Science & Technology

CSAC
Chemical Security Analysis Center

FISCAL YEAR 2023 ANNUAL REPORT

APPROVED FOR PUBLIC RELEASE

CSAC
Chemical Security Analysis Center

The Department of Homeland Security (DHS) Science and Technology Directorate (S&T) Chemical Security Analysis Center (CSAC) is the Nation's only federal studies, analysis, and knowledge management center for assessing the threat and hazard associated with an accidental or intentional large-scale chemical event or chemical terrorism event in the United States.

CSAC's mission is to assess and address chemical threats to the homeland.

CSAC accomplishes its mission by:

Collecting, consolidating, curating, storing, and sharing chemical data

Generating science-based assessments and recommendations and identifying emerging trends based on vetted data

Identifying, prioritizing, and addressing data gaps through high quality chemical research, development, test, and evaluation

CSAC serves the Homeland Security Enterprise and its stakeholders by staffing and operating a 24/7 Technical Assistance program that provides operational support and subject matter expertise, designing and executing laboratory and field tests and providing a comprehensive knowledge repository of chemical threat information that is synthesized and updated with data from scientific, operational, and private-sector sources.

CSAC INCLUDED IN THE 2023 NATIONAL DEFENSE AUTHORIZATION ACT

In late December, President Biden signed the National Defense Authorization Act (NDAA) for Fiscal Year (FY) 2023 into law, marking a significant milestone in the nation's commitment to comprehensively address chemical security threats. The NDAA includes provisions granting full legislative authorization to CSAC, the sole federal laboratory dedicated to assessing large-scale chemical incidents and acts of chemical terrorism. It employs scientific experimentation, data, analysis, and knowledge management to inform emergency planning and response efforts, embodying a unique partnership between DHS and the U.S. Army. The recent opening of CSAC's Chemical Security Laboratory (CSL) signifies the strength of this mission partnership.

The NDAA amends Title III of the Homeland Security Act of 2002 (6 U.S.C. 181 et seq.), adding at the end the following new section: SEC. 323. CHEMICAL SECURITY ANALYSIS CENTER.

President Biden signs US 2023 National Defense Authorization Act into law

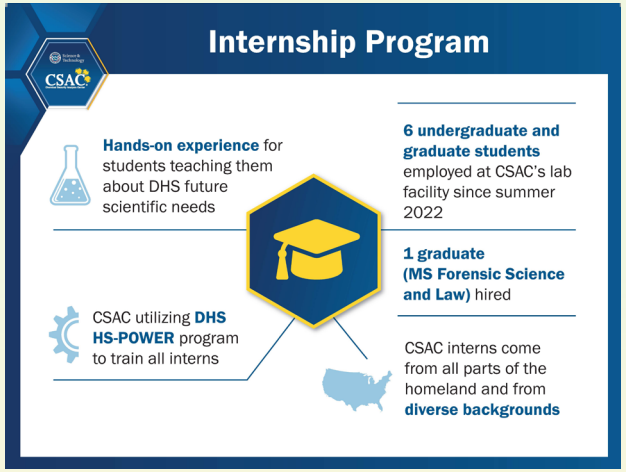
Established in 2006, CSAC has steadfastly supported homeland security for more than 18 years, playing a crucial role in supporting emergency response planning and providing DHS agencies and partners with essential chemical expertise and advanced analyses. Its contributions have ranged from addressing illicit opioids to preparing for chemical releases, enhancing aviation security, and safeguarding the food supply. Due to its strong track record and 24/7 responsiveness, CSAC has become the go-to resource for the emergency response community, offering rapid and reliable information on chemical threat scenarios.

> **"CSAC provides DHS agencies and partners with the chemical expertise and advanced analyses needed to consider likely scenarios, evaluate risk mitigating measures, minimize anticipated response time, and ultimately save lives."**
>
> *– Paul Strang, Director (Acting) of the S&T Directorate's Office of National Laboratories*

The NDAA legislative authorization acknowledges the critical role of CSAC in ensuring the safety and security of the nation against chemical threats.

