecraft. Our engineers design test tanks to match closely the internal design features of spacecraft tanks, while providing access for sensors and allowing visual observations.

D015818_8722



In the early 2000s, SwRI established a Spinning Slosh Test Rig (SSTR) to test fluid dynamic effects in full-scale models of spacecraft fuel tanks. Engineers tested this tank from the Genesis spacecraft to ensure that the spacecraft will remain stable during orbit insertion.

DM137099

DETAIL

Computational fluid dynamics is the science of numerically solving fluid motion equations to produce quantitative predictions and/or analyses of fluid flow phenomena.

SLOSH MODELING

Using computational fluid dynamics (CFD), engineers can better understand the effects that specific flight dynamics and tank configurations have on liquid motion. CFD predicts parameters, requiring less slosh testing to verify that new tank designs and internal structures suppress liquid sloshing. The result is accelerated advances in tank design at reduced cost. For example, CFD simulations can estimate the model inputs, such as frequency and damping ratio, needed for GNC simulations. CFD simulates the performance of propellant sloshing mitigation approaches and has become indispensable for evaluating new tank designs while minimizing costly testing.

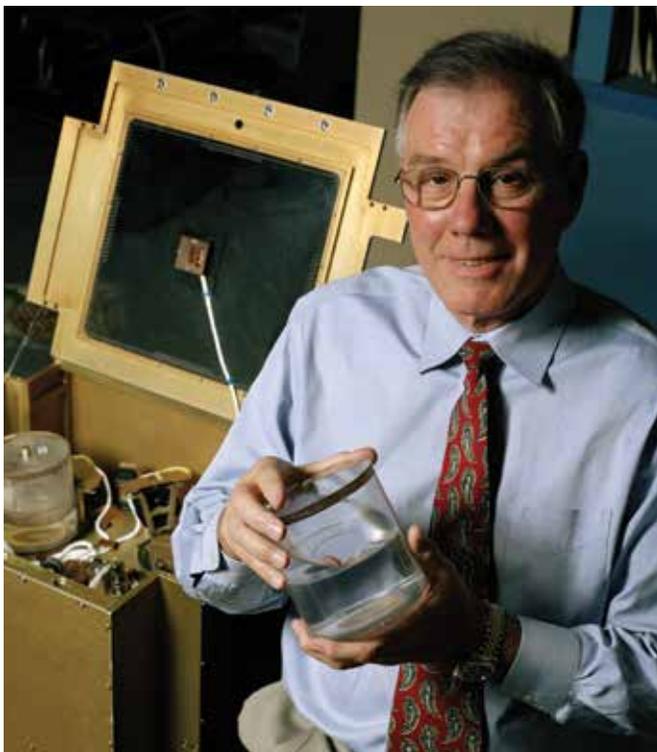
These new modeling methods are also useful for estimating the distribution of propellant in the tanks. Today's launch vehicles no longer use expendable single-use tanks. Instead, these very large reusable tanks now return to Earth, landing with very small amounts of propellant inside. In this situation, as well as air-launched vehicles, the vehicle experiences a near zero-g freefall state for a period of time, allowing the propellant to move freely throughout the tank. This means there is no guarantee that the liquid propellant will be present at the tank sump when the engines need to be started. CFD simulations can model the propellant movement in the tank during the vehicle freefall to help the vehicle designers provide for the propellant to be at the bottom of the tank when the engines need to start. Otherwise, the engines will ingest vapor instead of liquid fuel, which could cause a catastrophic landing.

SOFTWARE SOLUTIONS

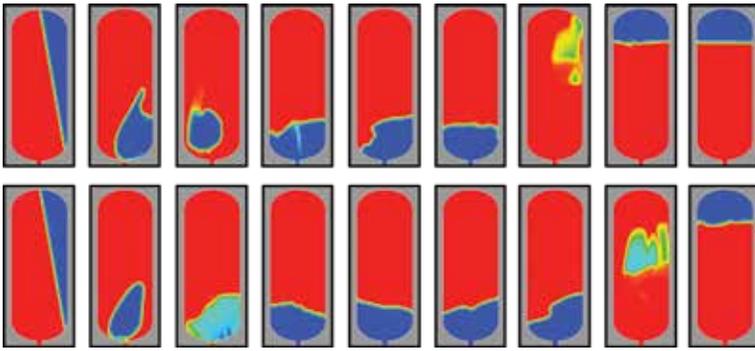
Engineers are also applying other software modeling approaches to propellant system development. For instance, boil-off gas in cryogenic tanks occurs when heat transfer raises the temperature of the liquid, allowing small amounts of it to return to its vapor phase. This evaporation raises the pressure inside the cryogenic tank during storage and transportation and must be vented overboard to maintain acceptable temperatures and pressures. In addition, a pressurant gas is typically added to the tanks during engine operation to keep pressures from dropping too low. Managing this complex thermodynamic and heat transfer problem often requires a separate pressurization system. SwRI uses software to model this thermodynamic system throughout the vehicle flight plan, assessing how various trajectories with different flight times and Sun exposure could contribute to boil-off and pressurant gas requirements. The large number of conditions evaluated improve confidence in the design and reduce the number of needlessly conservative assumptions.

Additionally, a tank's feedline, the critical path from the tank to the engine, can affect pump operations. Feedline pipes are designed to be as compact as possible to save weight and, as such, include twists and turns between the tank and the engines that can contribute to pressure loss and flow distribution problems. CFD modeling of these systems is critical because there is no available test data to understand how closely coupled twists and turns in the feedline

Retiree Dr. Franklin Dodge holds one of the tanks used in SwRI's liquid motion experiment conducted onboard the space shuttle in 1997. The scale-model experiment led to the development of a full-scale spinning slosh test facility.



DE137685



SwRI uses CFD simulations to analyze fluid motions in an air-launched rocket. The images illustrate how the liquid (red) and the vapor (blue) move around the tank in respect to the outlet.

affect overall system performance. The feedline is connected to both the vehicle structure and the engines, creating a feedback loop between structural vibrations and engine thrust fluctuations, also called pogo. With simulation capabilities, a wide range of operational scenarios can be investigated quickly as the vehicle development progresses to avoid or mitigate pogo. Engineers can also use CFD to evaluate and adjust mitigation scenarios based on their performance over a wide range of operating conditions.

TOMORROW'S LAUNCH TECHNOLOGY

Using today's modern simulation capabilities, tomorrow's launch vehicles can be designed in less time and at lower cost than 40 years ago. Much more analysis can be done during design, and many more operational scenarios can be investigated. Modern modeling reduces risks by asking "what if?" and assessing the likelihood and impact of a particular scenario. The detailed models make higher confidence predictions, which lead to less conservative assumptions and more realistic requirements. Forty years ago, for example, only a handful of cases could be

modeled with limited assumptions. The worst case was often used to direct vehicle requirements with additional safety margins. Now, detailed models can identify arcane worst-case scenarios and evaluate the likelihood and impact on vehicle design. At SwRI, we realize and emphasize that using these simulations for launch vehicle development is made possible by the decades of experience and test data compiled in the past. These data and the expertise that goes with them are critical to ensuring the modeling work is accurate.

Most of the earliest generation of propellant dynamics engineers have retired, and many next-generation launch vehicles are being developed by the emerging commercial space industry. Without transitioning this information to a new generation of engineers, decades of experience learned throughout the space program would be lost. SwRI is committed to passing this knowledge along through training and technology transfer.

Questions about this article? Contact Musgrove at grant.musgrove@swri.org or 210.522.6517.

ABOUT THE AUTHOR
Grant Musgrove manages the Propulsion and Energy Machinery Section in SwRI's Mechanical Engineering Division. He specializes in thermal-fluid dynamics, heat transfer and propulsion systems, particularly using experimental and computational methods in rotating machinery applications.

DM24327_6813



This IS Rocket Science!

Learn about launch vehicle liquid propellant system design and analysis

SwRI is offering a launch vehicle propulsion short course for participants with an engineering background. Attendees will develop an understanding of the propellant system needed to support the design, test and operation of launch vehicles, including in-depth understanding of liquid propellant dynamics and how they affect launch vehicle design. The course covers liquid propellant slosh concepts and how to use analytical, computational and experimental methods to characterize slosh parameters for guidance, navigation and control simulations.

