NSF Convergence Acceleration Workshop

Research Track: Chemical Sensing Innovation:

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Executive Summary

This report summarizes discussions and findings from a recently concluded NSF Convergence Accelerator workshop titled: "Frontiers in Chemical Sensing: Synthetic, Neuromorphic, and Cyborg Systems". The main objectives of the workshop were:

1) Identify the most important recent research advances in biological olfaction, material science, bioelectronics, manufacturing, genetic engineering, and AI/ML/Data Science that when integrated would push current boundaries in miniaturized, non-invasive chemical sensing;

2) Seed the transition of convergence research in the above-mentioned disciplines into tools and solutions that address national-scale societal challenges.

The highly interdisciplinary workshop included participants from academia, industry, and various federal research and funding organizations. In this report we summarize discussion points and findings from the workshop. Specifically, participants identified five thematic areas encompassing key societal challenges that would immediately benefit from advanced, robust chemical sensing technologies:

1) Environmental Chemical Sensing
2) Agriculture, Food Production, and Quality Control
3) Security and First Responders
4) Point-of-Care Applications
5) Personalized Chemical Sensing

Findings from a SWOT (Strengths, Weakness, Opportunities, and Threats) analysis for each of these application domains are summarized in this report. In addition, we list potential milestones and deliverables for short- (9 months) and longer-term (three years) projects in these areas. Finally, participants identified and discussed cross-cutting issues common across sensing applications and technologies.

Our charge

The NSF's Convergence Accelerator initiative tasks stakeholders to identify and elaborate on meeting societal challenges through collaboration and integration across disciplines, sectors, and technologies. We designed this workshop to bring together researchers, innovators, business leaders, and other key stakeholders to contribute their expertise on how to harness recent advances in biological, physical, chemical, and data science engineering to build the next generation of chemical sensors. To meet NSF's criteria for the Convergence Accelerator, we focused on ideas that:

- Address a specific and significant societal need;
- Have a high likelihood of success based on recent advancements in related fields and/or technologies;
- Are likely to be achievable within 3-5 years.

A total of 68 professionals registered for the four-day workshop. Participants included researchers from diverse fields including material science, chemistry, physics, chemical engineering, biomedical engineering, mechanical engineering, neurobiology, molecular biology, AI/ML/neuromorphic engineering, instrumentation engineering, and genetics. Researchers and policy makers from industry, academia, and various federal agencies, including NASA, ONR, NIH, NIST, DTRA, and DARPA were also in attendance. Before discussing specific areas of research focus, we asked participants to work together to answer the following questions:

- What are the pressing societal needs that can be met by chemical sensing technologies?
- Where are chemical sensors likely to have the greatest impact?
- What are the most promising recent advances in chemical sensors?

From these discussions we identified five thematic areas that encompassed the majority of recent interest, enthusiasm, and progress. Participants then worked to define key objectives within these themes, as well as strengths, weaknesses, opportunities, and roadblocks relevant to current research. Each theme is presented in detail below, including short- (9-month) and longer-term (3-year) milestones. Finally, we asked participants to reflect on the insights collected over the course of the workshop and articulate a "Grand Challenge" to the field of chemical sensing. We set no specific guidelines, but all were encouraged to consider what they think would help focus the field and/or develop a set of standards to promote convergence and accelerate progress within NSF's 2-3 year time horizon.

Significance and Critical Needs

Societal challenges/problems that could be addressed through advances in chemical sensing

As humans, we are severely limited in our ability to sense our chemical surroundings. We possess among the most limited olfactory sense across all mammals; ~650 fewer functional olfactory receptors than canines (Ache and Young, 2005) and ~800 - 900 fewer than mice or rats (Ache and Young, 2005). As a result, there are vast amounts of information about our environment—and ourselves—that are inaccessible to us without technology-based chemical sensors. Indeed, as our understanding of the universe of chemical signaling grows, we are ever more aware of the potential for novel chemical sensors to help keep us safe and healthy and to monitor larger scale environmental changes. We asked participants to identify current real-world challenges or problems that could be addressed with chemical sensing technology, and what the impact would be for society were that technology to exist. Responses coalesced around 10 topics:

- Disease exposure: Our highly interconnected society makes it critical to detect disease exposure and identify outbreaks early enough to prevent rapid spread. In addition to detecting certain organic compounds that indicate the presence of disease, chemical sensors can be used to track changes in a local environment following exposure to correlate markers with the development of respiratory disease.

- Food safety and quality control: Massive amounts of food are transported and stored all across the country. Monitoring that food for bacteria or mold that can be harmful if ingested is critical to maintaining the safety and quality of our food supply. Most tests of food safety and quality that are currently available involve complex laboratory assays or human tasting panels, both of which can be resource- and time-intensive. Novel chemical sensors could not only allow rapid monitoring of food quality but also reduce food waste. The latter has been classified as a 'wicked problem' by the NASA convergence acceleration workgroup[1].

- Hazard detection: One of the greatest potential impacts of advanced chemical sensing technology is improved hazard detection. Industrial applications could include detecting the presence of dangerous volatile organic compounds (VOCs)

[1] https://twitter.com/i/status/1434201624168304646

or leaks in a nuclear plant, or using advanced robotics to determine their source. Advanced sensors guided by robotic navigation could also replace canines trained to detect and locate explosives or other key chemicals in emergencies.

- Indoor environment monitoring: The COVID-19 pandemic highlighted the importance of monitoring indoor environments in keeping people safe. Existing and novel chemical sensors could be used to help us measure and understand how contaminants are carried on air currents to better align federal regulations with data-backed recommendations. Indoor sensors could also be used to monitor for bacteria or mold that can adversely impact human health and quality of day-to-day life.

- Personalized sensors: There is enormous potential to design and develop small, portable, and affordable chemical sensors for personal use. Applications may include monitoring one's personal chemical environment for pollutants, toxic gasses, infectious agents, or allergens.

- Clinical screening: There are numerous reports of volatile biomarkers that correlate with disease conditions in humans. Advanced chemical sensors could make such data actionable by alerting physicians to some of the earliest signs of disease or dysfunction, e.g., changes in gut bacteria.

- Supply chain safety and security: With technological advances to improve portability, reliability, and durability, chemical sensors can be deployed throughout the industrial chemical supply chain to ensure authenticity and support trust verification.

- Coastal waters monitoring: Harmful algal blooms have become more common in recent decades as a consequence of our changing climate. Overgrowths of some species of dinoflagellates or diatom (so-called "red tides") can devastate marine life and present hazards to human health and coastal economies[2]. Chemical sensors could be used to monitor coastal conditions to either detect the onset of harmful algal blooms earlier or even to predict when one is likely to occur based on environmental factors.

- Underwater detection: In addition to these specific areas of interest, participants noted that one of the greatest challenges in the field currently holding back progress is in designing sensors to operate reliably and effectively across diverse environments. What exactly this entails obviously varies depending on the sensor, the substrate, and the environment within which the sensor must operate. For example, for oceanographic applications, we need suitable underwater submersible technologies that house and protect the chemical sensor and associated electronics. Focusing efforts on developing a set of technological advances, for instance enhancing the diversity and durability of chemical transducers, that can improve the robustness and/or performance of chemical sensors across many different applications, has the potential to move the entire field forward.

Significant recent advances in chemical sensing technology

Fields associated with chemical sensing, i.e., biological olfaction and AI/ML related to chemical informatics, are moving at break-neck pace. Our growing understanding of the exquisite sensitivity and precision of chemical sensing in biological organisms intersects with key advancements in machine learning (ML), artificial intelligence (AI) and micro-engineering, generating exciting opportunities to integrate these advances in meaningful ways and drive the field forward in a non-

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[2] NOAA. Historical Maps and Charts audio podcast. National Ocean Service website, https://oceanservice.noaa.gov/podcast/july17/nop08-historical-maps-charts.html, accessed on 11/30/22

incremental fashion. Participants noted several specific recent advances in chemical sensing technology that are particularly relevant to some of the most pressing needs for chemical sensors:

- Brain-machine interfaces (BMIs): Recent advances in miniaturizing electrode arrays to allow for monitoring neural responses in behaving animals, as well as novel neural signal processing algorithms, and proof-of-concept data on innovative chemical sensors have laid the foundation for developing BMI-based approaches to chemical sensing. In these approaches, the biological organisms' capability to detect and recognize chemical cues are exploited by tapping into their neural or behavioral signals. This idea has been demonstrated recently using both vertebrates (Shor et al., 2022) and invertebrates (Saha et al., 2020; Farnum et al., 2023; Neta et al; 2023).