PREPARING THE FUTURE OF CHEMICAL DEFENSE

Developing the Next Generation: CSAC invested in educating science, technology, engineering, and mathematics (STEM) college students on chemical defense and opportunities at DHS and CSAC. Building on prior success, the intern program was expanded at CSAC where the lab hosted four Oak Ridge Institute for Science and Education (ORISE) interns, while also transitioning a former 2022 ORISE intern to a full time CSAC staff position, underscoring CSAC's commitment to building and developing talent.



> **"I had the unique opportunity to support CSAC's mission through meaningful lab work contributions. The opportunity to network and learn from the accomplished and established staff at CSAC was unparalleled."**
>
> *– Ms. Julianna Firek, former intern, recent graduate of Duquesne University's Master of Forensic Science & Law program, and current CSAC staff member*

Ms. Julianna Firek presenting at Coppin State University.

STEM Outreach to Diverse Institutions: CSAC's College Outreach Program was heavily engaged in building a STEM pipeline for college students. Led by Dr. David Reed and Ms. Julianna Firek who conceptualized and launched this initiative, CSAC presented its college lecture series to students, faculty, and staff at Duquesne University; University of Maryland Baltimore Campus; and three Maryland Historically Black Colleges and Universities—Coppin State University, Morgan State University, and Bowie State University.

BUILDING THE MATRIX

Through matrixed intra-S&T collaborations within the Office of National Laboratories (ONL), CSAC staff branched out into emerging areas of research to develop more in-house, organic capabilities. Multi-lab efforts enabled CSAC to help achieve ONL's vision of strengthened partnerships within the geographically dispersed S&T Laboratory enterprise.

Protecting the Nation's Food Supply: Ms. Jessica Cox and Dr. Carol Brevett engaged with Plum Island Animal Disease Center and S&T Food, Agriculture, and Veterinary Defense regarding a strategic path forward to mitigate the food adulteration threat. The focus included the need for protection of the U.S. food supply by protecting plants and animals from disease and integrating the roles of other sectors such as water, information technology, chemicals, and plastics.

CSAC efforts in protecting the Nation's food supply included identifying current and emerging chemical hazards and threats, generating data to understand these threats, and sharing knowledge with the Homeland Security Enterprise. Working collaboratively with the food industry, academia, and federal partners, CSAC led outreach efforts to increase the security of the U.S. food supply.

Ms. Jessica Cox was recognized by DHS S&T during Public Service Recognition Week for "skillful management of Food Defense and Security initiatives and assessments" for CSAC. This work has been recognized across DHS and highlighted in the Homeland Security Special Edition of *USA Today*.

Key presentations included:

- The impact on risk of experimentally-determined toxicity and organoleptic values of priority chemicals in various food matrices at the classified interagency 2023 Chemical and Biological Warfare Weaponization and Consequence Assessment Modeling Symposium.
- "Food Adulteration Events and Chemical Toxicity" to the Food Safety Professionals Group describing CSAC's forward-looking focus on potentially harmful chemicals such as Teflon, perfluorooctanoic acid (PFOA), per-/poly-fluoroalkyl substances (PFAS), and nanomaterials.

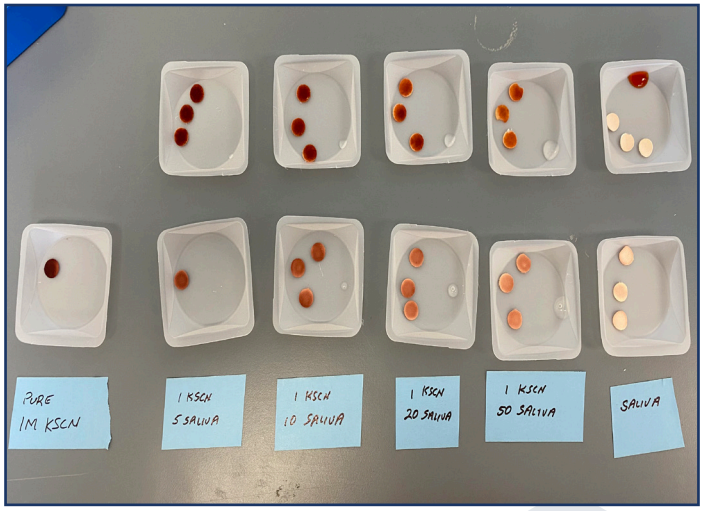
BUILDING THE MATRIX (CONT.)