- Propellant Tanks • Pressurization Systems
- Slosh Baffling • Feedline Dynamics
- Start Slump • Water Hammer • Pogo
- Propellant Modeling • Cryogenics
- Computational Fluid Dynamics
- Phase Change • Thermodynamics
- Boil-Off Prevention

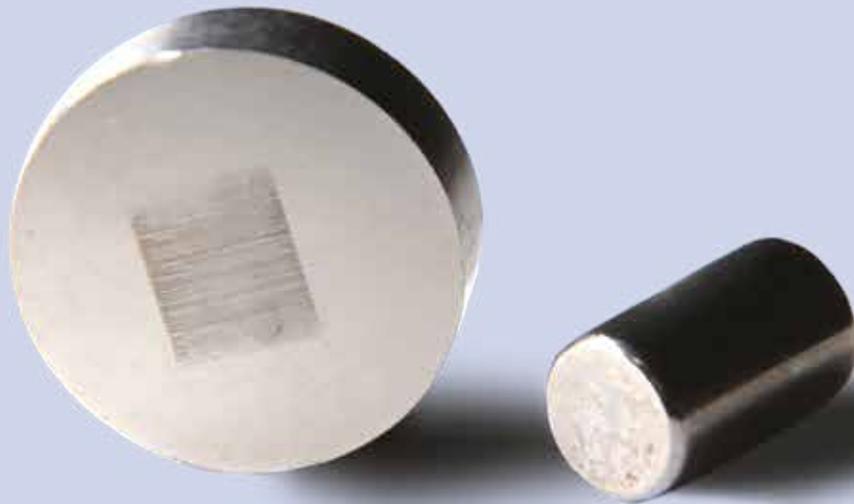
October 19–21, 2020

Due to the global COVID-19 pandemic, the course will be offered as a virtual training class.

To register, contact Grant Musgrove at grant.musgrove@swri.org or call +1-210-522-6517.



IMPROVING MILITARY FUEL TESTS



A new bench test uses small test specimens to characterize the lubricating properties of diesel fuels used in military vehicles.

DM24321_5265

Engineers in SwRI's Fuels and Lubricants Division are working to improve fuel lubricity laboratory bench tests to accelerate fuel qualification and lower costs. Standard ASTM lubricity tests for diesel and aviation fuels had numerous issues and often gave vague, inconclusive results. The SwRI team is developing new laboratory bench methods that could save the industry significant time and money qualifying lubricating fuels.

"Both ASTM D6079 and D5001 were developed to address advances in fuel system hardware," said Lead Engineer Gregory Hansen. "The increased capability and complexity of the systems required fuels with increased lubricating characteristics. Some of these lubricity requirements are satisfied with additives while others required more robust hardware."

The tests are commonly required for fuels used by military vehicles and aircraft. Both tests use small specimens to test the fuels on a laboratory bench rig. These screening tests are quite good at detecting large changes in fuel composition, however, D6079 is particularly insensitive to small amounts of additive.

"At times, we could run one of these tests and the results would show no difference between a fuel with no additives and fuels with the maximum amount of additives," Hansen said. "But there was no bench-scale alternative. Until now."

Laboratory tests require a fuel sample of about 50 mL and last one to two hours. In contrast, more accurate full-scale fuel pump tests involve running fuel through an engine rig for thousands of hours, usually at least 40 continuous days. This requires roughly 1,000 gallons of fuel and staff supervision around the clock.

"A full-scale pump test is by nature more expensive and time-consuming," Hansen said. "They replicate the actual engine operation with complete fuel system hardware and can take months to complete a single test."

SwRI has developed a new laboratory instrument that more accurately assesses the lubricity of diesel fuels, contributing to a more timely, cost-effective qualification process.

DM24321_5170

Beginning in 2016, Hansen began tweaking the standard laboratory tests, altering the conditions and the specimen geometries to see if he could improve correlations with the full-scale pump tests and improve confidence in laboratory efforts.

"We had some pretty encouraging results almost right away," he said. "Full-scale pump testing will not disappear as hardware, fuels and additives continue to evolve. But lowering the amount of pump testing required can accelerate project timelines and save money."

In 2018, Hansen began collaborating with the military on a custom bench instrument for the new, modified fuel tests. That device is now completed, and Hansen and his team are gathering data and preparing for the long process of introducing these new tests to the industry.

"These tests are very much new and improved," he said. "Because the tests are initially focused on diesel-powered ground vehicles for the military, the process would be to write an official military standard that would be adopted into a performance specification for certain types of fuel purchases. Once the industry has experience supporting the new testing methods, the standard would be introduced as a new ASTM method for the commercial market."



SwRI TACKLES MASK SHORTAGES

SwRI has taken techniques and technology developed to support clean air initiatives and applied them to address mask shortages during the COVID-19 pandemic. Our engineers and scientists have pioneered measuring and characterizing fine, ultrafine and nanoparticle mass and number in vehicle emissions. This expertise put us in a unique position to help characterize the filtration performance and flow of emergent supplies of face masks and N95 and KN95 respirators acquired during the COVID-19 crisis. Turns out, the airborne viral particles are roughly the same size as the particles our emissions specialists measure in vehicle exhaust. The team is doing this work for companies and health organizations.

SwRI's state-of-the-art particle calibration laboratory includes instruments to measure particle number, surface area, mass, size and morphology. The Institute-developed universal particle generator creates a variety of particles for research and instrument calibration, allowing us to determine what level of protection new supplies of facial masks could provide and if they meet standards.

DM24333_5811



N95 masks
Filter 95% particles
Good breathability

Flow rate = breathability
N95 have very high flow rate

SwRI generates particles
Specific size distribution
for testing and calibration

SwRI counts particles
Upstream & downstream
of filter material

American Association for Laboratory Accreditation
SwRI's laboratory is the only facility fully accredited to ISO/IEC 17025

SwRI particle size capabilities
Measure 10-10,000 nanometers (nm)
COVID-19 Virus: 70-100 nm

SwRI certified mask decontamination technique
Allowing safe reuse of N95 masks

SwRI certified filtration performance
Identified media combinations with 99% filtration efficiency

SwRI testing revealed
8 out of 11 KN95 respirator samples were counterfeit and failed to meet the U.S. standards

DM24333_6022





DRUG-ELUTING IMPLANTS

Improving convenience,
compliance & costs

By Sandra Drabik, Ph.D.

Nonadherence to prescribed treatment is thought to cause at least 100,000 preventable deaths and \$100 billion in preventable medical costs every year.

Medication noncompliance is an extremely common public health issue, affecting as many as 40% to 50% of patients prescribed medications to manage chronic conditions such as diabetes or hypertension. This nonadherence to prescribed treatment is thought to cause at least 100,000 preventable deaths and \$100 billion in preventable medical costs every year. Barriers to medical adherence range from lack of motivation to complexity of treatments to unpleasant side effects and inconvenience.

The medical community has been investigating the controlled release of pharmaceuticals for decades to address some of these issues. Using medicinal chemistry and proper formulation, chemists can control the release of orally administered drugs, creating more feasible once-a-day or once-a-week dosing options. However, all oral dosage forms — tablets, capsules and liquids — still experience cyclic high and low blood concentrations depending on the time from the last dose, where highs can result in side effects and lows impair clinical results. These swings are particularly problematic over longer treatment durations.

Some orally delivered drugs, for example, degraded by the harsh acidic environment in the stomach, can be coated to protect the active ingredients until they enter the lower digestive system, where the coatings then degrade in a neutral pH environment and release the drugs where they can be safely absorbed. Another common issue related to oral drug delivery is the need to maintain drug-blood concentrations in the therapeutic window, a narrow “sweet spot” of efficacy and safety, requiring several doses per day.

One solution that can address all these problems is a drug-eluting implant that can provide months to years of sustained, nonfluctuating release. Over the past 20 years, Southwest Research Institute has been developing subdermal drug-eluting implants for a variety of applications. SwRI has developed a flexible platform produced by hot melt extrusion where the drug or active ingredient is mixed with a binder and then extruded in a rod-like format that can be inserted just below the skin. Drug-eluting implants offer efficient, effective controlled release of pharmaceuticals with compliance assured.

IMPLANT IMPACT

In addition to offering several advantages over more conventional treatments, implantable devices allow site-specific drug administration, delivering a drug where it is most needed. For example, implants to treat brain tumors or prostate cancer *in situ* could significantly lower doses of a drug necessary while minimizing potential side effects.