- Diversity of Electronic noses technology (e-noses): Recently developed e-nose technologies include plasmonic sensors, surface acoustic waves, quartz crystal microbalances, colorimetric sensors, MEMS-based chemiresistive technologies, miniaturized instruments (e.g., GC-MS), surface-enhanced Raman spectroscopy, and electrochemical sensor arrays, among others (Li et al. 2019; Lee et al 2021; Pena-Pereira et al. 2021; Ozer et al. 2021). Notable progress over the last 5-10 years has resulted in diverse sensor transduction mechanisms, enhancing the potential to detect and recognize chemical targets of various types.

- Gene editing: The recent advances in CRISPR-based gene editing approaches make it possible to tweak a biological sensor array and potentially create designer transgenic animals that are exquisitely sensitive to select chemicals. This will be necessary to fine-tune the general-purpose biological sensor array (a vertebrate nose or an invertebrate antenna) in an application-specific manner.

- Synthetic biology: Expressing biological transducers or other biologically-derived materials *in-vitro* has also been successfully exploited in e-nose technology. Of particular interest is the ability to express olfactory receptors in heterologous mediums such as cell cultures, or in combination with biocompatible semiconductor technologies (Kwon et al., 2015).

- Data science and Artificial intelligence/Machine learning: With the rise of technologies that generate extremely large data sets have come advancements in how to handle and process such large datastreams. This is also true for artificial olfaction. Recent progress in data preprocessing and inferring techniques that led to breakthroughs in computational vision and speech processing can and should be used as templates for similar advances in the chemical sensing field. Particularly important will be methods that allow seamless integration of data from multiple different types of sensors, and methods through which to rapidly recalibrate replacement sensors. We currently lack data from sensors operated in real-world scenarios, which are necessary to determine how we may adapt existing methods and/or develop new methods appropriate for chemical sensing.

- Largescale manufacturing capabilities: To accelerate technology transfer from the lab to the real-world, we need to develop large sensor arrays that can be manufactured at scale. Developing disposable sensor arrays, either through additive manufacturing methods or standard lithographic methods, should make it possible to deploy different sensing technologies more widely and at lower cost.

Despite these critical advancements, human-built chemical sensors are limited in their ability to replicate the high dimensionality of chemical sensing/olfaction; capture the enormous, ill-defined, and dynamic chemical sensing space; or recognize chemical cues independent of extrinsic perturbations (i.e., differences in environmental or temporal contexts, or changing ambient conditions). For context, there are ~1000 genes in the human genome that encode olfactory receptor proteins (approximately one out of every 30 genes plays some role in olfaction; Ache and Young; 2005). Although most of these genes are psuedogenes, the human olfactory epithelium does employ ~300-350 different types of olfactory receptor proteins (Ache and Young; 2005). Even relatively simple organisms, like fruit flies, have 55-60 different olfactory receptor proteins (Ache and Young; 2005). In contrast, state-of-the-art chemical sensor arrays have fewer than 50 sensors, which generally perform worse than their biological counterparts in both selectivity and sensitivity (Raman et al., 2011). Moreover, current artificial intelligence/machine learning methods cannot accommodate signal drift or non-stationary data distributions. Finally, whereas we have pattern recognition models that work remarkably well for visual data, the same approach applied to olfactory data has been less successful.

Identifying opportunities for convergence

Given the challenges and recent advances noted above, we next explored the points at which the two lists overlap. Specifically, where can novel chemical sensing technology be immediately applied to help address a real-world need? Below we list a few such opportunities for convergence.

Applying what we have learned about chemical sensing in biological systems to:

- **Increase the number of different compounds detectable via chemical sensors:** As noted earlier, the biological sensor arrays are large and diverse, employing a number of olfactory receptors to detect and recognize various chemical species. Thus, enhancing diversity among sensors and sensing mechanisms is an area that requires integration across material and biomolecular sciences. Taking advantage of the rich repertoire of synthetic transducers and bio-derived transducers that are sensitive to and selective for a variety of chemical species is one important area of research convergence.

- **Build better artificial intelligence models**: The challenges posed by high-dimensional, dynamic data obtained from chemical sensors requires that we adapt recent advances in AI/ML algorithms, such as deep learning neural networks and other novel dimensionality-reduction approaches. Neuromorphic approaches that seek to model neural information processing principles directly, provide an alternate approach to statistical algorithms. These areas are ripe for breakthrough and require large datasets from sensor arrays that are operated in realistic environments.

- **Build multimodal electronic noses:** Biological olfaction tends to use information such as vaporization rates, air turbulence, presence of information from other kind of sensory information to improve recognition and performance. An electronic nose that is similarly multimodal would improve on current technology, and represents a key area of convergence. While tranducers that detect these various environmental cues are already available, integrating them in a suitable framework is an area of integration and acceleration.

- **Build animal-machine hybrid devices:** Recent proof-of-concept results demonstrate that bio-hybrid systems that directly tap into the capabilities of biological olfaction are viable. Integrating advances in electronics, instrumentation, robotics, and data sciences, building functional animal-machine chemical sensing systems and validating their performance in different application domains remains a high-priority goal that can be achieved within the next two-three years.

Applying advancements in instrumentation to improve:

- **Durability:** Build sensors that can withstand harsh environmental conditions such as those experienced in industrial or under-water settings.
- **Longevity:** Prolong functional sensor duration either through refreshable sensor arrays (i.e., self-cleaning sensor surfaces or disposable sensor arrays) or recalibration approaches that compensate for reasonable sensor drift.
- **Efficiency:** Design sensors that use less power to increase lifespan and therefore viability for use-case scenarios.
- **Modularity:** Build modular sensors with parts that can be replaced as needed.

Applying advancements in data science and AI/ML to improve:

- **Sensor fusion/networks:** As mentioned before, developing distributed sensing frameworks within which information from different types of chemical and non-chemical sensors are integrated to enhance the sensing performance is a promising area of convergence.
- **Availability of datasets:** Unlike other sensory modalities, we still lack operational sensor data with which to develop novel algorithms and signal processing approaches. An immediate need in the field is to obtain application-specific datasets that can then be used to develop and train machine learning models that enhance sensor performance.

Theme Recommendations

We identified five themes encompassing the areas where research readiness and enthusiasm converged with technology readiness and societal need. We then asked participants to answer the following questions specific to each of those themes:

- What is the key objective of developing these types of sensors?
- What are the strengths (knowledge we have), weaknesses (knowledge we need), opportunities (questions/challenges that can be addressed right now), and threats (critical limitations and roadblocks to progress) related to this theme?
- What opportunities are there for convergence in this area?
- What key advances make this area ready for acceleration?
- What are some 9-month and/or 3-year milestones that pertain to this theme?

Theme A: Environmental Chemical Sensing

Climate change and chemical pollution are two defining and urgent issues of our time. Climate change is expected to worsen the frequency, intensity, and impact of extreme events such as wildfires and hurricanes. Importantly, our ability to sense chemical pollutants, monitor changes in our atmosphere and large bodies of water, and predict extreme events is limited. We need to improve upon and develop novel environmental chemical sensing technologies to inform climate and pollution policy and workplace improvements.

Goals and objectives

Measure and track changes in the concentration profiles of volatile organic compounds (VOCs). Changing levels of VOCs, such as CO_2 and methane, reveal how the climate and atmosphere are changing at the global and local level. The next generation of chemical sensors optimized for detecting VOCs in the environment will help inform those tasked with making decisions based on the current state of the climate. We can also use such data to develop ML/AI algorithms that predict the occurrence of extreme events such as volcano eruptions, forest fires, and red tides. An early warning system for extreme events that uses chemical sensing technology could inform evacuation and other countermeasures and have a great societal impact. Toward this end, biologically-inspired solutions, such as bio-hybrid sensors, could be used to detect such events. Indeed, certain insects can detect specific chemicals present in smoke from far off distances (Gee, Nature 1999), which could be exploited to develop forest fire detection solutions. Developing capabilities to tap into the biological chemical sensing capabilities, and determining the limits of detection (sensitivity and distance) will be crucial to advance stand-off detection technology that can be used in face of extreme events.