Photo credit: USDA

CSAC developed new testing methods and protocols in the CSL to generate food-related data needed for S&T Probabilistic Analysis for National Threats Hazards and Risks (PANTHR) and Tools for Integrated Evaluation of Risk (TIGER) and provided results to the U.S. Department of Agriculture Food Safety and Inspection Service.

CSAC researchers analyzed data, along with U.S. Army Medical Research Institute of Chemical Defense, on chemical adulterants in food to assess risk more accurately, as part of the Solubility, Toxicity and Organoleptic Profile of Toxic Chemicals of Interest (STOP-TIC) project.

Advancing Chemical Defense Technology: Dr. Dave Reed partnered with S&T's National Urban Security Technology Laboratory (NUSTL) to spearhead advanced development of the Rapid Cyanide Detection (RAPCYD) field test kit. NUSTL's relationship with New York City emergency response entities will enable CSAC collaboration with the Fire Department of New York (FDNY) for proof-of-concept testing in FY 2024.



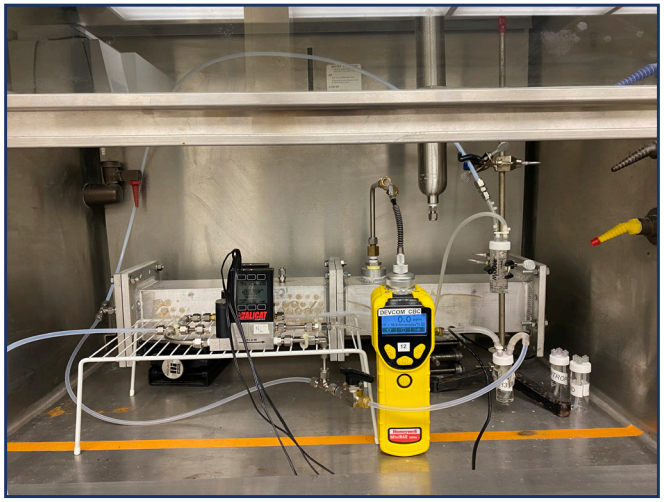
From right to left, the first RAPCYD test strip is the color of natural saliva. As the concentrations of cyanide increased, the color became a more intense red, which is the farther left strip. The two rows represent the reproducibility of exposure.

Drs. David Reed, George Emmett, and Rabih Jabbour from CSAC developed the RAPCYD presumptive cyanide exposure test, a rapid and cost-effective method for detecting cyanide exposure using a biomarker, crucial for early diagnosis and treatment. This field-deployable test takes seconds and costs very little, making it a potentially invaluable tool for first

BUILDING THE MATRIX (CONT.)

DHS was granted a patent for "Detecting Cyanide Exposure Based on Thiocyanate Measurement". The patent was conceived by Drs. David Reed, George Emmett, and Rabih Jabbour from CSAC.

responders, particularly firefighters and fire smoke victims who may have been exposed to cyanide. The test strip for identifying cyanide exposure is designed for nationwide deployment, aiding rapid assessment during mass casualty events involving toxic gases. CSAC is collaborating with various entities, including the FDNY and the Johns Hopkins Burn Center, for proof-of-concept testing in FY 2024.



A flow cell for challenging detectors with controlled concentrations of toxic industrial chemicals.

Evaluating Chemical Detection Technology: CSAC continues to evaluate detection capabilities for environmental monitoring for chemical threats, providing insights into the current capacity to detect explosives, illegal drugs that have been diluted with cutting agents, and toxic industrial chemicals.

Dr. Jerry Cabalo's work evaluating handheld detectors determined that few existing detectors can identify low-purity materials, a growing concern for DHS considering the prevalence of fentanyl, which is often cut with other substances. Dr. Cabalo's work provided insight into the current capacity for Customs and Border Protection to detect illegal drugs that have been heavily diluted with cutting agents. His work also provided awareness of current detector capabilities and limitations, and potential next steps toward future improvements.