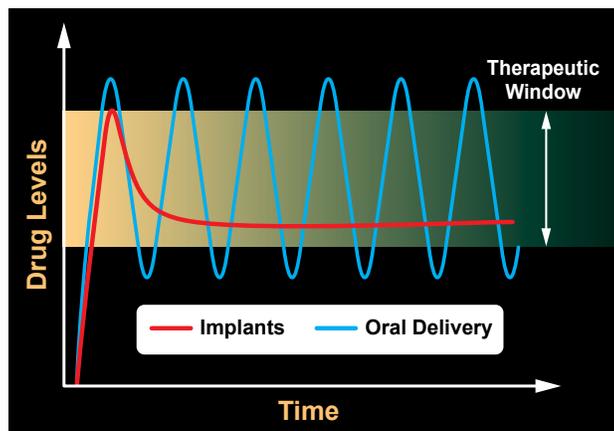
Implantable devices also allow sustained release of drugs, avoiding the peaks and valleys in drug levels. An implant typically releases an initial burst of the drug and thereafter maintains blood levels of the drug at constant concentrations. They maintain the effective therapeutic range while minimizing side effects that are associated with transient high levels. In addition, implants typically require less of the drug to maintain a therapeutic dose because the compound is released directly into the tissues and is absorbed into the bloodstream without having to pass through the digestive system, potentially reducing undesirable side effects.

Drug eluting implants also offer the advantage of improved bioavailability. In pharmacology, bioavailability is the fraction of an administered drug that is absorbed and reaches the circulatory system. For example, when a medication is delivered intravenously, it has 100% bioavailability. Poor water solubility affects up to 40% of potentially valuable drug candidates. Drugs administered through implants are better absorbed, requiring lower dosages and improving bioavailability.

But perhaps the most important advantage of drug-eluting implants is patient compliance. An implant releases a continuous level of medication, overcoming intentional and unintentional nonadherence, both of which lead to substantial advancement of disease, increased healthcare costs and higher risk of death.

Trained medical staff place the flexible, rod-like devices beneath the skin using a trocar surgical instrument in a simple outpatient procedure under a local anesthetic. Multiple rods may be implanted into an individual patient’s upper arm or alternative location depending on the dose required.

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An oral delivery drug will typically be dissolved in a few minutes but may take a few hours to reach therapeutic levels in the bloodstream. After the peak concentration is reached, the drug will slowly get broken down by metabolic processes, and blood levels will fall out of the therapeutic window. Properly formulated subdermal implants can offer sustained, controlled, nonfluctuating release within the therapeutic window.

DETAIL

A trocar is a cannular medical instrument that functions as a portal for the subsequent placement of other devices, such as surgical instruments or drug implants.



SwRI uses a hot melt process in a CGMP-compliant cleanroom to produce drug-eluting platforms. The active ingredient and a polymer are combined and extruded in a thin tube that is cut into matchstick-sized subdermal implants. These rods can be inserted just below the skin for convenient, consistent dosing over extended periods of time.

Implants can be resorbable and dissolve over time in tissue, or can be removed, with advantages and disadvantages to both methods. For example, removable implants can be retrieved if an adverse reaction occurs, while resorbable implants do not require a second procedure after treatment.

DETAIL

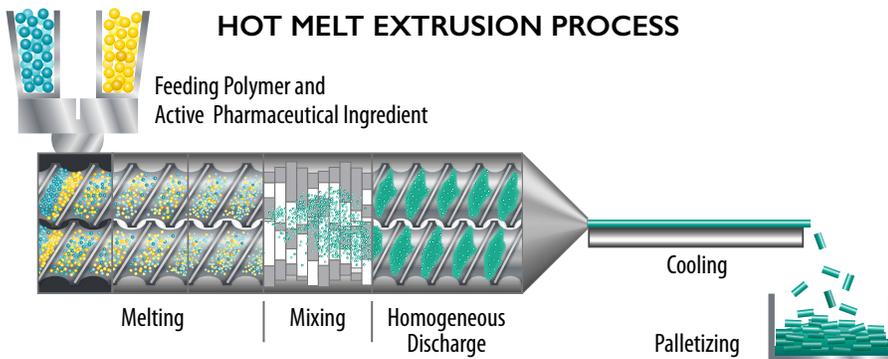
A gravimetric feeder is a self-calibrating system that determines the amount of material to be dosed by weight.

SwRI produces implants in a Current Good Manufacturing Practice (CGMP)-compliant ISO 7, class 10,000 clean room. Gravimetric feeders supply the active ingredient or drug and a binder, typically a polymer, into the extruder. The resulting strand is then collected on a conveyor belt while cooling. The strands are cut to the appropriate length, washed, weighed, packaged and sterilized. After quality control inspections and delivery to our clients and other research collaborators, they are used in Food and Drug Administration clinical trials.

APPLICATIONS

Existing and developing therapeutic areas for drug-eluting implants include opioid addiction, Parkinson’s disease, thyroid insufficiency, birth control, antivirals and malaria as well as veterinary applications. SwRI has worked with a variety of clients to address public health problems to overcome treatment-specific challenges using drug-eluting implants. For example, in 2018, over 46,000 Americans died of opioid-related overdoses. Patients with opioid dependence find that medication-assisted therapies — such as daily methadone or buprenorphine — reduce withdrawal symptoms while controlling cravings. SwRI has helped develop an FDA-approved buprenorphine-releasing implant that can provide up to six months of a constant level of drug therapy. This alleviates the need for daily dosing or visits to drug treatment facilities, which greatly improves compliance and quality of life during recovery.

SwRI is also researching implantable drug delivery formulations for chemoprophylactics to prevent malaria. Malaria kills



Hot melt extrusion processes heat and mix a drug or active ingredient with a binder, which is then extruded in a long strand, cooled and cut into a rod-like format that can be inserted just below the skin.

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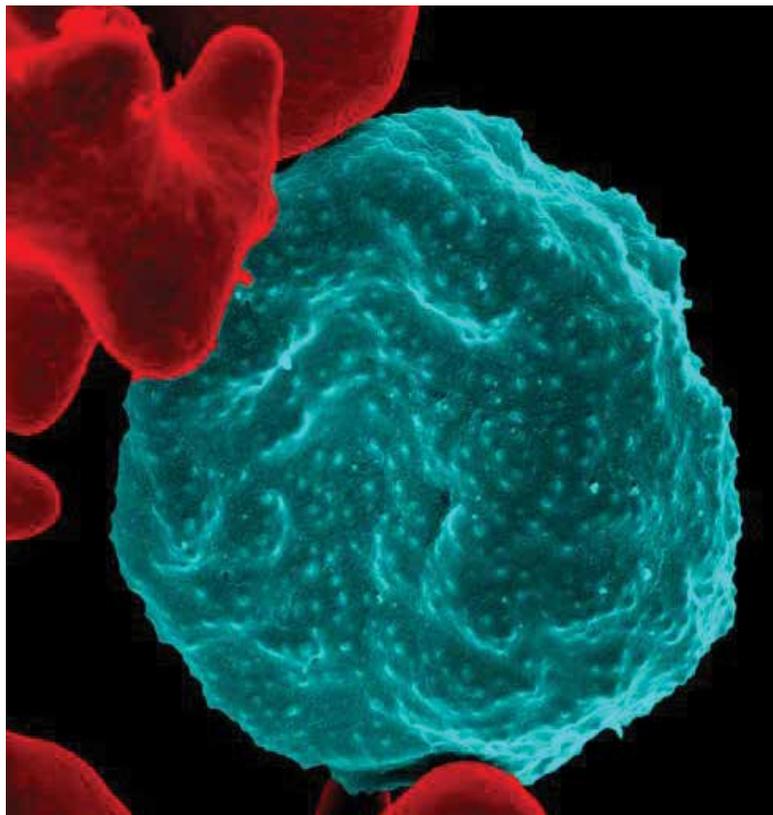
over 400,000 people per year. United States armed service personnel are often deployed to malaria-endemic regions and are at risk for contracting the deadly disease. Currently, the prevention of malaria involves the use of a variety of drugs taken before, during and after travel, with many significant side effects including nausea, vomiting, abdominal pain, headache, insomnia, dizziness, loss of balance and ringing in the ears. As a result, compliance is an issue, with many either skipping doses or stopping the medication too early. Successful military operations in malaria-endemic regions often require daily supervised administration to ensure service members take their medications. If these drugs could be delivered by an implant, compliance would be assured. Another scenario where implants would be advantageous is when special forces are deployed under conditions that make it difficult if not impossible to administer a daily supply of the medications over long periods in austere conditions. Having the drug automatically delivered over extended periods of time is of great interest to the U.S. Department of Defense.

In collaboration with the Experimental Therapeutics Branch at the Walter Reed Army Institute of Research, SwRI produced drug-eluting implants to prevent malaria infection. Our military collaborators implanted matchstick-sized rods containing a widely used malaria protection drug in mice and monitored blood levels of the compound over eight weeks. The drug was released in a consistent and steady manner. By comparison, the half-life of an oral dose of the same medication is approximately two to three days in mice. To demonstrate that these blood levels protected the mice from infection, they were exposed to malaria 12 weeks after implant insertion and were compared to a control group without the implant. The unprotected mice all acquired malaria, while the treated mice all avoided infection.