Monitor air, water, and soil for pollutants and toxins. The World Bank estimates the global economic costs of pollution at $225 billion[3]. The next generation of chemical sensing technologies will need to be able to rapidly detect pollutants to support informed policy, manufacturing, and waste management decisions to minimize impact on the environment and human health. For example, landfill emissions have a critical impact on environment quality, and chemical sensors for VOCs and ammonia emissions are needed to evaluate whether the amount of emission and its spread are reaching concentrations that are regarded as immediate danger to life and health[4]. Such technologies cannot be limited to VOC detection; liquid-based sensing will be key in monitoring local water supplies and water waste. A related objective in this theme is to develop chemical sensors for environmental toxins that can monitor their distribution over space and time. Toxins have recently been linked to cancer, heart problems, and many other issues (Cohen and Jefferies, 2019). However, our ability to rapidly detect the source of these toxins is currently limited (McKone TE, Huey BM, Downing E, et al., 2000).

Monitor for hazardous chemicals in the workplace. According to the Occupational Safety and Health Administration (OSHA), an estimated 32 million workers in >3.5 million workplaces in the United States are regularly exposed to hazardous chemicals[5]. Chemical sensing is already implemented in some cases. For example, an optoelectronic nose was used to differential 19 toxic industrial chemicals (Lim et al., 2009). Microelectromechanical systems (MEMS)-based microsensor arrays can detect toxic chemicals in complex settings with interferences and background gases (Raman et al., 2009). However, OSHA identifies a large repertoire of chemicals as toxic gases[6], and novel technologies are needed to sense a large fraction of these chemicals. Implementation will be another challenge. Barriers to adoption include high cost and the logistical burden of implementing a new system into an existing workflow. Policy changes and regulatory efforts may also be necessary to enforce adherence.

Integrate multiple sensors to increase impact. Participants noted that creating and expanding the range of sensors that can be integrated within the "internet-of-things" will be critical to achieving the full potential of the next generation of chemical sensors. This type of integration, whether on a local or more global scale, would make it possible to consider data from multiple sensors to inform decisions or train AI/ML models.

Current limitations

Sensor selectivity and sensitivity. Some of the most advanced chemical sensors currently available do not have sufficient sensitivity to detect pollutants and toxins at relevant concentrations. In other cases, sensors are limited in their dynamic range and selectivity. Given the dynamic nature of the environment, new technologies will need to account for variables

[3] https://www.worldbank.org/en/news/press-release/2016/09/08/air-pollution-deaths-cost-global-economy-225-billion. Accessed 11/30/22.
[4] https://www.compostfoundation.org/Portals/2/COTC%20Reports/CCREF%20Emissions%20Paper%20(NPR).pdf?ver=2020-07-23-135819-210. Accessed 11/30/22.
[5] https://www.osha.gov/news/newsreleases/trade/03012012. Accessed 11/30/2022
[6] https://www.osha.gov/emergency-preparedness/guides/toxic-industrial-chemicals. Accessed 11/30/2022

including temperature, humidity, wind flow, and soil composition. Accounting for humidity and other ambient condition changes—interfering gases in particular—remains a critical issue.

Localization issues. Although we understand how sound and light propagate, measuring and predicting three-dimensional fluid and gas flow is challenging, particularly within the parameters of a sensor operating in situ. Future research will need to focus on understanding how to optimize selectivity and sensitivity amid dynamic sensing environments.

Scalability. Given the scale of global climate monitoring, efficient sensor production will be critical. Currently, manufacturing chemical sensors at scale is limited, as lab-based solutions do not necessarily scale well. Indeed, the path towards producing the large-scale arrays needed for environmental monitoring needs to be paved. Technology developments, such as ink-jet printing or localized heat-induced growth or directed self-assembly (Guo et al., 2022), will be needed to be further refined to reduce production costs and increase production efficiency.

Longevity. Providing sensors with an adequate power supply, especially in remote areas away from power lines, remains a challenge. Furthermore, sensors often experience drift and a limited lifespan. Bio-hybrid sensors in particular have limited lifespan and durability (Saha et al., 2022). Both biologically inspired and synthetic sensors require appropriate calibration, but we are lacking methods to automate this process. Before widespread implementation of environmental chemical sensors can become a reality, these issues of sensor power supply, longevity, and stability will need to be addressed.

Data integration. The large quantities of data that can be collected from multiple, inter-connected sensors will require advancements in data integration techniques. Methods to handle large data sets and build statistical and bioinspired models are well developed (Raman et al., 2011). Methods for drift compensation, rapid sensor recalibration, and transfer of trained models to fresh sensor arrays need further development.

High-impact deliverables

Bio-hybrid sensor platforms. Biologically-inspired chemical sensing solutions at the environmental level are likely to make a significant impact on society in the years to come. There are also some existing technologies that could be scaled to meet the needs of environmental applications. Participants foresee capitalizing on the complexity of biological olfactory and gustatory sensory systems of various species by engineering brain-computer interfaces to create other hybrid designs. For example, proof-of-concept studies demonstrating feasibility in using invertebrate- and vertebrate-based hybrid systems for chemical sensing have emerged (Saha et al., 2020; Shore et al., 2022; Anderson et al., 2020). Gene-editing techniques, which have advanced significantly in recent years (Dierick et al., 2021), can be leveraged to improve hybrid sensors. Participants identified several short-term, high-impact deliverables, including cyborg mouse and insect models in which olfactory receptor neuron activity is artificially boosted to increase sensitivity to chemicals of interest (< 3 years timeframe). A long-term goal (3-5 years timeframe) would be to perfect gene-editing techniques to create reliable bio-hybrid sensors for these environmental objectives.

Neuromorphic sensors. Recent improvements in the availability and affordability of robotic and neuromorphic technologies can be leveraged toward the environmental chemical sensing goals outlined above (Imam and Cleland, 2020; Drix and Schumker, 2021). Specifically, participants identified the development of neuromorphic platforms and the application of photonics to integrate sources and sensing elements on chips as two feasible short-term deliverables. Combining neuromorphic platforms with active sensing and multi-modal signal integration approaches are another area of potential impact (< 3 years timeframe).

ML systems and novel algorithms for data integration. Recent advances in ML, AI, and data science methods have provided a critical opportunity for improvements in data integration. The localization and mapping of the chemical environment is a good first step to achieving the long-term objectives of monitoring the environment for changes in climate and pollutants on a large scale. Participants highlighted the potential of swarm intelligence and the internet-of-things to create a network of chemical sensors to monitor environmental changes. Short-term deliverables for improvements in data collection and integration in environmental chemical sensing include collecting and organizing relevant data from a variety of chemical sensors, and customizing conventional ML systems for olfaction to meet environmental objectives. A longer-term goal is to develop algorithms based on the circuit architecture of the olfactory system to integrate environmental chemical sensing data (3-5 years timeframe).

Theme B: Agriculture, Food Production, and Quality Control

The quality and volume of our food supply are critical to support global health and economic growth. One of the most critical issues we face today is food insecurity, with individuals or even whole populations lacking sufficient access to safe and nutritious food. Indeed, NASA has identified food insecurity as a "wicked problem[7]", meaning that the complexity of the problem is so great that there is no discernable solution or stopping point. However, chemical sensing technology in agriculture, food production, and quality control has the potential to be transformative in terms of improving global food access. Chemical sensors to detect food spoilage and monitor plant health already exist but are not widely implemented. For example, although we know the presence of certain biogenic amines in edible items leads to food poisoning (Tabanelli, 2020), detecting these chemical species remains an unmet need. Participants identified several goals and objectives for the next generation of chemical sensing technology that will improve performance and practicality, towards the ultimate goal of increasing and broadening implementation. We now have a foundational understanding of the composition and metabolic pathways of volatiles produced by plants and can manufacture sensors that are highly sensitive to these volatiles. This is an easy target for further improvement in chemical sensing for applications in sustainable agriculture, and food safety and quality control processes.

Goals and objectives

Improve agricultural productivity. Chemical sensing technologies can be used to improve agriculture practices. For instance, tracking changes in plants' VOC profiles can help farmers determine optimal harvest time (Brillli et al., 2019) or identify the sex of a chick while still inside the egg (Xiang et al., 2022). Chemical sensors could also be integrated with other smart agriculture practices (i.e., high-control greenhouses, Cui et al., 2021) to improve agricultural infrastructure to increase productivity, for example by determining the optimal chemical environments for vertical farming or autonomous agriculture systems to enrich yield. Participants also noted the goal of leveraging genetic engineering in plants to effectively work as chemical sensors themselves, or to emit chemicals that impact neighboring plants to improve agricultural production (Kos et al., 2013). As a secondary objective, sensors that detect chemical emissions by plants in real time could enable new research into plant communication by VOCs.