In response to a requirement from the U.S. Coast Guard, CSAC subject matter experts evaluated a Small Business Innovation Research project funded by the S&T Mission Capability Support - a colorimetric sensor for class identification of toxic industrial chemicals. CSAC's technical validation and feedback facilitated development of two colorimetric class sensors for gases that affect pH and reductant gases at half the level for immediate danger to life and health.

EMPOWERING WOMEN IN STEM

CSAC is intentional about creating an environment where women, and other underrepresented groups, thrive, hold pivotal positions, and are assured equitable access to leadership roles. The women of CSAC, providing technical expertise and core capabilities, comprise nearly 40% of the laboratory's workforce with over 230 combined years of expertise in program management and STEM. Strengthening our diverse workforce in this way is essential to promoting innovation and driving technological relevance, and more broadly drives sustained economic growth.

Ms. Helen Mearns (left) mentors women and girls.

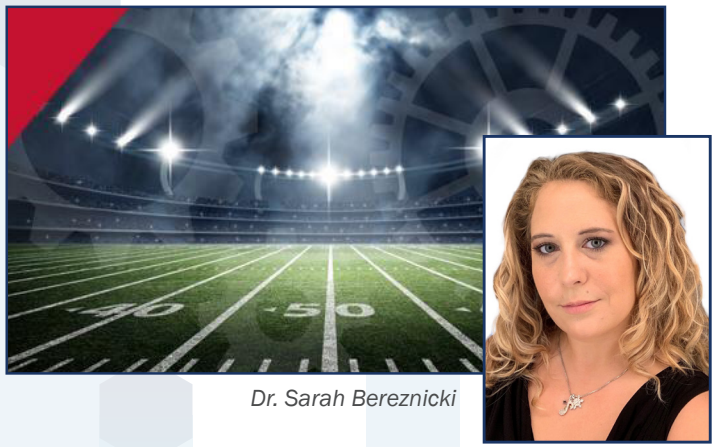
In celebration of International Day of Women and Girls in Science, Ms. Helen Mearns shared her involvement in tutoring and mentoring women and girls in her community. "As a woman blazing trails in my field," Ms. Mearns said, "I feel a vital responsibility to make sure not only that CSAC maintains the talent and capabilities necessary to support the Homeland Security mission, but that we serve as an example for other agencies to follow." Ms. Mearns mentors women and girls of all ages from elementary school to adult. She listens, encourages, and relates science to everyday life.

For Women's History Month, Ms. Jessica Cox shared advice and discussed her career path on the "Now Live! Minisode 9: And the Rest Is History" featuring Women in Science at S&T. Ms. Cox's advice to a new generation of girls in science is, "Do it! That's number one." As Ms. Cox joined the workforce, there were very few women in science. Her first jobs were not an easy battle gaining the respect she deserved in a male-dominated workplace. "Science needs men's views on things, and women's views on things", Ms. Cox said, also stating "If you're passionate about what you want, there's nothing that should stop you."

EMPOWERING WOMEN IN STEM (CONT.)

At Civilian Research and Development Foundation Global's annual Breaking Barriers event, Ms. Helen Mearns presented on Building an Inclusive Future of Scientific Progress. The event supported The Women in Science and Security Initiative that focuses on promoting the active involvement and leadership of women in STEM and chemical, biological, radiological, and nuclear (CBRN) security fields. Ms. Mearns also shared her background and experience, why she became a STEM mentor, and her advice to others interested in mentoring women in STEM.

Dr. Sarah Bereznicki was featured on the Tech Speak "Minisode 10: Providing the Best Information to Save Lives". In this podcast, Dr. Bereznicki explains how CSAC modeled indoor and outdoor threat scenarios for events leading up to, and including, the Super Bowl LVII. CSAC develops realistic scenarios which provide information on impact, resource demands, and response limitations which prepares and informs the planners and provides a basis for tabletop exercises. "Not everybody is aware the Super Bowl is not just the event in the arena, it ends up becoming a culmination of events in that city over a week-long period. We've done multiple events and multiple types of scenarios, and they are excited about that." The results of 100s and 1000s of scaled scenarios provide medical mitigation insight, key takeaways to plan for future events, and save the lives of attendees, emergency responders, and people in the community.



