**TITLE**: Innovative AI-based chemical vapour detection platform for monitoring busy spaces

**STEP 1**

1. **Proposal Value Proposition Statement**

We plan to synergize low-cost commercial sensors, reliable data acquisition, seamless integration with existing networks and AI-based analytics, to establish a comprehensive and adaptable system to address pressing challenges in air monitoring for chemicals of interest in busy spaces and detection applicable to both the civilian as well as military sectors. The collated data from all sensors within the network are pushed to the end user for decision making. Networked sensor platforms can be statically deployed for defence on fixed locations or deployed on mobile platforms for dynamic threat data collection. This project holds the promise of reshaping our understanding of low-level detection of chemicals of interest, empowering informed decision-making, and contributing to a safer healthier future.

1. **Abstract**

Expanding from our successful AirU network (NSF and DARPA SIGMA+ funded), this project will develop ChemAirU, a low-cost modular platform capable of detecting and monitoring toxic chemical compounds. The success of our sensor network will rely on the convergence of: (1) low-cost commercial sensing elements implemented in a commercially available air quality sensor platform, (2) high spatial coverage through easy to deploy monitoring platforms, (3) compatibility with several communication protocols to ensure seamless integration with network infrastructures, (4) artificial intelligence-based algorithms to identify chemical compounds of interest and aggregate the data from a variety of sensors to perform appropriate background removal. Our approach is targeted towards the capability to detect excursions of chemicals of interest in the atmosphere of busy spaces through the implementation of an AI-based analytical approach that evaluates baseline background during various environmental conditions.

**Our proposed idea**

To detect toxic gases under realistic scenarios, we will enhance the capabilities of the AirUPro air pollution monitors, currently deployed in complex urban environments, to screen a large panel of toxic gases with a high selectivity and a sensitivity at ppb levels. We propose an integrated chemical sensor array continuously detecting toxic gases down to low part- per-billion traces. The specificity for detecting and identifying specific gases will be achieved through the development of a machine-learning intelligence capable of adapting to the local environmental and chemical background conditions that could obscure any release of chemicals of interest. The data will be real-time reported to a central node either through cellular and/or secured WiFi connections for further processing and threat signature identification. The collated data from all sensors within the network are pushed to the end user for decision making. The sensor nodes can be either stationary or mobile.

The current state of the art for relatively low-cost air monitoring systems relies on gas sensors of relatively low specificity. To increase the probability of correctly detecting and identifying gas species, we propose a unique three-fold approach that builds on the available AirUPro air monitoring platform currently in use for environmental pollution monitoring: 1) large panel chemical screening utilising an array of commercially available chemical sensors implemented in the AirUPro, 2) The creation of an innovative AI solution trained on controlled laboratory and real-world chemical exposures to alleviate sensor cross sensitivity and environmental conditions, and perform individual chemical identification, 3) The integration capability of multiple sensor nodes into a spatial network either through WiFi or cellular connectivity to allow for a large spatial and temporal air monitoring network that allows for environmental (temperature, humidity, particulate matter) baseline correction that could otherwise interfere with the ability to detect gases of interest.

**Background**

Current sensor technologies for chemical detection typically fall into four categories: spectrometric, optical, microelectromechanical systems (MEMS) and chemiresistive.

Spectrometric methods like Ion Mobility Spectrometry (IMS) and Mass Spectrometry (MS) are considered gold standards but face challenges in miniaturization, cost, and reliance on power-intensive vacuum and radioactive sources. Both techniques rely on separation of ionized molecules by mass and charge. As these systems shrink, they tend to lose mass resolution which can be problematic since many separation technologies are likely to separate by volatility, which is generally correlated to mass. Furthermore, these technologies require vacuum, which is power intensive, and ionization sources, which are frequently radioactive. Field-portable systems tend to be very expensive (>$35k for IMS, >$100k for MS); in practice, samples are usually collected in a canister and sent to a contract lab for analysis, at a high cost per sample and with delays of days to weeks before results are available.