The best applications for the drug-eluting implants are lower-dosage, longer-term treatments with compounds that are not too water-soluble. Continuous, subcutaneous administration of therapies offers many advantages, including increased compliance, optimum therapeutic levels to curb side effects and a convenient treatment regime that offers a better quality of life for patients. SwRI continues to help collaborators and clients formulate drug-eluting platforms that can be implanted and essentially forgotten, while ensuring effortless, efficient and effective treatment for a range of chronic conditions or continuous protection against disease.

Questions about this article? Contact Drabik at sandra.drabik@swri.org or 210.522.6419.

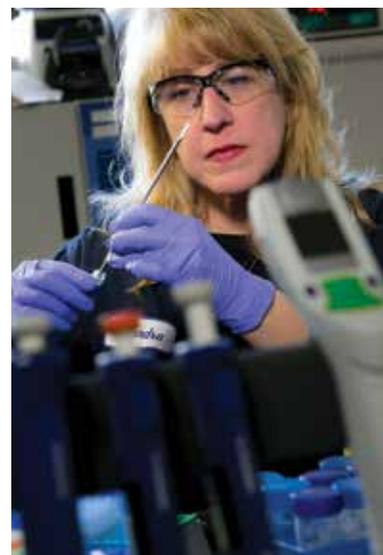
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SwRI is developing and testing antimalarial implants to prevent the deadly mosquito-borne parasitic disease. This colorized scanning electron micrograph shows the rough surface of a blood cell infected with the parasite in blue in contrast to uninfected cells with a smooth red surface.

ABOUT THE AUTHOR

Dr. Sandra Drabik manages the controlled substances and Current Good Manufacturing Practices programs in the Chemistry and Chemical Engineering Division. In addition, Drabik oversees drug development projects, researching capsules, tamper-resistant formulations, injectable and implantable drug products, and components for preclinical trials through phased clinical trials to commercial production.



D022898_1560

SMALL SATELLITE MISSIONS MOVE FORWARD



“While spacecraft are constructed out of aluminum and exotic metals, they are initially made of requirements documents.”

PUNCH MISSION ACHIEVES MILESTONE

The Polarimeter to UNify the Corona and Heliosphere (PUNCH) mission achieved an important milestone, passing NASA’s critical System Requirements Review/Mission Definition Review (SRR/MDR). SwRI is leading PUNCH, a NASA Small Explorer (SMEX) mission that will integrate understanding of the Sun’s corona, the outer atmosphere visible during eclipses, with the tenuous “solar wind” filling the solar system.

“For over 50 years, we’ve studied the solar corona by remote imaging and the solar wind by direct sampling,” said PUNCH Principal Investigator Dr. Craig DeForest of SwRI’s Space Science and Engineering Division. “PUNCH will bridge that gap by imaging the solar wind itself as it leaves the outermost reaches of the Sun’s corona.”

The solar wind, a supersonic stream of charged particles emitted by the Sun, fills the heliosphere, the bubble-like region of space encompassing our solar system. Its boundary, where the interstellar medium and solar wind pressures balance, ends the sphere of the Sun’s influence.

PUNCH is a constellation of four separate suitcase-sized satellites scheduled to launch in 2023 into a polar orbit formation. One satellite carries a coronagraph, the Narrow Field Imager, that images the Sun’s corona continuously. The other three each carry SwRI-developed wide-angle cameras, Wide Field Imagers (WFI), optimized to image the solar wind. These four instruments work together to form a single field of view spanning 90 degrees of the sky, centered on the Sun.

“Preparing for the SRR/MDR review was an unexpected challenge,” DeForest said. “Team members had been working at home, yet they met the challenge and presented their design in written and oral presentations culminating in the positive decision from our review board.”

SRR/MDR is a major milestone of mission development. It checks the flow of engineering and mission definition as activities segue into the design phase.

“I’m very proud of this team for what they’ve accomplished during less than ideal collaboration conditions,” said DeForest. “While spacecraft are constructed out of aluminum and exotic metals, they are initially made of requirements documents.”

TRACERS HELIOPHYSICS MISSION ENTERS PHASE B

NASA has approved the Tandem Reconnection and Cusp Electrodynamic Reconnaissance Satellites (TRACERS) mission to proceed to Phase B, which marks the transition from concept study to preliminary flight design. The satellites, led by the University of Iowa (UI) and managed by SwRI, are set to launch in late 2023.

In addition to providing mission management and science services to UI, SwRI is developing the Analyzer for Cusp Ions (ACI) instrument, which will study how the magnetic fields of the Sun and the Earth interact through novel measurements in the polar cusps. Under a subcontract to Millennium Space Systems, SwRI is also managing the development of its two satellite bus platforms, supporting instrument integration and testing, and conducting mission operations.

TRACERS will use two satellites to observe particles and fields at the Earth’s northern magnetic cusp region — the region encircling the Earth’s poles where our planet’s magnetic field lines curve down toward Earth. Here, the magnetic field allows particles from the boundary between Earth’s magnetic field and interplanetary space to access the atmosphere.

“TRACERS is an exciting mission,” said SwRI’s Dr. Stephen Fuselier, the mission deputy principal investigator and leader of the development of the ACI instrument. “We had the opportunity to do a test run of the mission and ACI when we flew NASA’s TRICE-2 rockets in the cusp in 2018. The data returned from that single pass through the cusp were amazing. We can’t wait to get the data from thousands of cusp passes.”

The cusp provides easy access to the Earth’s boundary with interplanetary space, allowing a unique perspective on how magnetic fields all around Earth interact with those from the Sun. In a process known as magnetic reconnection, the field lines explosively reconfigure, accelerating particles to velocities reaching a significant fraction of the speed of light.

“Over the planned one-year mission, the identical satellites will be outfitted with a combined total of 10 instruments to measure the plasma and fields in over 3,000 cusp crossings,” said SwRI’s Ron Black, the TRACERS mission manager. “This will allow us to determine reconnection variability over a wide range of solar wind conditions.”

TRACERS’ principal investigator is Dr. Craig Kletzing from the University of Iowa in Iowa City.

DEFENDING AGAINST AN ELECTROMAGNETIC PULSE

While the COVID-19 pandemic is disrupting life around the world, for the San Antonio Electromagnetic Defense Initiative Task Force, the pandemic is highlighting vulnerabilities that could be amplified by a different type of disaster. The task force is preparing for the emerging threat of an electromagnetic pulse (EMP), a manmade or natural burst of powerful electromagnetic energy that could cause long-term, widespread power outages. An EMP, in the form of a nuclear blast or solar event, could prove deadly by dismantling critical national infrastructure, including transportation, health care and food and water supplies for weeks or months.

“Take the current COVID-19 crisis as an example. The inconvenience of social distancing and stay-at-home orders have had a devastating impact on the economy and our way of life,” said Jody Little, a manager in SwRI’s Defense and Intelligence Solutions Division, who is providing leadership on two task force steering

committees. “Now, take away all power, water, gas, communications and other conveniences. This disastrous scenario could play out during an electromagnetic event if we are not prepared.”

SwRI is a founding member of the San Antonio Electromagnetic Defense Initiative, established by the U.S. Air Force and Joint Base San Antonio (JBSA) in March 2019 in response to federal requirements to coordinate a national resilience against an EMP. The local initiative supports collaboration among the city’s government, military, research, academic, business and utility partners to prepare San Antonio for an electromagnetic event, with a key focus on domestic electromagnetic spectrum operations (DEMSO). DEMSO will establish policies and doctrine to ensure continued commerce, comfort, sustained military operations and a swift recovery after an EMP event. Little is chair of the DEMSO steering committee.

“The purpose of DEMSO is to create electromagnetic defense policies and ensure a well-defined doctrine is inserted into emergency plans,” Little said. “We are also looking beyond our local community and envision being the blueprint for national policy by providing direction, examples and lessons learned.”

In May, the Department of Defense (DOD) designated JBSA and San Antonio as a national pilot program for grid resilience and long-term power outages, the first national test site for electromagnetic defense. In June, the Office of the Undersecretary for Defense for Research and Engineering designated Joint Base San Antonio an official 5G experimentation site for two major DOD program trusts, 5G Core and Security and 5G in Telemedicine. The combination of these two major program thrusts will make JBSA the largest DOD 5G experimentation site in the DOD portfolio.





SUPPORTING SATELLITE SERVICING

SwRI developed critical docking system avionics for a satellite life-extension service vehicle, shown here in a laboratory demonstration.

Using critical docking avionics provided by SwRI, the first Mission Extension Vehicle (MEV-1) successfully docked with a client satellite on February 25, 2020. SpaceLogistics, a wholly owned subsidiary of Northrop Grumman, selected SwRI's Rendezvous and Docking Avionics Unit (RDAU) for its MEV-1 docking system.