Monitor environmental impact of agriculture and food production. Agricultural practices, especially those conducted at scale, can have a tremendous impact on the environment and are a major contributor to climate change[8]. Technology to

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[7] https://appel.nasa.gov/2010/02/25/ao_1-4_f_wicked-html/ (accessed 01/12/2022)

[8] https://ccafs.cgiar.org/media/press-release/agriculture-and-food-production-contribute-29-percent-global-greenhouse (accessed 12/01/2022)

detect plant distress as a result of changing conditions could be helpful to track the effects of climate change. There is also the potential to apply chemical sensors to track pesticides and herbicides with known deleterious effects on biodiversity and/or human health [e.g., glycophosphate spray linked to pollinator death (Motta et al., 2018), dithiocarbamate linked to Parkinsons; (Goldman, 2014)]. Thus, an important goal is to develop sensors to monitor for these chemicals. Finally, participants note a key area for technological integration in this field: the use of optical chemical sensors in conjunction with other chemical sensing technologies to create satellite maps of crop health, potential contamination, toxins, and pollutants.

Identify food spoilage and contamination to limit waste. Food spoilage and waste take a large toll on the global food supply, with a third of the food produced being wasted globally[9]. Chemical sensing technologies can be leveraged to identify spoilage early, monitor food quality in transport, and assess food quality using chemical sensing beyond what is accessible to human olfaction. Food processing factories can introduce contamination into the food supply and are a source of toxic substrates and products. Chemical sensing technologies can be developed with the goal to regulate food production to minimize contamination and waste and monitor food processing factories for flammable and toxic substrates and products (e.g., in fermenters and methane digesters).

Current limitations

Limited dataset of relevant odorants. There are several limitations that are currently impeding the development and widespread implementation of chemical sensing technologies in agriculture, food production, and quality control. First, there are limitations in the data necessary to develop these technologies. There have been great advancements in ML and AI techniques in recent decades. However, the application of these techniques to chemical sensing in agriculture and food supply is limited by data scarcity. Therefore, the primary limitation in this field is inadequate data pertaining to relevant odorants. To effectively monitor plant health to improve agricultural practices and identify problems early in the food supply chain, we need to correlate the bouquet of volatiles and other signals to plant health or specific toxins/stressors. Furthermore, we do not know *what* needs to be detected to ensure plant health and food quality, and to detect food spoilage. VOC fingerprinting, in which a pattern of multiple chemicals is detected and linked to a particular outcome, will likely lead to more powerful sensing technologies compared to those that detect a single chemical. Finally, variability in background volatiles, some of which may be geographically dependent, will complicate chemical sensing in this field and is a barrier that novel sensors and data interpretation technologies will need to address.

Sensor portability and deployment. A second set of limitations centers around sensor deployment. Large-scale agriculture, in which fields can extend for miles, requires sensors to be highly sensitive, portable, and fast to identify and localize abnormalities. Drones with attached chemical sensors (e.g., portable gas chromatography-mass spectroscopy, sensor array, and ion-mobility spectroscopy) are promising deployment vehicles for agricultural settings. However, we need a greater understanding of how the sensors will perform under those conditions. Alternatively, sensors could be developed with a greater standoff detection range to cover larger areas. One solution to improving deployment of chemical sensing technologies that was discussed was to integrate chemical sensors into existing infrastructure. Technology is limited by a trade-off among sensitivity, portability, and detection speed. Consequently, a close collaboration among end-users, data scientists, and engineers will be essential to clarify the specific needs for each application and modify sensor development and deployment accordingly.

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[9] https://www.worldbank.org/en/topic/climate-smart-agriculture (accessed 12/01/2022)

High-impact deliverables

Reducing the cost of crops, improving yield, and limiting food spoilage and waste increases food accessibility. Moreover, detecting and limiting pesticide and heavy metal toxins in the food supply is likely to have a great impact on human health. With these high-impact goals in mind, participants noted the following deliverables: On a 9-month time scale, work should focus on evaluating chemical sensing technology to detect plant-emitted volatiles in a greenhouse setting, correlating specific biomarkers with different toxins or stressors, and generating large datasets of odorants relevant to plant health, food quality, and food spoilage. High-impact deliverables possible on a 3-year time scale include validating whether plant health and pathogen infection can be monitored with chemical sensor technology, developing AI to interpret large datasets of food-relevant odorants, and creating chemical sensors tuned for specific biomarkers to detect toxins or stressors.

Theme C: Security and First-responders

Chemical sensing technologies can be used to assess environments and identify dangerous situations. According to a report from the Centers for Disease Control and Prevention, in the 57,975 chemical incidents reported from January 1991 to September 2009, the top five chemicals associated with chemical injury were carbon monoxide, ammonia, chlorine, hydrochloric acid, and sulfuric acid; totaling $45 million in damages annually (Anderson, 2015). Proof-of-concept sensing technologies have been demonstrated for a number of toxic industrial chemicals (TICs) and toxins, such as ammonia, hydrogen cyanide, chlorine, arsine, phosgene, etc. (Lim et al., 2009; Raman et al., 2009). To assess dangers in public spaces and in emergency situations we need to monitor for illicit and toxic substances, localize explosives and other hazards, and be able to assess danger in rapidly changing catastrophic environments. Participants in the workshop agreed that there is great benefit to expanding the use of chemical sensing technologies in security and first response in emergency situations.

Goals and objectives

Improve safety and performance of first responders. Chemical sensing technologies can be implemented to improve the safety and performance of first-responders in emergencies. To this end, goals and objectives include developing technologies that rapidly and reliably assess the environment to provide actionable information to first responders. For example, portable chemical sensing technology could be developed to help firefighters detect the presence of dangerous toxins. These technologies could be wearable or be designed to go into hazardous environments ahead of first responders. In the same vein, chemical sensing technologies could be used to monitor the health and safety of first responders themselves, and that of the public, in dangerous conditions. Here, there is an overlap with the point-of-care theme discussed below, as technologies developed for health monitoring could also be utilized by emergency medical services in the field to rapidly diagnose and monitor. Importantly, any technologies developed to be used by first-responders in the field will need to be portable, compatible with other first-responder gear, fast, and easy to use.

Threat monitoring. There is a need for chemical sensing technologies to monitor for threat agents and other hazardous conditions in public spaces and public utilities. Goals include: improving industrial hazard monitoring, i.e., monitoring for TICs, toxic industrial materials (TIMs), and diesel and gasoline fumes; developing chemical sensing technologies for threat agents, such as explosives, in urban settings; and detecting illicit products and elements in the environment and public water sources. As a crossover with the agriculture theme, chemical sensing technologies could also be used to detect invasive pests at border crossings. Chemical sensing technologies may be uniquely beneficial for identifying and monitoring illicit drug manufacturing sites and shipping containers. Dogs are currently used to “follow the trail” of an odorant, but current training methods are limited by the availability of odorants. To this end, there is an opportunity to develop non-toxic simulants of toxic smells and employ virtual scent generation and virtual reality to better train animals used for these purposes. Eventually, future synthetic chemical sensor technologies may replace canine models.

Improve safety and performance of the military. Finally, chemical sensing technologies also have the capability to improve the safety of the military in the field. Joong Kim (Office of Naval Research; ONR) provided a key note talk that provided details regarding challenges in field deployment and other considerations/constraints that needs to be considered for field operation. Such deployment are by necessity not within the 3 year time line of interest to the NSF convergence acceleration program.

Current limitations

Canine sensors. We currently rely on animal sensors, specifically dogs, for many security applications such as the identification and localization of explosives and illicit substances. These canine models are limited and involve a large financial and time investment for training. Efforts to reduce training time and cost could help ease the burden; however, synthetic and/or bio-hybrid chemical sensing technologies are likely to replace these models in the future.

Complexity of real-world environments. Current chemical sensors are limited in their ability to handle the complexities of the field and the highly dynamic situations in which they are needed. Variations in humidity, temperature, and background interferences can affect sensor performance. In real-world deployment, sensors will be exposed to background odors and interfering substances, which, in many instances, will be geographically dependent. This is a massive hurdle for the field to overcome. A focus should be on validating and testing new or existing technologies in harsh realistic environments prior to deploying for security or first-response applications.