Dr. Sarah Bereznicki

Ms. Helen Mearns is the recipient of the 2023 Bernard F. Langer Nuclear Codes and Standards Award. Established in 1977 and presented by the American Society of Mechanical Engineers (ASME), the award honors an individual who has been instrumental in the development and promotion of ASME Nuclear Codes and Standards. Ms. Mearns has participated on the ASME Committee on Nuclear Air and Gas Treatment since 1995 where she led the team that established a new code section on Sand Filters such as those used


ASME

THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS

2023

Bernard F. Langer Nuclear Codes and Standards Award

awarded to

Helen A. Mearns

For contributions to the nuclear power plant industry through the development and promotion of ASME Nuclear Codes and Standards

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EMPOWERING WOMEN IN STEM (CONT.)

at the Savannah River National Laboratory and where she is involved in the code sections for High Efficiency Particulate Air (HEPA) filters and filter media. Among other uses, HEPA filters are used on air transportation to filter cabin air and grew in importance during the COVID-19 pandemic. This year, due to heightened awareness of the dangers resulting from PFAS, filter media manufacturers are performing research on new solutions that will meet the rigorous requirements of the relevant ASME code sections.

Through an upskilling initiative offered by CSAC's partner, U.S. Army Combat Capabilities Development Command Chemical Biological Center (DEVCOM CBC), Ms. Lindsay Evans attended a three-part series and four-day intensive course on Artificial Intelligence and Machine Learning. The three-part series, provided by faculty from Carnegie Mellon School of Computer Science, included ten-week sessions on Programming with Python, Artificial Intelligence, and Machine Learning: Fundamentals and Algorithms. Later, Lindsay followed up the series with a four-day intensive course on Machine Learning with Python. CSAC values growth and professional development, and these courses have assisted in understanding the impact of emergent technologies on chemical threats.

Ms. Helen Mearns is the chemical defense delegate of the U.S. to the North Atlantic Treaty Organization (NATO) Hazard Management Panel (HMP) where she participated in the Fall 2022 meeting in Prague, Czech Republic, and the Spring 2023 meeting in Paris, France. The HMP includes a team of experts meeting on Allied Engineering Publication 58, "Combined Operational Characteristics, Technical Specification, Test Procedures and Evaluation Criteria for Chemical, Biological, Radiological, and Nuclear Decontamination Equipment", the plenary session of the HMP, and a session to develop standard operations. CSAC is collaborating with the United Kingdom Defence Science and Technology Laboratory (UK Dstl) on the revision of test methods and procedures and hazard and risk management to achieve the NATO objective of interoperability of equipment.

INTEGRATING JACK RABBIT PROGRAM DEVELOPMENTS

CSAC assessed the evolving chemical landscape and identified chemical risks due to growing global interest in alternative zero carbon emission energy sources, including ammonia. The potential impact from a large-scale release of ammonia is being addressed to enhance preparedness in the event of such an incident. CSAC evaluated the secondary hazards in collaboration with DEVCOM CBC to understand the evaporation of anhydrous ammonia from concrete and the resultant potential airborne hazard. CSAC's Controlled Environment Reactivity Test (CERT) project reached a critical milestone for assessing the removal of ammonia by reaction with environmental materials and concluded a multi-year effort for the Jack Rabbit program. The four materials tested, in addition to multiple materials from prior phases, were representative of what might be found along transportation routes and provided critical data leading to an understanding of how ammonia contamination might be mitigated were there to be a large release. The tests were conducted under a range of environmental conditions to assess removal for a variety of seasons and locations.

Plants after exposure to Ammonia in the CERT Chamber.

CSAC was once again well represented at the 27th Annual George Mason University Conference on Atmospheric Transport and Dispersion modeling. Drs. Shannon Fox, Sun McMasters, and Patrick Goalwin, and Mr. Ray Jablonski led Jack Rabbit III Special Sessions in collaboration with the Defense Threat Reduction Agency (DTRA), further expanding the partnership with Air Products, Maritime Planning Associates, the UK Health Safety Executive, the UK Dstl, and the Agency for Defense Development of South Korea.