MEV-1 is the industry's first satellite life-extension vehicle, designed to dock to geostationary Earth-orbiting satellites nearly depleted of fuel. Once connected to its client satellite, MEV-1 uses its own thrusters and fuel supply to extend the satellite's lifetime. When a satellite no longer needs service, MEV-1 will undock and move on to the next client satellite needing support.

"Keeping satellites running beyond their typical 15-year design life is an efficiency measure," said Larry McDaniel, who led the program in SwRI's Space Science and Engineering Division. "There's value in keeping satellites running beyond their design life when they are continuing to function well overall but are unable to maintain orbit unassisted."

The SwRI-developed RDAU manages critical, real-time information to facilitate MEV-1 satellite docking. The highly configurable, programmable data processing platform provides advanced on-orbit capabilities, including high-speed signal processing. The SwRI RDAU includes vision-processing capabilities, supporting multiple camera interfaces. This provides high-performance processing and field-programmable gate array (FPGA) platforms for camera-data routing and image processing.

"We designed the RDAU with an image-processing FPGA that can be programmed in space," McDaniel said. "Usually you can only program these on the ground, prior to launch. With our system, MEV-1 operators will be able to add new system capabilities by reconfiguring the FPGA on orbit, a first for this particular device."

The 2,330-kilogram MEV-1 launched last October and has since been using its electric propulsion system to reach geostationary orbit. Now connected to the client satellite in a stacked configuration, the spacecraft will undergo a series of tests and checkouts.

SwRI Supports Medical Manufacturing

SwRI has helped forge the Medical Manufacturing Alliance of South Central Texas. Made up of economic development, manufacturing and research organizations, MMASCT was initially launched to help meet needs for locally manufactured medical supplies in response to the COVID-19 pandemic.

The alliance is an active collaboration between the San Antonio Manufacturers Association (SAMA), Texas Manufacturing Assistance Center (TMAC) South Central Region, SwRI, Fusion Success Group and Bexar County's Economic and Community Development Department.

Alliance members began sharing resources with local manufacturers in response to social distancing orders and a spike in demand for personal protective equipment (PPE) and essential medical supplies.

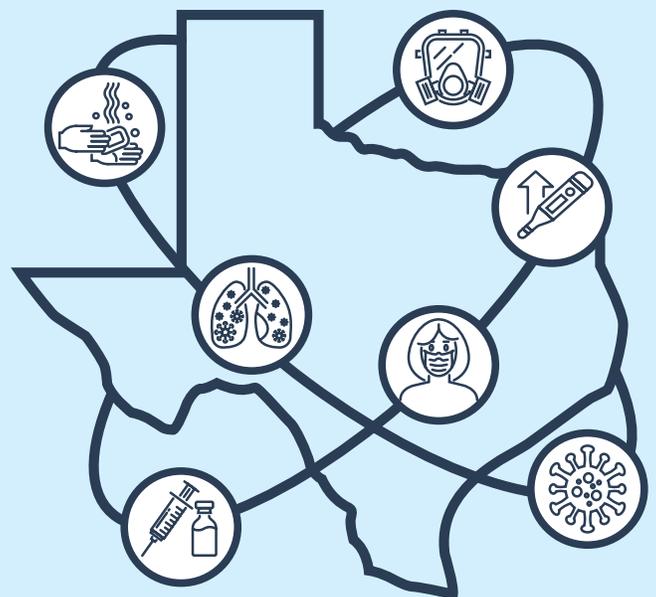
"The immediate focus is to help the regional manufacturing sector to identify products and source materials so they can retool plants to meet these needs," said Bill Rafferty, who leads the TMAC South Central Region office based at SwRI.

The alliance is also helping local manufacturers identify the health and safety standards for face masks and other medical equipment. In cases where items are still useful but not yet approved with official agencies, the alliance is recommending labeling to alert health care professionals and end users.

SwRI supports the alliance by testing equipment, evaluating materials and conducting collaborative research with several local and national universities and research institutions.

"We have already seen a number of innovations through our collaborative research efforts," said Executive Vice President and COO Walt Downing, P.E. "There is a great deal of ingenuity and capability to meet demand for medical equipment and build in some support for a local supply chain across several manufacturing sectors."

SAMA is providing a series of webinars and panel discussions to help manufacturers navigate this pandemic.





D024291_1059

After screening millions of compounds as potential treatments for COVID-19, SwRI conducts cytotoxicity testing on the most promising candidates.

ACCELERATING COVID-19 DRUG DEVELOPMENT

SwRI scientists are using Department of Defense supercomputers to virtually screen millions of drug compounds in pursuit of possible treatment options for the novel coronavirus. The Henry M. Jackson Foundation for the Advancement of Military Medicine awarded SwRI a \$1.9 million, one-year contract to support efforts to develop a COVID-19 therapy.

Working with the DOD High Performance Computing Modernization Program, SwRI is using its Rhodium™ 3D drug development software to screen millions of potential drug compounds. Supercomputers speed up the process, increasing screening capacity from 250,000 compounds a day to more than 40 million compounds in a week.

“This grant will enable SwRI to collaborate to develop safe antiviral drug therapy treatment options for COVID in record time,” said Dr. Joe McDonough, director of SwRI’s Pharmaceutical and Bioengineering Department.

As a drug development tool, Rhodium helps scientists predict how protein structures in infectious diseases will bind with drug

compounds to find viable candidates to develop into therapies.

“Rhodium is helping us quickly identify highly probable compounds from databases with existing drug candidates to narrow down our focus,” said Dr. Jonathan Bohmann, who is leading the COVID-19 drug screening work. “As we identify potential candidates, we have moved them on to testing.”

SwRI uses laboratory tests to assess the toxicity of compounds to help narrow down potential treatment options. Once compounds are tested and meet the criteria set for safety and efficacy, SwRI will be involved in formulation development and production scale-up for the compounds. The Institute has previously used this process to develop drug treatment therapies for Ebola virus, malaria and other infectious diseases.

“This is definitely a priority project, and we understand the urgency,” said Nadean Gutierrez, who is managing the project. “Once compounds have been identified by Rhodium and then passed toxicity testing, they move to the Texas Biomedical Research Institute for the next steps in testing.”

NASA Bets on Lunar LASVEGAS

NASA has awarded SwRI \$3 million to develop a lunar version of its Laser Absorption Spectrometer for Volatiles and Evolved Gas (LASVEGAS) instrument. This spectrometer can precisely measure the volatile compounds present in planetary atmospheres and surfaces — critical information for space science and exploration.

“LASVEGAS is about half the size of a paper towel roll. It’s extremely compact, low mass, low volume and low power — all important characteristics for spaceflight,” said SwRI’s Dr. Scot Rafkin, principal investigator of the instrument. “It can be deployed on the smallest of rovers or landers as well as carried in a single hand by an astronaut sauntering across the lunar surface in search of water ice, methane and other useful resources.”

The instrument measures gases from planetary atmospheres such as Mars to understand their composition. It can also heat a thimble-sized sample of a planetary surface such as the icy surface of Jupiter’s moon Europa or from lunar soil to determine the composition of released gases.

NASA’s Maturation of Instruments for Solar System Exploration (MatISSE) program provided \$3 million in 2019 to develop the LASVEGAS instrument for application to Europa and similar icy worlds. In 2020, SwRI received an additional \$3 million from the agency’s Development and Advancement of Lunar Instrumentation (DALI) program to adapt the design to operate on the Moon’s surface.

The gas flows into a small, cylindrical chamber where laser light of different wavelengths is bounced back and forth between mirrors on each end. As the light passes repeatedly through the gas in the sample, the different molecular species in the gas absorb the light differently depending on the wavelength. Then the laser light is directed onto a detector that measures its intensity to determine the abundance of the volatile compounds. Each molecular species in the gas has a distinct “fingerprint” of absorption, revealing its overall abundance.

COMPARING INTERNATIONAL FIRE CODES

SwRI conducted room burn tests to better understand how country-specific fire codes in the U.S., France and the United Kingdom affect the fire safety of home furnishings and their contributions to flashover. Flashover occurs when temperatures at the ceiling reach 1,000° C and all the combustibles in the room ignite.

Reducing the rate for flashover can save lives, allowing significantly more time for people to escape a fire. The study found the American- and French-furnished rooms reached flashover in just five to six minutes, whereas the United Kingdom-furnished room took 22 minutes to reach flashover. Upholstered furniture from the U.K. is treated with the most fire-retardant protection, which also resulted in lower smoke toxicity measurements than the U.S. and French tests.