Sensor longevity. Sensors used in the field will need to be operational with a limited power supply and without experiencing sensor drift. While biohybrid models that rely on insect antennae or vertebrate noses do not have these issues, longevity is still an issue. For example, insect antennae present a straightforward strategy for detecting several chemical species, but excised antennae are only operational for a few hours, severely limiting their impact. Other BMIs also experience drift in electrodes, leading to slowly changing signals analogous to the non-stationary datastreams from synthetic sensor arrays.

Difficulties with signal localization. Localizing hazardous substances is an important objective in security and national defense. As mentioned earlier, modeling diffusion of chemicals in urban settings is a non-trivial problem. Distributed sensor networks will be needed, as will methods to fuse information from multiple sensors to develop a concentration profile. In some tasks, localization may require milli-second sensor reaction times.

Sensor deployment. Most current sensors, e.g., chemiresistors, require periodic recalibration, which is impossible to perform in the field. Chemical sensor systems used by first responders and the military will need to be made into field-ready portable systems that are easily operated to reduce the strain on emergency personnel. These sensors will be deployed in highly dynamic situations and will require adaptive technologies and feedback control methods to recalibrate and change the mode of operation. For example, modulating sampling frequency based on relevant input could improve the lifetime of the sensor. Alternatively, the use of disposable sensor arrays obviates the drift problem entirely. Therefore, these technologies will need to be developed and calibrated with the specific end-user in mind.

Generalizability. Sensors used for security and first response in emergencies will be deployed in resource-limited settings, making the development of multi-use systems that provide multiple types of information to reduce the load on the first-responders an important strategy. First responders do not always know the conditions that they are facing, so there is a benefit to increasing the generalizability of the sensors. However, the technology must balance generalizability and specificity, alongside other factors such as portability, durability, and power supply.

Legal issues. Without established standards for the use of chemical sensors in the field, the ability for data procured from these sensors to be used in a court of law will be limited. While these issues and those related to ethics are important, they were not considered in detail in this workshop.

High-impact deliverables

Bio-derived sensors. Participants identified bio-derived sensors as an important opportunity to improve the sensitivity, localization, and speed of sensors in this field. One promising avenue of investigation is the use of insect swarms with surgical implanted trackers to detect and localize odorant signals. Recent improvements in the lifetime of trackers would potentially allow these swarm-based sensors to function for longer periods of time. Insects and swarm-based sensors may ultimately replace checkpoint-based security. There is also proof-of-concept for the use of insect antennae integrated into autonomous drones (Anderson et al., 2020), and entire insect-machine hybrid system systems integrated into autonomous robots (Saha et al., 2020). In combination with gene-editing techniques to develop insect antennae designed to detect specific odorants, this technology could be further improved and developed to detect hazardous substances in real-world applications. Participants identified the development of gene-edited insect antennae that can detect specific odorant receptors as an important and attainable first step that could be accomplished on a 9-month timeline. Bio-hybrid sensors could also be developed using an entire insect rather than just its antennae, allowing longevity and robustness of operation while exploiting the entire neural information processing machinery. In parallel, a high-throughput system to implant electrodes into insect brains or antennae would improve the scalability of these technologies. These advances could then be combined to develop a functional prototype of a single-odorant (e.g., TATP or 2,4-DNT) bio-hybrid detector as a longer-term goal (3 year timeframe).

Novel sensor development. The field can take advantage of the latest advances in integrated photonics and semiconductor processes to produce novel sensor technologies on a large scale. Participants suggested that low-cost portable sensors for use by HazMat teams may be a highly impactful and attainable goal (< 3 year timeframe).

Olfactometer for animal sensor training. Another immediate goal identified by the participants was a prototype for a virtual scent generator that can mix odorants at varying dilutions. As a longer-term goal, this prototype could be used for virtual scent generation and the development of virtual reality training programs for animals-based chemical sensors (3 year time frame).

Theme D: Point-of-Care Applications

Participants in the workshop agreed that chemical sensing technologies could have numerous point-of-care applications, providing more information on the health and disease state of patients with non-invasive techniques. Indeed, chemical sensing technologies are already applied, albeit to a limited extent, to monitor intoxication and other health indications. This is an area of study ripe for investigation as there is already a plethora of literature on known biomarkers for various disease conditions (Turner and Magan, 2004).

Goals and objectives

Diagnosis. Chemical sensing technologies with point-of-care applications have the potential to be leveraged for rapid non-invasive diagnostic applications to improve health outcomes by detecting diseases early in disease progression or at a pre-symptomatic stage. Recent advances toward this goal include: detecting VOCs in breath to diagnose COVID-19 (Chen et al., 2021) or certain cancers (van Geffen et al., 2019), demonstrating that VOC analysis is a feasible diagnostic tool to improve the speed of detection of communicable diseases and other health conditions. To this end, chemical sensing technology should be developed to detect clinically relevant patterns in an individual's odor profile using samples from breath, saliva, sweat, skin, feces, etc. This odorant fingerprint could serve as a baseline, or to track what happens after a patient consumes a reagent to stimulate a reaction. Understanding disease-relevant odorant fingerprints will also inform our understanding of disease biology.

Epidemiological monitoring. Chemical sensing technologies that detect communicable diseases on the individual level could be modified to monitor disease spread in populations, e.g., wastewater detection or indoor air monitoring.

Health and disease monitoring. Beyond diagnosis, chemical sensing technology can be used to non-invasively monitor the progression of chronic diseases and conditions over time. For example, a recent study demonstrated that e-noses could differentiate among different categories of asthma patients based on systemic inflammatory markers, circulating eosinophil and neutrophil counts, and oral corticosteroid use (Licht and Grasemann, 2020). The galvanic skin response (changes in skin conductance with sweat secretion) is currently used as a non-invasive measure of arousal to investigate stress and anxiety (Markiewicz et al., 2022). However, this technology could be improved by adding chemical sensors that analyze the *contents* of the sweat. Further, chemical sensing technologies could leverage recent advances in microbiome research that have identified markers associated with diabetes, alcoholism, cancer, Parkinson's disease, COVID-19, epilepsy, ebola, inflammatory bowel disease, asthma, cystic fibrosis, strep throat, ulcers, depression, and stress and anxiety disorders. By collecting VOC and odorant fingerprint data on an individual overtime, providers may be able to detect longitudinal changes in secondary metabolites that are indicative of microbiome alterations associated with disease. Accordingly, novel algorithms would be required to analyze the complex datasets involved in these analyses to identify functionally-relevant changes over background noise.

Current limitations

Data interpretation. We are currently limited in our ability to correlate data from analyzing breath and other personal odorants to clinically-relevant information, e.g. to inform a diagnosis. Further, variations in personal VOC fingerprint overtime are not understood, making it difficult to appreciate whether monitoring at a single or multiple time points is needed. We need more data, as well as more work to determine the best analyses for these data, including ML algorithms and similar techniques for handling large datasets.

Dearth of target odorants. In many cases, the target odorant or pattern of odorants identifying a particular health state is unknown. There is currently an unmet opportunity to replicate or harness the innate abilities of biological organisms in the field of chemical sensing for medical purposes. We can train animals, such as dogs, to detect medical conditions. For example, seizure-alert dogs can detect seizures seconds to minutes before they strike[10]. Recent reports argue that dogs can sniff out COVID infection[11]. However, we are limited in our understanding of *what* the dogs are sensing. Disease state is likely more represented by an odorant fingerprint (collection of odors) than through the detection of a specific biomarker (or set of biomarkers). Moreover, non-relevant odors (background odors) dependent on foods eaten, general metabolic state, personal hygiene, and other factors, can confound the final odorant fingerprint, further obfuscating the target.

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[10] https://www.epilepsy.com/recognition/seizure-dogs (accessed 12/01/2022).

[11] https://www.npr.org/sections/goatsandsoda/2022/06/16/1104931711/dogs-trained-to-sniff-out-covid-in-schools-are-getting-a-lot-of-love-for-their-e (accessed 12/01/2022)

Regulatory and ethical concerns. Healthcare applications require diligent regulatory procedures before implementation. Regulatory approval for sensing systems that utilize pattern recognition rather than the precise identification of a disease marker is uncharted territory. Moreover, there are unresolved ethical issues pertaining to odorant fingerprints. For example, the personal ownership rights of the air space surrounding an individual are unresolved, making data acquisition, privacy, and testing of an individual's airspace open topics of debate. Therefore, ethicists and legal experts need to comment on intended technologies and their applications.