CSAC and the Ammonia Safety and Training Institute (ASTI) collaborated in a Tabletop Exercise (TTX) to assess the feasibility of implementing an ammonia release response Concept of Operations (CONOPS) Template. The TTX, conducted under a DHS Cooperative Research and Development Agreement (CRADA) with the ASTI CEO and Drs. Sun McMasters, Patrick Goalwin, and Sarah Bereznicki of CSAC in conjunction with the Crisis Communication Workshop in Pendleton, Oregon showcased the practical application of ChemResponder in enhancing the efficiency of emergency response efforts. The TTX centered around a case study of a past anhydrous ammonia release incident at Millard Refrigerated Services in Theodore, Alabama, in 2010. During the exercise, the value of the Federal Emergency Management Agency ChemResponder as an emergency response tool became evident, highlighting the importance of integrating such real-time information-sharing tools into emergency response CONOPS.

CHEMICAL DEFENSE PREPAREDNESS AT HIGH-PROFILE EVENTS

By special request, in December 2022, CSAC partnered with the Phoenix, Glendale, and Scottsdale Fire and Emergency Services agencies to prepare for potential chemical releases at Super Bowl LVII and related events. In conjunction with a multi-agency security team, CSAC developed and modeled realistic scenarios covering multiple venues and multiple threat agents, each of which would challenge the response efforts in different ways.

The modeling and analysis, produced by Mr. Ray Jablonski, Ms. Lindsay Evans, Dr. Sarah Bereznicki, and Mr. Dennis Howell, included potential public health impacts from the release of ten different materials. The ten materials covered the range of simple to more complex attacks for three major outdoor events and two indoor venues, including the venue of Super Bowl LVII at the State Farm Stadium. The planners expressed their appreciation for the analysis and used the results to inform emergency planning and response agencies. The results led first responder agencies to adopt several changes to pre-event CONOPS to enhance readiness.

State Farm Stadium in Glendale, Arizona.

DEVELOPMENT AND DEPLOYMENT OF HExCAT MODELING TOOL

CSAC developed the Homeland Explosive Consequence and Threat (HExCAT) Modeling Tool in 2020 to provide emergency managers with capabilities to streamline decision making and emergency response planning. HExCAT is a unique modeling system that can estimate scenario-specific hazards and potential outcomes, helping emergency managers plan for and mitigate the impact from explosive devices, given the inherent uncertainty in these attacks. On September 26, 2023, HExCAT patent no. 11766294B1 was awarded to CSAC and its co-contributors.


US011766294B1

(12) United States Patent
Gooding et al.

(10) Patent No.: US 11,766,294 B1
(45) Date of Patent: Sep. 26, 2023

CSAC scientists Ms. Rachel Gooding, Dr. David Reed, and Mr. Alex Dolan provided valuable insight on HExCAT's consequence modeling methodology and integrated medical response module at the Vulnerability Assessment Protection Options (VAPO) Technical Exchange Meeting hosted by DTRA. The probabilistic assessment of human health impact and structural damage integrated with a medical response module provides a unique capability to the explosives modeling community. The presentation and ongoing work with the VAPO technical team have highlighted how HExCAT could best be used, independently or in conjunction with other types of analysis, to support decisions. This exchange is part of CSAC's transition strategy for this capability.

CSAC demonstrated the HExCAT tool to stakeholders during the biannual full-scale exercise sponsored by the DHS Cybersecurity and Infrastructure Security Agency (CISA) Exercise Division. Scenarios for this exercise included an improvised explosive device at a public transit station at the sporting complex, an active shooter, and a vehicle ramming occurring at simultaneous sporting events. The scenarios included representatives from the National Hockey League at Little Caesars Arena, National Football League at Ford Field, and Major League Baseball at Comerica Park. HExCAT was used to deconstruct the scenario to estimate the potential casualties, response requirements, and identify choke points and limitations in the response. The exercise showcased the power of a HEXCAT analysis to better plan for a response, as well as provide an opportunity for the HEXCAT team to better understand the needs and thought processes of first responders to guide future development.