“Most countries test upholstered furniture for fire performance, however, fire preventative measures and testing standards applied to consumer products vary greatly by country,” said Dr. Matthew Blais, director of SwRI’s Fire Technology Department and lead author of a paper outlining this research published in the journal *Fire Technology*.

SwRI fire engineers conducted nine room burns to better understand the variances in fire standards from different countries and to study how quickly flashover occurs in a realistic environment. Each of the three identically furnished sets of rooms contained a three-cushion couch, a chair and a flat panel television. SwRI purchased these specific items from each respective country. Each room setup also included an identical coffee table, end table, curtain, bookcase and books, all purchased in the U.S. Because these items are typically not treated with a fire retardant, the fire performance should not vary from country to country. The Institute conducted the room burn tests using the international standard for full-scale room test specifications, ISO 9705.

When the living room furnishings are the first item ignited in a fire, there tends to be a higher incidence of death. SwRI selected three ignition sources of increasing strength, with two representing the passing level for the U.K. standard and one exceeding that requirement to ensure the ability to measure smoke toxicity. For each room configuration, ignition started in the center couch cushion.

The U.S. and France use a smolder-only flammability test standard while the U.K. combines a smolder and open flame ignition test to evaluate the flammability. “In the U.S. and other countries, there is a push to eliminate chemical flame retardants due to an anti-chemical movement,” Blais said. “This study shows the impact of country fire codes only requiring smoldering ignition compared to a country testing with open flame ignition. When an open flame standard is applied to consumer products that have been treated with fire preventative material, the results show the room would reach flashover at a much slower rate, allowing people five to six times more time to escape from a house fire when the first item ignited is a couch.”

Karen Carpenter, assistant director of Fire Technology, and Kyle Fernandez, a fire technology engineer, also collaborated on the study and paper titled “Comparative Room Burn Study of Furnished Rooms from the United Kingdom, France and the United States” (DOI 10.1007/s10694-019-00888-8).

The North American Fire Retardant Alliance and the American Chemistry Council funded the research.

To see a video about this fire study, visit <https://youtu.be/wlnAAxOKYLg>.



Proposed SwRI/UNH Mission Leaps Forward

NASA has selected SwRI and the University of New Hampshire to continue developing a mission to look for evidence of distant energetic events, such as the birth of black holes. NASA's Astrophysics Missions of Opportunity program selected the "Large Area burst Polarimeter" (LEAP) program for a mission concept study.

Mounted on the outside of the International Space Station, LEAP would study energetic jets such as those erupting from the explosive death of a massive star or the merger of compact objects such as neutron stars. LEAP's ability to measure the polarization of gamma-ray bursts (GRB) could resolve competing theories about the nature of the jets. LEAP would complement NASA's Imaging X-ray Polarimetry Explorer (IXPE), scheduled to launch in 2021, which will study lower-energy X-ray phenomena.

"Gamma rays are the smoking gun for some of the most energetic events in the universe," said Dr. Mark McConnell, director of SwRI's Earth, Oceans and Space (SwRI-EOS) Department at UNH's Durham, New Hampshire, campus. "When a very massive star explodes in a supernova and then collapses into a black hole, it ejects jets with energies that can exceed anything observed in the universe since the Big Bang. LEAP will measure the resulting GRB with previously unachievable precision."

LEAP will improve our understanding of the role that magnetic fields play in these systems, especially with regard to the formation and sustainment of the high-speed jets that are responsible for what we see. It should also reveal how the observed gamma radiation is produced within the jet.

LEAP is a single instrument with nine polarimeter modules based on well-established, flight-proven technologies. It will measure gamma-ray burst polarization while self-sufficiently providing the source localization required to analyze polarization data. These data will allow LEAP to differentiate between classes of GRB models. Detailed time-resolved and/or energy-resolved studies will be conducted for the brightest GRBs.

NEW EMISSIONS RESEARCH FACILITY

SwRI has launched a new automotive emissions aftertreatment catalyst testing facility, expanding the capacity and capabilities of its state-of-the-art Universal Synthetic Gas Reactor (USGR®) technology. These systems simulate real-world exhaust gas conditions to quickly and accurately characterize catalyst performance.

"SwRI's USGR system allows our clients to quickly determine catalyst performance under a variety of conditions and at a lower cost than with traditional engines or burner systems," said Dr. Cary Henry, an assistant director in SwRI's Powertrain Engineering Division. "Accurate control of gas composition and advanced measurement techniques like SPACI-IR (spatially resolved capillary inlet infrared spectroscopy) enable us to develop kinetic models for reactions and understand how aging and chemical contamination affect catalyst materials."

Catalytic aftertreatment equipment use a porous ceramic core treated with reactive chemicals that process exhaust and remove potentially harmful gases and particulates to help engines meet increasingly strict emissions regulations. Testing core samples of material used in three-way catalysts, diesel oxidation catalysts, diesel particulate filters, selective catalytic reduction (SCR) compounds and ammonia slip components shows how products perform under different operating conditions. Clients receive the technical information needed to help them develop new catalyst technology and materials.

The Catalyst Technology Center includes two new USGR systems, bringing SwRI's testing capacity to six systems. The facility allows SwRI engineers to conduct several tests in parallel, improving turnaround time and lowering testing costs.

SwRI's USGR systems can operate under a wide range of flowrates (7.5 to 65 L/min) and temperatures (100° to 1,200° C) and are capable of continuous automated testing for up to 60 hours. The system supports as many as 13 metered gases, which can be introduced simultaneously, as well as water or hydrocarbon injection. Testing can be tailored to clients' needs, but standard tests include reverse and forward light-off tests, four-step protocol for SCR and V-volatility testing approved by the Environmental Protection Agency. The facility also supports thermal and chemical aging experiments.

SwRI uses its novel Universal Synthetic Gas Reactor (USGR®) technology to simulate real-world exhaust gas conditions to quickly and accurately characterize catalyst performance.



D024358

MODELING MARS' INHOSPITABLE CLIMATE

An SwRI scientist modeled the climate of Mars to understand if hydrated salts or brines on the surface of the Red Planet could harbor life. The results suggest that hydrated salts and brines on Mars are not supportive of life. For example, if the dark streaks shown here are formed by the flow of briny water, then that briny water would be too cold to support life.

An SwRI scientist modeled the atmosphere of Mars to help determine that salty pockets of water present on the Red Planet are likely not habitable by life as we know it on Earth. A team that also included scientists from Universities Space Research Association (USRA) and the University of Arkansas helped allay planetary protection concerns about contaminating potential Martian ecosystems.

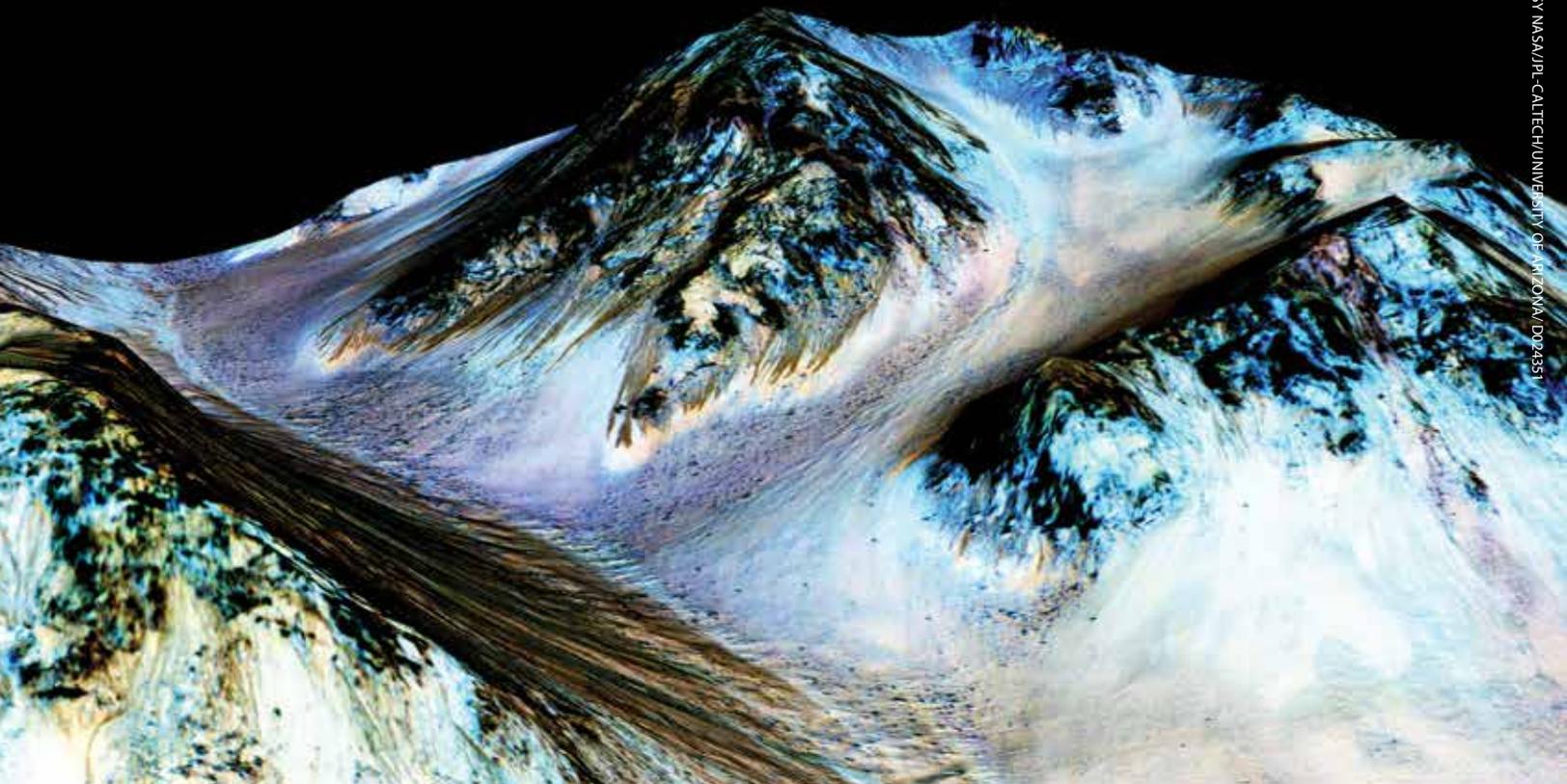
Due to Mars' low temperatures and extremely dry conditions, a droplet of liquid water on its surface would instantly freeze, boil or evaporate — unless the droplet had dissolved salts in it. This brine would have a lower freezing temperature and would evaporate more slowly than pure liquid water. Salts are found across Mars, so brines could form there.