High-impact deliverables

Data collection, integration, and analysis. Many short-term, high-impact deliverables for point-of-care applications center around data collection and analysis. AI, ML, and computational systems allow for deeper analyses of odorant fingerprint data than those performed in the past and need to be applied to a greater extent in this field. Investigations need to correlate odorant data with clinically-relevant measures. Further, data matrices that explain health-related phenomena and show an emergence of a clear signal should be created. Finally, efforts should be focused to identify clinically-relevant targets for which sensors need to be developed (< 3 year time frame). On a longer timescale, efforts must focus on problems in which clinical targets are unknown (i.e., odor fingerprint recognition; 3 – 5 year time frame).

Sensor development. Participants in the workshop agreed that novel sensors need to be developed to meet the point-of-care goals described above. There is an opportunity to extract the biological sensing elements, such as the olfactory receptor proteins, from animals and integrate this biologically derived component with a synthetic device to create bio-hybrid sensors. Novel synthetic sensors could also be developed using recent advances in miniaturizing instruments or through recent advances in nanomaterials. One 9-month deliverable would be a proof-of-concept model showing the feasibility of detecting specific disease or health states using odorant profiles. On a longer timescale, the focus must be on quantifying diagnostic performance within more complex operational settings (3 year time frame).

Theme E: Personalized Chemical Sensing

In the current era of personal health tracking devices and personal smart devices, one can easily imagine how many of the chemical sensing applications discussed above could be modified and marketed for personal use. For example, chemical sensing technologies used to monitor exposure in the chemical workplace could be adapted to monitor an individual's exposure throughout their day; food spoilage monitoring technologies could be implemented in a personal kitchen; early-warning sensors used by first responders in hazardous situations could be modified for the home; and point-of-care applications could be integrated into the numerous methods available for personal health tracking. In fact, incorporating chemical sensors into wearables is already an active area of research (Sempionatto et al., 2020). The recent miniaturization and cost reduction of many technologies and developments in ML and AI, combined with cloud data storage and the societal move toward personalization and targeted medicine/health, make personalized chemical sensing an area ready for acceleration.

Goals and objectives

Monitoring personal exposure to hazardous chemicals, toxins, and pollutants. People exposed to radiation in the workplace often have wearable radiation tags to track their exposure. However, there are no existing commercial technologies that provide inexpensive monitoring of individual exposure to TICs, toxins, and pollutants.

Identification of hazards in the home environment. Chemical monitoring in the home is not a novel concept. Carbon monoxide and smoke detectors are present in nearly every residence. However, the number of hazardous chemicals and substances detected by these sensors could be greatly expanded. According to the Environmental Protection Agency, 4.6 million asthma cases are attributed to mold exposure in the home (Muddari and Fisk, 2007). Chemical sensing technologies for the early detection of antigens of interest, such as mold, could allow for early intervention and prevention of unnecessary exposure. Further, multifunctional sensors could be integrated into the personal environment through clothing, furniture, infrastructure, etc.

Home assessment of personal food quality and freshness. Chemical sensing technologies developed to assess food quality and warn of spoilage on a large scale could be modified for home use to prevent food waste and poisoning. With 48 million cases of food poisoning per year in the United States, accounting for 128,000 hospitalizations and 3000 deaths[12], chemical sensing technologies for common causes of food poisoning in the home could have a great impact.

Personal health and hygiene tracking. There are many ways in which chemical sensing technologies developed for point-of-care applications could be modified for personal use. The tremendous growth in personal health tracking devices have shown that many have a desire for greater data on their personal health. Furthermore, VOCs from breath, urine and skin may be used to monitor the health and compliance of individuals suffering from a chronic disease. Another personal application of chemical sensing technologies is in the development of methods to detect and warn individuals of personal odors, such as bad breath. Participants in the workshop agreed that there were many ways in which these technologies could be integrated for personal use.

Pooled data to reveal local patterns. An aggregation of the chemical sensing data from individuals may reveal trends or problems at a local level. For example, these data may enable the faster detection of neighborhood ground pollutants, localized disease propagation, and pandemic monitoring and provide valuable information for targeted decision making in response to pandemics or other threat responses.

Current limitations

Since many of these goals and objectives overlap with the themes already discussed, personalized chemical sensing technologies are also prone to the same limitations. There are, however, some barriers and limitations that are inherent to personalized technologies. Personalized sensors must be easily mass-produced at relatively low cost. Data privacy concerts are also of special interest. As with any personal data, there would need to be new considerations for data privacy and laws regarding data use by corporations and governments. In some cases, the goals of the individual consumer, industry, and academic researcher do not always align. Getting personal chemical sensing technologies into the hands of consumers will require teams of sensor designers, electronic engineers, software programmers, academic researchers, and commercial businesses.

[12] https://www.fda.gov/food/consumers/what-you-need-know-about-foodborne-illnesses (accessed 12/01/2022).

High-impact deliverables

Nine-month milestone. A necessary first step to pursue the goals listed above would be the creation of a functional group of multidisciplinary researchers, both academic and private, and the definition of an end goal or product. There are many options for what a first product could be. However, although a high-impact deliverable would be ideal, the greater impact will be in generating an operating procedure modeling the multidisciplinary and integrative approach needed to develop a personalized sensing technology, identify the intended market, and implement the technology, while also tracking and studying any unintended consequences. A crucial part of the short-term goal will be to investigate any regulatory procedures relevant to the intended technology. Ideally, this effort would result in the design and creation of a 1st-generation prototype.

Three-year milestone. A more long-term goal would then be to implement widespread consumer adoption of the new technology. Depending on the technology chosen and its applicability to the public, the target market could be monumental, comparable to personal cell phones or home smoke detectors.

Cross-cutting challenges

In considering the specific themes above, participants noted several areas of overlap. Specifically, there are common challenges that appear in more than one theme. Meeting these challenges is likely to be particularly impactful, with broad applications that can meet more than one societal need.

Detection standards

Unlike face-detection or speech recognition, chemical sensing targets are diverse and often not well defined. In many cases, the target is not a single compound but a collection of compounds at specific relative concentrations, forming an odorant fingerprint. A common challenge in creating and implementing chemical sensing technologies, therefore, will be precisely defining the sensing target, including relevant concentrations. Sensors often require a tradeoff among sensitivity, specificity, and speed of detection. A precise definition of the requirements of the sensors for any given objective will be necessary to guide sensor development.

Data standards

A crucial need in the field is to standardize datasets and evaluation metrics to allow comparison across different e-nose technologies. Participants made it clear that currently there is a lack of data to develop and test AI/ML algorithms. Nonexistent are datasets from sensor arrays operated in realistic real-world conditions and/or over long periods of operation. Therefore, the following cross-cutting measures were identified as high priority:

- Build better ML models and artificial intelligence systems;
- Collect rich datasets covering a wide range of chemical events to power ML and AI algorithms;
- Obtain datasets that reflect real-world operating conditions;
- Ensure greater crosstalk among chemometrics labs, the ML and AI community, and practitioners working in real-world scenarios.

Participants noted a potential stumbling block in striving towards these goals: the interests of academic researchers and company researchers are not necessarily well-aligned. Some effort will be required to generate collaborative, productive working relationships.

Deployment challenges

Several practical challenges associated with instrumentation, packaging, and deployment were identified as cross-cutting challenges faced by all chemical sensing technologies:

- Miniaturization of sensor arrays;
- How to enhance the lifespan and reliability of sensors;
- How to get sensors installed and monitored in remote places;
- Adapting size, weight, and power to specific applications;
- Manufacturing at scale;
- Operating in harsh conditions.

Potential Partnerships

It is worth noting that participants from other federal agencies had expressed interest in the chemical sensing innovation idea and with some expressing explicit interest in collaboration with NSF. Of particular note are

- NASA Wicked Problem Working Group. Gary Hunter and Vikram Shyam had initiated a collaborative invitation to the NSF program managers to explore further possible areas of join exploration
- Venna Misra (NCSU) represented DARPA's interest in this space and will presenting the findings from the convergence accleartion workshop to DARPA.
- Rhea Brooking-Dixon (DARPA) shared information about ongoing DARPA SIGMA + program releated to this workshop[13].
- Other federal agencies including Jennifer Soliz (DTRA), Joong Kim (ONR), Steve Semancik (NIST), Shawn Mulvaney (NIH) participated in the workshop.
- There was strong interest in industry partners to acceleratre lab-grown technologies through product development, rigourous testing and evaluation phases (for example see[14]).