Optical techniques, including infrared spectrophotometry and fluorescence, offer selectivity but struggle with vapor-phase detection and specificity. Infrared techniques generally provide a signal based on the vibrational or rotational absorptions of a molecule, which produces a unique signature of a chemical. Infrared techniques offer good selectivity but are better suited to interrogating solid-state materials rather than the vapours required by this program. Poor sensitivity for vapor-phase detection is another drawback. Fluorescence sensors (*e.g.*, amplified fluorescence polymers) offer excellent sensitivity to vapor-phase molecules, but their specificity is typically insufficient for identification. Sensing is often based on fluorescence quenching (*i.e.*, a decrease in light emission). Colorimetric sensing relies on the changing colour of sensor molecules when exposed to an analyte. Most colorimetric sensors work for liquids or solids but are relatively slow and exhibit poor selectivity toward vapor-phase analytes. In general, colorimetric sensors lack selectivity and may require more than 64 different sensors in an array to provide sufficient differential sensing for identification. Moreover, the colour change is usually permanent, so the sensors must be replaced after they are triggered.

MEMS-based sensors show promise but are still primarily in the research phase. While there are a variety of different configurations and devices, in general, they rely on a structure that vibrates at a certain resonant frequency with adsorption of a chemical changes the resonant frequency. MEMS-based sensors offer no intrinsic selectivity and must be functionalized.

Chemiresistivesensors include electrochemical-, inorganic-, and organic-based techniques. Electrochemical cells are standard technologies for monitoring industrial spaces for toxic chemicals for compliance with Occupational Safety and Health Administration regulations. They are very inexpensive, but they are prone to limited sensitivity and marginal selectivity. Sensors based on metal oxides and other inorganic semiconductors (*e.g.*, silicon, gallium arsenide) operate at elevated temperatures, which is power intensive. Metal oxides interact strongly with water and, as a result, are very sensitive to humidity (1). Furthermore, these materials lack intrinsic selectivity and must be functionalized. The functional groups help but fail to block all nonspecific interaction (2). Organic nanofibers are self- assembled from building-block molecules that are functionalized which promise to interact more specifically with certain chemicals or classes of chemicals. Once assembled, the nanofibers are coated onto an electrode pair to create a chemiresistive sensor. While promising devices, organic nanofibers still suffer from large cross-sensitivities, large device to device variations and strong sensitivity to humidity and temperature.

**Statement of Work**

**Work Package 1:** *ChemAirU Pilot Deployment*

To demonstrate ChemAirU network's viability for busy space chemical monitoring, a pilot infrastructure will be manufactured and deployed at the University of Utah. This initiative involves deploying AirU Pro instruments that are tailored to the defence community needs. A robust cloud-based platform, supported by TELLUS AirView technology, will manage collected data and provide real-time air quality metrics visualization.

*Task 1.1: ChemAirU Hardware*

We will acquire production AirUPro devices from TELLUS and specifically customize them for the ChemAirU pilot application. AirUPro features a modular architecture that allows users to tailor sensor configurations according to specific project requirements. This flexibility ensures that the monitoring device remains aligned with evolving needs, providing a cost-effective solution that can be easily scaled or modified without replacing the entire system. AirUPro devices are typically configured to monitor CO, H2S, CH2O, PM2.5, VOCs, SO2, NO2 and O3. We will complement these capabilities by increasing the number of electrochemical sensors on the AirUPro device (using chemical sensors sourced from Alphasense UK), in order to test across all four categories of toxic gases of interest to this competition: Acid/base (H2S, HCl, HCN, SO2, NH3), Reductant (H2, CO), Oxidants (O3, H2O2 Cl2) and Halo organics (Cl2, VOCs, C2H4O). Beyond this list of primary targets, we expect the system to provide detection and identification capability to more than 25 compounds at the ppb level as listed below, including by not limited to the following species (5-Ethylidine-2-norbornene, 1,6-Dichlorohexane, Perfluoro(methylcyclohexane), Dichlorvos, Perfluoro-1,3-Disopropyl fluorophosphate, Bromonitromethane). Once the units will be received, we will expose three units to laboratory testing and the remainder in outdoor and indoor busy spaces.

Success criteria: Timely delivery and installation of six AirUPro as part of pilot deployment.

*Task 1.2: Cloud-based infrastructure deployment and API delivery to Data analytics partners*

We will establish a robust cloud-based infrastructure to handle the data collected from the monitoring network. ChemAirU will be supported by TELLUS AirViewTM technology. AirView presents integrated air quality metrics in a real-time visualization map, making it easy to visualize and interpret. The platform employs statistically modelled regions (using Gaussian process modelling – see Task 3.3), enhancing accuracy and reliability. Through localized anomalies notifications, AirView empowers stakeholders to take informed actions to protect health and well-being. This infrastructure will allow for secure storage, real-time data processing, and efficient management of the air quality data. Furthermore, the infrastructure will provide a well-designed *Application Programming Interface* (API) to access and analyse the collected data. The API will be used to develop and refine the AI-based identification methodologies. It can also be shared with other performers to enable them with seamless data sharing and analysis, fostering collaborative efforts and deriving valuable insights to address the busy space chemical monitoring challenge effectively.