“Our team looked at specific regions on Mars — areas where liquid water temperature and accessibility limits could possibly allow known terrestrial organisms to replicate — to understand if they could be habitable,” said SwRI’s Dr. Alejandro Soto, a senior research scientist and co-author of a study published in *Nature*

Astronomy. “We used Martian climate information from both atmospheric models and spacecraft measurements. We developed a model to predict where, when and for how long brines are stable on the surface and shallow subsurface of Mars.”

Mars’ hyper-arid conditions require lower temperatures to reach high relative humidities and tolerable water activities, which are measures of how easily the water content may be utilized for hydration. The maximum brine temperature expected is -55° F — at the boundary of the theoretical low temperature limit for life.

“Even extreme life on Earth has its limits, and we found that brine formation from some salts can lead to liquid water over 40% of the Martian surface but only seasonally, during 2% of the Martian year,” Soto continued. “This would preclude life as we know it. These new results reduce some of the risk of exploring the Red Planet while also contributing to future work on the potential for habitable conditions on Mars.”



FUEL PROCESSING CAPABILITIES EXPANDED

SwRI has expanded its capacity to develop and certify fuels from alternative sources with a new, custom fixed-bed reactor. The SwRI-designed system can be used for refinery processes, such as hydrotreating and hydrocracking, to produce stable fuels ready for vehicle use.

Hydrotreating is an established refinery process for reducing sulfur, nitrogen, oxygen and olefins in fuel and lubricant products. Refineries use hydrocracking to adjust the properties and boiling point ranges of crude oil fractions into products such as gasoline, kerosene, jet fuel and diesel.

“Developing reliable biofuels can help reduce the world’s reliance on fossil fuels,” said Eloy Flores III, assistant director of SwRI’s Chemical Engineering Department. “SwRI is a leader in developing fuels from unconventional sources, producing biofuels that meet Environmental Protection Agency specifications. The Institute also is home to one of the few laboratories in the United States to register alternative fuels for integration into the mainstream vehicle fuel supply.”

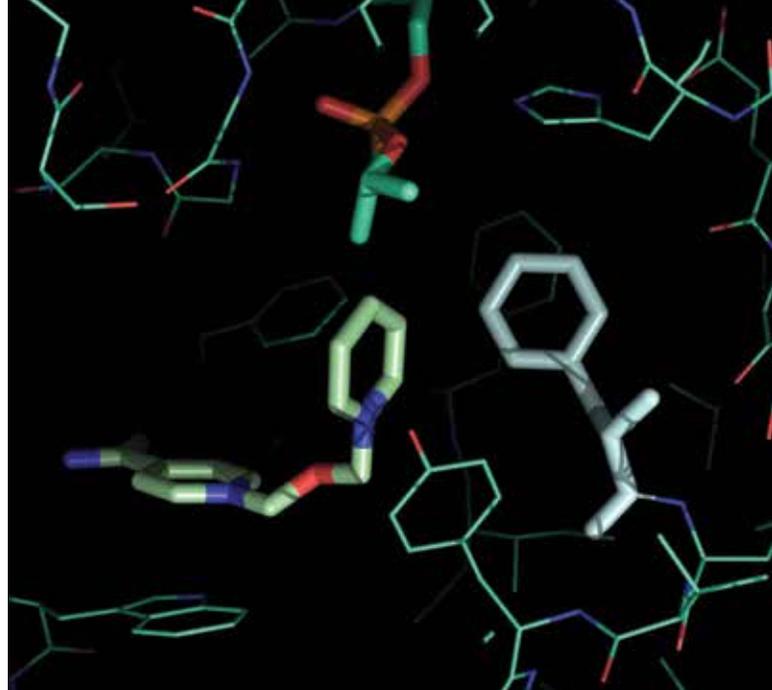
Alternative or biofuels are developed by converting raw materials such as corn, algae, plastics, wood or even heavy crude oil into refined fuel. SwRI’s new reactor includes a large reactor bed and two additional smaller units to develop processes to produce fuel samples. The pilot system can process and produce up to two drums of specification fuels per day, operating at up to 3,500 psig and 550° Celsius.

“Combining the large reactor bed with smaller units allows us to handle various feed materials ranging from Fischer-Tropsch waxes to naphtha,” Flores said. “We help our clients take an unconventional feedstock, such as pyrolysis oils, and produce biofuel blends that can be used in cars, buses, trucks and jets. Our goal is to provide more efficient scale-up and proof-of-concept techniques for processing fuels and other chemical products for our clients.”

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SwRI-developed Rhodium™ software helps scientists discover nerve agent antidotes that penetrate the central nervous system. This 3D display illustrates how a potential antidote interacts with an agent.

DEVELOPING NERVE AGENT ANTIDOTE

SwRI has received funding from the Medical CBRN Defense Consortium (MCDC) administered by Advanced Technology International to develop a nerve agent antidote for emergency use on the battlefield or to protect public health.

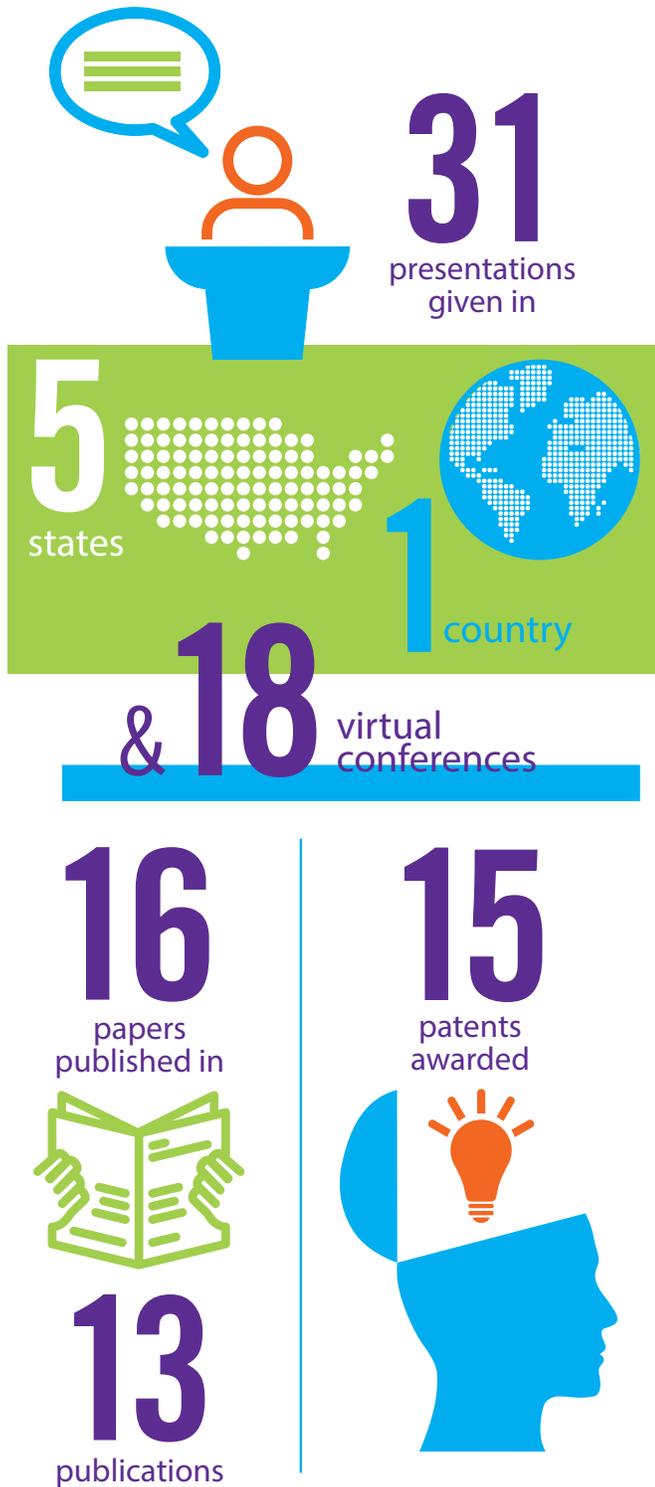
The use of nerve agents continues to be a significant threat to both military and civilian populations. This prototype medication could serve as a countermeasure against a nerve agent attack. SwRI will lead the development of the antidote under the \$9.9 million, five-year program. It will collaborate with the University of Pittsburgh on the synthesis and compound design, through the support of the Defense Threat Reduction Agency (DTRA).