CISA Exercise Division at Comerica Park in Detroit, Michigan, home of the Detroit Tigers.

RESPONDING TO CHEMICAL INCIDENT REQUESTS FOR INFORMATION

In FY 2023, CSAC responded to 26 Requests for Information (RFI) to provide 24/7 Technical Assistance for chemical incidents, subject matter expertise, and other chemical questions. Nine of those RFIs were in support of national level Interagency Modeling and Atmospheric Assessment Center (IMAAC) events. CSAC highlights include:

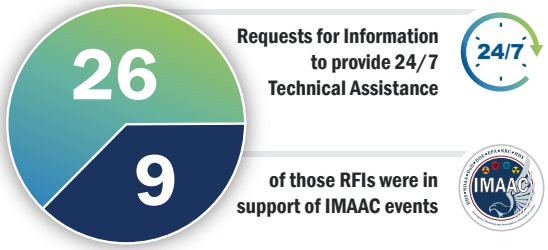

Photo credit: NTSB

- Generated a bulletin for IMAAC "Chemical Considerations for the Train Derailment and Fire in East Palestine, OH, February 3–8, 2023" which described the chemical incident and hazards related to the spillage of vinyl chloride.
- Provided information on the chemical hazards associated with combustion products related to burning oil (hydrogen sulfide, sulfur dioxide) and reviewed the IMAAC modeling results for the Environmental Protection Agency Region 5 concerning an oil refinery fire in Oregon, Ohio.
- Provided chemical hazard and vulnerability information to the 61ST Civil Support Team in Arkansas on Earthquake Mission Support.
- Developed and delivered a tool to the U.S. Secret Service to determine stand-off distances necessary to reduce exposure to chemicals used by protestors in various riot scenarios.
- Provided information on fentanyl syntheses to U.S. Immigration and Customs Enforcement including reaction pathways for fentanyl, fentanyl analogs, and fentanyl precursors.
- Generated a report for the Mid-Atlantic High Intensity Drug Trafficking Area on the accuracy of xylazine test strips after interferences were identified for known components in street drugs.
- Performed evaluations for the Committee for Foreign Investment in the United States regarding implications of the purchase of U.S. companies by international entities, explaining the significance of the transfer of chemical-related capabilities and technology.

CSAC EXPANDED LABORATORY SPACE AND CAPABILITIES

In FY 2023, CSAC's CSL, a partnership with DEVCOM CBC leveraging the Army's more than a century of experience with hazardous chemicals, doubled in size, adding a 3D printing capability. The additional space underscores CSAC's continuing partnership with DEVCOM CBC and includes new collaborations with their scientists in areas of filtration, decontamination, and detection of hazardous chemicals.

The additional space enables the CSL to perform more experiments on chemicals of concern to DHS. CSL researchers expanded the characterization of hazard chemicals in different environments and background matrices, generating experimental data which will improve the underlying model and risk assessment studies. CSL capability improvements include the ability to test and evaluate nanomaterials to determine their feasibility in defense of the Homeland.

***Above**: Scientists work in a chemistry lab at Aberdeen Proving Ground's Edgewood Arsenal near the end of World War 1. Edgewood became home to the nation's Chemical Warfare Service where it conducted the U.S.'s defensive and retaliatory chemical weapons program. **Middle**: One of CSAC's FY 2023 ORISE interns, Mr. Jasen Mabus, collaborated with DEVCOM CBC's Dr. Samir Deshpande using Artificial Intelligence and Machine Learning to process data generated from E-nose detection devices. **Below**: CSAC hosts S&T Under Secretary Dr. Dimitri Kusnezov in the Chemical Security Laboratory.*

FORGED GROWING RELATIONSHIPS WITH KEY PARTNERS

Experts from CSAC participated in the Non Conventional Threats (NCT) USA Conference in Aberdeen, Maryland. The event was co-sponsored by DEVCOM CBC and the Chemical, Biological, Radiological, Nuclear and Explosives (CBRNe) Society and featured experts and decisionmakers representing multiple sectors within the national CBRNe community. CSAC Director, Dr. Shannon Fox, was joined by Deputy Director, Ms. Helen Mearns, and Dr. Rabih Jabbour at the event. Dr. Fox participated in a panel on "Homeland Defense Response from Emerging Threats," and discussed CSAC's capabilities and efforts in chemical defense. The conference was attended by more than 500 delegates including representation from 11 NATO allies and exhibits from 44 companies with capabilities spanning CBRN mission areas such as medical mitigation, detection, protection, and hazard management.