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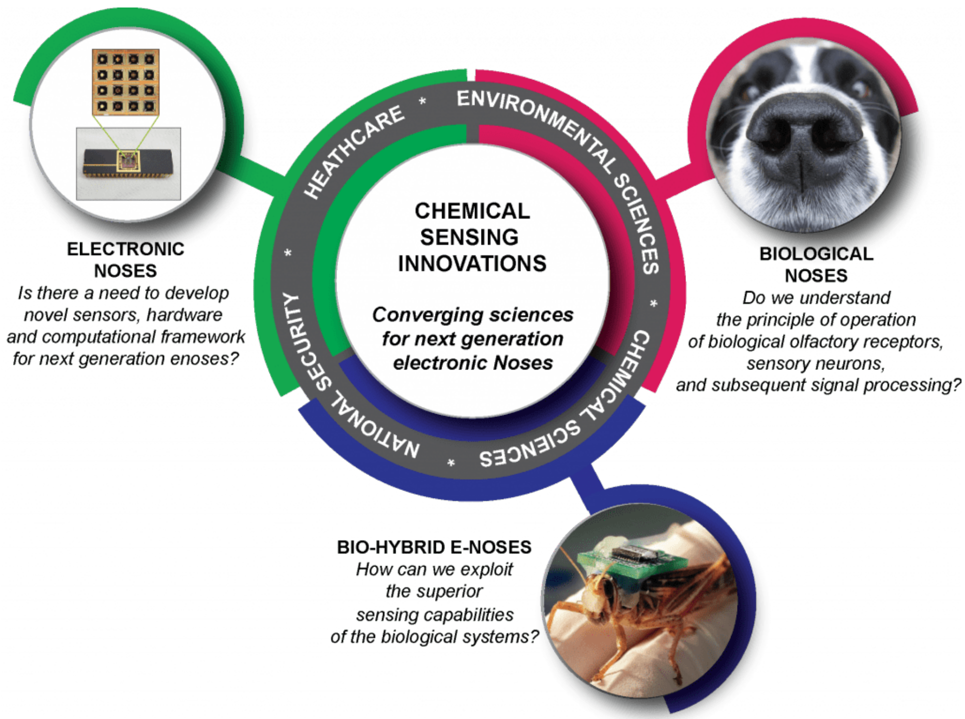
[13] https://www.dropbox.com/s/i9ykvmdr1edhsqa/SIGMA%2B%20Overview%20-%20NSF%20Workshop%202022.pdf?dl=0

[14] https://www.dropbox.com/s/eo79osb89n3un8s/MRIGlobal%20Introduction%3B%20NSF%20Workshop-KRS%20%20-%20%20Read-Only.pptx?dl=0

Concluding Thoughts

For all themes, a grand challenge for the next 2-3 years is developing a standardized data format and handling method, similar to the NIH's standard for MRI and other imaging data. It will also be critical to establish a central hub for access and distribution of standardized datasets.



Chemical Sensing Innovation: Towards next generation of electronic noses. [Picture Courtesy: Nicole Moore, WUSTL]

Appendices

Program committee:

Member name	Institution	Expertise
Barani Raman	WUSTL	Biological and artificial olfaction
Shantanu Chakrabartty	WUSTL	Neuromorphic sensing and computation
Srikanth Singamaneni	WUSTL	Material science and biosensing
Alexandra Rutz	WUSTL	Bioelectronics and biomaterials
Yeuhda Ben-Shahar	WUSTL	Biology and Genetic Engineering
Dima Rinberg	NYU	Neuroscience and Chemical Sensing
Ken Suslick	UIUC	Chemistry and Chemical Sensing
Nicole Moore	WUSTL	Research Development

Other Support: Gabrielle Edgerton and **Sarah Daniel**, Editors, Red Pen Scientific Inc.

Key Notes Talks:

Audrey Odom (Children's Hospital Philadelphia): *Need for chemical sensing technologies in biomedicine*

Hossam Haick (Israel Institute of Technology - Technion): *Challenges and Opportunities in designing next generation electronic noses*

Joong Kim (Office of Naval Research): *Need for chemical sensing technologies in defense and homeland security*

Ken Suslick (Univeristy of Illinois at Urbana-Champaign): Chemical sensing and societal impact

Dima Rinberg: Brain machine interfaces for chemical sensing

Participants: Session 1 (October 18, 2022)

Name (Original Name)	Affiliation	Expertise
Chetan Singh Thakur	Indian Institute of Science	Neuromorphic Sensors and Engineering
M. Dougherty		Artist and Researcher
Perena Gouma (Pelagia Gouma)	Ohio State University	Chemical Sensing
Jacob Rosenstein	Brown University	Microelectronics and sensing systems
Pao Lin	Texas A&M University	Miniaturized chemical sensor
*Joong Kim (Joong Kim)	Office of Naval Research	Standoff Detection of Explosives and Chemical Hazards
Pamela Abshire	University of Maryland	Integrated Circuits, Biosensors
Conor Sharp	Booz Allen/Defense Threat Reduction Agency	Chemical Sensors and Sensor Materials
Jon Evju	Carrier FSAS	Chemical Sensors
Ettigounder Ponnusamy	Millipore Sigma	Green Chemistry
Stephen Semancik	National Institute of Standards and Technology	Miniaturized chemical sensor
Noah Michaeli	Bioconvergence R&D	Chemical sensors, Neuroscience/perception, Entomology
Sameer Sonkusale	Tufts University	Chemical sensors, Biomedical devices
Gert Cauwenberghs	University of California, San Diego	Neuromorphic Computing
Matt Wachowiak	University of Utah	Neurobiology
KI - Effie (Effie Kistner)	Know Innovation	Facilitator
KI - Sydnie Hammer (Sydnie Hammer)	Know Innovation	Facilitator
KI - Hana Mamnoon (Hana Mamnoon)	Know Innovation	Facilitator
KI - Malachi Greaves (KI - Malachi)	Know Innovation	Facilitator
Mitra Hartmann	Northwestern University	Biomechanics and airflow sensing
Barani Raman	Washington University in St. Louis	Biological and Artificial Olfaction
Nicole Moore	Washington University in St. Louis	Research Adminstration
Audrey Odom	Children's Hospital Philadelphia	Infectious Diseases
Jon Askim	Iridescent Sensors	Optoelectronic sensor arrays
Shantanu Chakrabartty	Washington University in St. Louis	Neuromorphic sensing
Brian H Smith	Arizona State University	Neurobiology
Shawn Mulvaney	NIH / NIBIB	Biosensors and diagnostic devices
Alexandra Rutz	Washington University in St. Louis	Bioelectronics & Biomaterials
Nabil Imam	Georgia Institute of Technology	Neuromorphic Computing
Srikanth Singamaneni	Washington University in St. Louis	Soft nanomaterials and Chemical Sensing
Gabrielle Edgerton	Red Pen Scientific	Scientific writer
Vipulan Vigneswaran	SRI International	Organometallic chemistry
Tahmid Latif	Wentworth Institute of Technology	Insect-machine interface
Dima Rinberg	New York University	Neuroscience
Floh Thiels	National Science Foundation	Program Manager
John Crimaldi	University of Colorado	Fluid mechanics
Kenneth Suslick	University of Illinois, Urbana-Champaign	Chemical Sensing
Alper Bozkurt	North Carolina State University	Bioelectricity
Alec Jorns	MRI Global	Mechanical Engineer
Ellen Briggs	University of Hawaii	Chemical sensors for seawater carbon
Saha Debajit	Michigan State University	Biosensing
Anne-Marie Dowgiallo	SRI International	Chemistry
Pradeep Fulay	National Science Foundation	Program Manager
Yehuda Ben-Shahar	Washington University in St. Louis	Geneticist
Christina HIldebidle	SRI International	Project Developer
Veena Misra	DARPA	Gas sensors, wearables
Melanie Anderson	University of Washington	Biohybrid Robots
Aleksandr Simonian	NSF/ENG/CBET	Program Manager
Vikas Bhandawat	Drexel University	Neurobiology
Halleh Balch	Stanford University	Nanophotonics & Microscopy
Gary Hunter	NASA	Smart Chemical Sensors
Grace Hwang	NSF	Program Manager
Tim Morley	Know innovation	Facilitator
Hossam Haick	Technion - Israel Institute of Technology	Chemical Sensors
Michael Schmuker	University of Hertfordshire	Olfaction in animals and machine
Lucas Lopez	Volatile AI	Chemical Sensor
Chris Rand	Aurora Scientific	Olfaction