“This antidote improves on the current standard of care, importantly, its ability to reverse the effects of the toxin in the central nervous system,” said Dr. Jonathan Bohmann, a principal scientist in SwRI’s Pharmaceutical and Bioengineering Department. “The antidote will eventually be administered through an autoinjector, which allows for rapid and effective treatment in the field. It would work much like an epinephrine auto-injector or EpiPen® administered during a severe allergy attack. The initial goal of the project is to support our warfighters; however, this treatment could also eventually be administered for civilian use.”

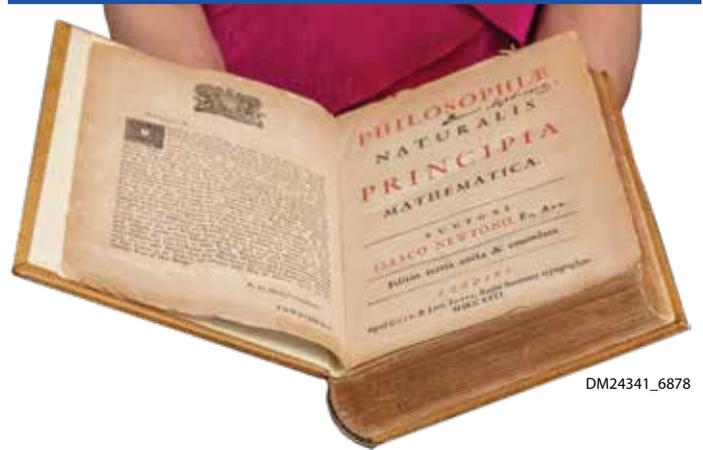
SwRI will use a computer-based drug design software platform called Rhodium™ to develop the antidote. SwRI developed Rhodium, a proprietary docking simulation software tool, to enhance drug design and safety while reducing costs and speeding up development time. The Institute offers Rhodium as a service to clients. Rhodium supports drug development and screening for antibiotics as well as preventative treatments such as vaccines. The software also predicts adverse drug reactions and side effects.

See *COVID-19 Drug Development* on p. 23 for more Rhodium news.

BY THE **NUMBERS** SPRING – SUMMER 2020



RARE TECHNICAL TEXTS



DM24341_6878

In 1947, Southwest Research Institute founded the first scientific and technical library in San Antonio. Originally known as the ESSAR (the phonetic SR abbreviation for scientific research) Library and renamed for our founder in 1969, the Thomas Baker Slick Library preserves, acquires, maintains and provides access to scholarly science and technical information.

Beginning in the late 1950s, former SwRI President Martin Goland and Library Director Ed Vaught began collecting landmark texts of science that laid the foundation for the research conducted at the Institute. The collection contains over 250 rare and unique works dating from the 16th to the 20th century.

In 2020, the library's Vasu Lyengar worked with hypersonics researcher Dr. Nicholas Mueschke to curate a collection of rare books that contain some of the founding principles for SwRI's aerospace and engineering dynamics research. SwRI's Rare Book Collection includes some original texts that lay out the principles for understanding the extreme physics and environments that aircraft endure. These early texts provide insights into the aerodynamics and compressible gas dynamics theory that has formed the foundation of hypersonic flight today. SwRI's groundbreaking hypersonics research will be featured in the Fall issue of Technology Today.



Vasu Lyengar and Dr. Nicholas Mueschke curated a display of rare books about the principles of aerospace.

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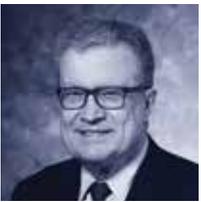
D024370

Dr. Robin Canup, assistant vice president of the Space Science and Engineering Division and head of SwRI's Boulder, Colorado, office, has been named one of two co-chairs for the National Academies of Sciences, Engineering and Medicine's (NAEM) newly launched Planetary Science and Astrobiology Decadal Survey. The survey will assess the state of planetary science, identify the most important scientific questions, rank the importance of future NASA missions and present a comprehensive research strategy for 2023 to 2032.



D024125_3543

Senior Safety Engineer Matthew Herron, P.E., CSP, CPE, has been awarded the 2020 Emerging Professional Award by the American Society of Safety Professionals (ASSP). The award recognizes Herron's leadership, volunteerism and desire to impact workplace safety. He is among five recipients chosen for the inaugural award from a field of hundreds of ASSP members who are under 40 years old or have fewer than five years of work experience in the occupational safety and health field.



D024362

Executive Vice President and COO Walt Downing is an Institute of Electrical and Electronics Engineers Distinguished Lecturer and IEEE Aerospace and Electronic Systems Society president. He presented "CubeSat Mission to Study Solar Particles (CuSP)" in an online virtual meeting on June 5, hosted by the IEEE Galveston Bay Section.



D024369

SwRI's Technology Today Podcast received an El Bronce Excellence Award from the Public Relations Society of America's San Antonio Chapter. The 2020 Del Oro Awards recognize the outstanding contributions of individuals in the public relations field. The podcast team includes Senior Communications Specialist Lisa Peña, Senior Specialist Ian McKinney (left) and Specialist Bryan Ortiz.

WEBINARS, WORKSHOPS and TRAINING COURSES HOSTED BY SWRI:

Gas Turbine RCFA Webinar, July 29, 2020. Free training.

Blade Aeromechanic Analysis Webinar, August 5, 2020. Free training.

Lean Six Sigma Green Belt Training, San Antonio, August 10–14 and September 21–25, 2020. SwRI's Texas Manufacturing Assistance Center is hosting this two-week workshop.

Fundamentals of Supercritical CO₂ Webinar, August 12, 2020. Free training.

Hydraulic Fracturing with Foams Webinar, August 19, 2020. SwRI is hosting this webinar.

Manufacturing Supervisor Certification Program, August and September. SwRI's Texas Manufacturing Assistance Center is hosting this five-day training in Austin and San Antonio.

Acoustic Induced Vibrations Webinar, August 26, 2020. Free training.

Transient Hydraulic Modeling Webinar, September 2, 2020. Free training.

Thermal Transient Modeling and Analysis Webinar, September 9, 2020. Free training.

Penetration Mechanics Short Course, San Antonio, September 14–18, 2020. SwRI is hosting this short course.

An Introduction to Lateral Rotordynamics Webinar, September 16, 2020. Free training.

sCO₂ Power Cycles Analysis and System Development Webinar, September 23, 2020. Free training.

Lean Manufacturing Certification Program, September–October 2020. SwRI's Texas Manufacturing Assistance Center is working with the San Antonio Manufacturer's Association to host this training program.

Turbine Case Design with ASME VIII-2 Webinar, September 30, 2020. Free training.

Launch Vehicle Propulsion Course, October 19–21, 2020. SwRI is hosting this virtual training event.

Southwest Research Institute
6220 Culebra Road
P.O. Drawer 28510
San Antonio, Texas 78228-0510
United States

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210.522.2122
ask@swri.org

swri.org



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