Ms. Helen Mearns and Ms. Rachel Gooding engaged experts from the joint Federal Bureau of Investigation (FBI), and the Transportation Security Administration (TSA) Terrorist Explosive Device Analytical Center, Improvised Explosives Detection and Synthesis (TIEDS) Center to discuss research on explosives synthesis, characterization, detection, and future opportunities for partnership. The TIEDS Center is an interagency partnership organization among S&T, the FBI, and the TSA that assesses the characteristics of improvised explosives and devices to evaluate detection technologies against existing and emerging explosive threats.

Attendees at the NCT USA conference expo, co-sponsored by DEVCOM CBC, networked and shared industry knowledge across organizations. (Photo by NCT Consultants) (Photo Credit: Courtesy)

ENHANCING CAPABILITIES THROUGH LABORATORY PIPELINE

To enhance CSAC's detection and predictive toxicology capabilities, Dr. Jerry Cabalo collaborated with experts from the Pacific Northwest National Laboratory (PNNL), DTRA, the National Institutes of Health, and U.S. Food and Drug Administration regarding new chemical detection instrumentation and algorithms. Headway was made on topics such as new methods for chemical signature prediction and chemical properties for emerging chemical threats including new fentanyl analogues.

Dr. Cabalo, in collaboration with PNNL, has constructed a software "pipeline" to automate the calculation of quantum mechanical properties of synthetic opioids. The properties include molecular structure, vibrational frequencies, gas phase infrared spectra, electron density, and electrostatic potential around the molecules. The objective is to use the calculated properties, along with available experimental results, to exploit machine learning to build mathematical models that are expected to be capable of predicting toxicological values for new and emerging opioids. To date, quantum mechanical calculations have been performed for ~300 fentanyl analogues and ~25 non-fentanyl synthetic opioids.

CSAC's Dr. Jerry Cabalo (left) collaborates with a PNNL scientist on chemical detection lab work.

KEY COLLABORATIONS ADVANCE INNOVATIVE SOLUTIONS TO CRITICAL INFRASTRUCTURE AND GFR THREATS

CSAC continued collaborations with the UK, and other international and interagency communities, regarding aviation hazard modeling and gas forming reactions (GFR) threats. Earlier in the year, CSAC hosted UK Dstl scientists on harmonizing approaches to modeling aviation threats, including assessment of health effects related to those threats, evaluation of potential mitigation strategies, and differences in the toxicity values used. The visit also captured how to best validate the models against the data from tracer trials or, in the absence of trial data, in comparisons to other models. The UK scientists shared the details of their model validation methods, which CSAC is adapting to the ongoing validation of B767 ground trials.

DHS S&T CSAC hosted scientists from the UK Defense Science and Technology Laboratory in a continued collaboration regarding aviation hazard modeling and validation.

CSAC scientists Ms. Rachel Gooding, Dr. David Bradley, Mr. Dennis Howell, Ms. Lindsay Evans, and Mr. Ray Jablonski participated in a GFR modeling workshop at DHS TSA with representatives from the UK, France, and interagency partners. The workshop showcased the work of analyzing the impact of the GFR threats on transportation targets. CSAC and the UK Dstl and Department for Transport presented complimentary briefs on the work accomplished since 2017 which has led to a cohesive scientific set of results on which policy decisions can be made in the U.S. and UK.

Demonstrating continued relevance to DHS and state, local, tribal, and territorial stakeholders, CSAC leveraged its extensive aircraft chemical release studies to develop Pharmaceutical-Based Agents (PBA) release consequences modeling for more general small indoor spaces. At the request of the DHS Countering Weapons of Mass Destruction Office and the Florida Department of Law Enforcement, CSAC modeled a low and high purity PBA release in an airplane and a conference room to capture potential consequences in spaces with higher and lower air change parameters.

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