Session 2 (October 24, 2022)

Name (Original Name)	Affiiation	Expertise
KI - Effie (Effie Kistner)	Know Innovation	Facilitator
KI - Sydnie Hammer (Sydnie Hammer)	Know Innovation	Facilitator
KI - Hana (Hana Mamnoon)	Know Innovation	Facilitator
KI - Malachi	Know Innovation	Facilitator
Nicole Moore	Washington University in St. Louis	Research Administrator
Barani Raman	Washington University in St. Louis	Biological and Artificial Olfaction
Brian H Smith	Arizona State University	Neurobiology
Kenneth Suslick	University of Illinois - Urbana - Champaign	Chemical Sensors
Dima Rinberg	New York University	Neurobiology
Tahmid Latif	Wentworth Institute of Technology	Insect - machine interface
Gabrielle Edgerton	Red Pen Scientific	Scientific Editor
Shawn Mulvaney	NIH/NIBIB	Biosensors and diagnostic devices
Sarah Daniel	Red Pen Scientific	Scientific Writer
Srikanth Singamaneni	Washington University in St. Louis	Soft nano materials and chemical sensing
Jacob Rosenstein	Brown University	Microelectronics and sensing systems
Matt Wachowiak	University of Utah	Neurobiology
Alec Jorns	MRI Global	Mechanical Engineering
Alexandra Rutz	Washington University in St. Louis	Bioelectronics & biomaterials
Vikas Bhandawat	Drexel University	Neurobiology
Noah Michaeli	Bioconvergence R&D	Neuroscience/perception, Entomology
Melanie Anderson	University of Washington	Biohybrid robotics
John Crimaldi	University of Colorado	Fluid dynamics
Ellen Briggs	University of Hawaii	Chemical Sensors for underwater sensing
Ibrahim Mohedas	NSF	Program Manager
Nabil Imam	Georgia Institute of Technology	Neuromorphic computing
Anne-Marie Dowgiallo	SRI International	Chemistry
Alper Bozkurt	North Carolina State University	Bioelectricity
Ettigounder Ponnusamy	Millipore Sigma	Green Chemistry
Veena Misra	DARPA	Gas sensors, wearables
Gary Hunter	NASA	Smart chemical sensors
Edda Thiels	NSF	Program Manager
Milutin Stanacevic	Stony Brook University (SUNY)	Bioelectronics
Christina Hildebidle	SRI International	Product Development
Grace Hwang	NSF	Program Manager
Jon Evju	Carrier FSAS	Chemical Sensors
Pao Lin	Texas A&M University	Miniaturized chemical sensors
Sameer Sonkusale	Tufuts University	Chemical sensors, Biomedical devices
Pelagia Gouma	Ohio State University	Chemical sensors, biosensors, biomedical diagnostics
Mitra Hartmann	Northwestern University	Biomechanics and airflow sensing
Mona Zaghloul	George Washington University	Electronics, Neural Networks
Yehuda Ben-Shahar	Washington University in St. Louis	Genetics
Shantanu Chakrabartty	Washington University in St. Louis	Neuromorphic sensors and analog computing
Tim Morley	Know Innovation	Facilitator
Michael Schmuker	University of Hertfordshire	Olfaction in animals and machines
Lucas Lopez	Volatile AI	Chemical Sensors
Chris Rand	Aurora Scientific	Neurobiology

Session 3 (October 26, 2022)

Name (Original Name)	Affiliation	Expertise
Chris Rand	Aurora Scientific	Neurobiology
Tim Morley	Know Innovation	Facilitator
Michael Schmuker	University of Hertfordshire	Olfaction in animals and machine
Lucas Lopez	Volatile AI	Chemical Sensors
Malachi Greaves	Know Innovation	Facilitator
Hana Mamnoon	Know Innovation	Facilitator
Effie Kistner	Know Innovation	Facilitator
Sydnie Hammer	Know Innovation	Facilitator
Grace Hwang	NSF	Program Manager
Jon Askim	Iridescent Sensors	Optoelectronic sensor arrays
Vikram Shyam	NASA	Wicked Problem Work Group
Dima Rinberg	New York University	Neurobiology
Sara Daniel	Red Pen Scientific	Scientific Writer
Gabrielle Edgerton	Red Pen Scientific	Scientific Writer
Alec Jorns	MRI Global	Mechnical Engineering
Anne-Marie Dowgiallo	SRI International	Chemistry
Alexandra Rutz	Washington University in St. Louis	Bioelectronics and biomaterials
Tahmid Latif	Wentworth Institute of Technology	Insect machine interfaces
Kenneth Suslick	University of Illinois Urbana - Champaign	Chemical Sensors
Pao Lin	Texas A & M University	Miniaturized chemical sensors
Shawn Mulvaney	NIH/NIBIB	Biosensors and diagnostic devices
Jacob Rosenstein	Brown University	Microelectronics and sensing systems
Noah Michaeli	Bioconvergence R&D	Chemical sensors, Neuroscience/perception, E
Vikas Bhandawat	Drexel University	Neurobiology
Saha Debajit	Michigan State University	Biosensing
Veena Misra	North Carolina State University	Gas sensorsa nd wearables
Gary Hunter	NASA	Smart chemical sensors
Ibrahim Mohedas	NSF	Program Manager
Jon Evju	Carrier FSAS	Chemical Sensors
Sameer Sonkusale	Tufts University	Chemical sensors, Biomedical devices
Melanie Anderson	University of Washington	Bio-hybrid robotics
Nabil Imam	Georgia Institute of Technology	Neuromorphic Computing
Milutin Stanacevic	Stony Brook University (SUNY)	Bioelectronics
Halleh Balch	Stanford University	Nanophotonics & Microscopy
Brian H Smith	Arizona State University	Neurobiology
Edda Thiels	NSF	Program Manager
Vipulan Vigneswaran	SRI International	Organometallic chemistry
Nicole Moore	Washington University in St. Louis	Research Adminstrator
Matt Wachowiak	University of Utah	Neurobiology
Yehuda Ben-Shahar	Washington University in St. Louis	Genetics
Shantanu Chakrabartty	Washington University in St. Louis	Neuromorphic Computing
Mitra Hartmann	Northwestern University	Biomechanics and airflow sensing

Session 4 (October 28, 2022)

Name (Original Name)	**Affiliations**	**Expertise**
Tim Morley	Know Innovation	Facilitator
Chris Rand	Aurora Scientific	Neurobiology
Michael Schmuker	University of Hertfordshire	Olfaction in animals and machines
Malachi Greaves	Know Innovation	Facilitator
Sydnie Hammer	Know Innovation	Facilitator
Hana Mamnoon	Know Innovation	Facilitator
Effie Kistner	Know Innovation	Facilitator
Nicole Moore	Washington University in St. Louis	Research Administrator
Gabrielle Edgerton	Red Pen Scientific	Science Writer
Jon Askim	Iridescent Sensors	Optoelectronic sensor arrays
Kenneth Suslick	UIUC	Chemical Sensors
Dima Rinberg	NYU	Neurobiology
Barani Raman	Washington University in St. Louis	Biological and Artificial Olfaction
Noah Michaeli	Bioconvergence R&D	Chemical sensors, neurobiology, entomology
Shawn Mulvaney	NIH/ NIBIB	Biosensors and diagnostic devices
Ellen Briggs	University of Hawaii	Chemical sensors for underwater
Alec Jorns	MRI Global	Mechanical Engineer
Grace Hwang	NSF	Program Manager
Jon Evju	Carrier FSAS	Chemical Sensors
Sara Daniel	Red Pen Scientific	Science Writer
Jacob Rosenstein	Brown University	Microelectronics and sensing systems
Halleh Balch	Stanford University	Nanophotonics and microscopy
Brian H Smith	Arizona State University	Neurobiology
Yehuda Ben-Shahar	Washington University in St. Louis	Genetics
Gary Hunter	NASA	Smart chemical sensors
Tahmid Latif	Wentworth Institute of Technology	Insect machine interface
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Veena Misra	NCSU	Gas sensors and wearable technology
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