Success criteria: Timely setup of data analytics cloud-based infrastructure.

**Work Package 2:** Chemical Monitoring Testing, Data Acquisition and Validation

The success of identification and monitoring of volatile chemicals with commercial gas sensors at ppb levels and a high level of specificity depends on acquiring refereed laboratory data sets and a unique AI-based data fusion approach.

*Task 2.1: Laboratory Sensor Calibration, Validation and Data Collection*

Laboratory testing will evaluate the functionality of AirUPro sensing elements. This sensor evaluation will include precision, accuracy, sensitivity, selectivity, sensor-to-sensor variation in performance, and performance under environmentally relevant conditions, including ranges of temperatures/humidity and mixtures of gases. To establish a benchmark, we will validate these sensors by generating target chemical vapours with certified chemical analyte permeation tube challenges or calibration gases. We will also evaluate complementary sensors to measure temperature, humidity. The laboratory test chamber (including flows, concentrations, temperature, and humidity), developed under the DARPA SIGMA+ program, allows calibration of multiple sensors at one time and enables 24-hour data collection, thereby facilitating the efficient collection of thousands of data points for integration into an AI-based model for the detection and identification of chemicals of interest in the vapour state. We propose to test with the chemicals already listed in task 1.1, although we can adjust this list as per the sponsor’s input. These chemicals will cover all four chemical categories put forward by the solicitation (see earlier for complete list).

Success criteria: Sensor response to certified chemical permeation tube challenges is 100%, with 95% proper chemical identification with downstream data analytics and machine learning processing.

*Task 2.2: Baseline data collection in busy spaces.*

Identification of volatile chemical species faces challenges due to the complex chemical background to be found in the environment, especially in busy spaces. Therefore, we will deploy six AirUPros (three indoors and three outdoors) across the University of Utah campus to be set up in busy spaces for a realistic background data collection (Research building with large amount of traffic and chemical laboratories, Student Union with large amount of traffic and food vendors, parking lots with large amount of vehicular traffic, parking garage with large amount of vehicular traffic). This data will subsequently be used, together with laboratory collected data for individual chemicals of interest, in the AI-based model for the identification of chemical species.

Success criteria: Data review of every deployed sensor node and either validation of the data received on current node configuration and location or redefine the deployment requirement. The devices that are not validated will be reconfigured with new chemical capabilities or at a new location.

*Task 2.3: Verification of sensor platform and AI-model Identification capability*

To test the functionality of the sensor platform and AI-based chemical identification model performance, we will expose the sensors deployed in busy spaces to the following calibration gases (SO2, CL2, NH3, formaldehyde, HCl). Sensor responses will be collected with the ChemAirU platform, transmitted to the cloud-based infrastructure via WiFi or cellular and subsequently fed into the machine-learning model for analysis. Data collection will be continuous over a period of several weeks with occasional challenges with the calibration gases. This will allow for background sampling, event detection and chemical species identification.

Success criteria: Sensor response to the chemical challenges is 100% with at least 80% correct identification of chemical species.

**Deliverable 1 – Month 1 – Progress report**

Status report on operation of the delivered ChemAirU (AirUPro specifically tailored to toxic gas detection) hardware and API access, demonstrating readiness to data collection.

**Deliverable 2 – Month 6 – Progress report**

Status report covering (1) Detailed laboratory testing results, (2) Data review of every deployed sensor node in busy location and either validation of the data received on current node configuration and location, (3) Status of development of data analytics and (4) Preliminary results of AI-based chemical identification.

### Reference List: (Optional)

(1) K. Le, A. Butterfield, K. Kelly, P-E. Gaillardon, K. Tingey, and T. Becnel, “Building Air Quality Sensors and Inspiring Citizen Scientists,” *Chem. Eng. Educ.*, vol. 52, no. 3, pp. 193–201, Jun. 2018.

(2) K. Kelly, W. Xing, T. Sayahi, L. Mitchell, T. Becnel, P.-E. Gaillardon, M. Meyer, R. Whitaker, “Community-Based Measurements Reveal Unseen Differences during Air Pollution Episodes,” *Environ. Sci. Technol.*, vol. 55, no. 1, pp. 120–128, Jan. 2021.

(3) T. Sayahi, A. Butterfield, and K. E. Kelly, “Long-term field evaluation of the Plantower PMS lowcost particulate matter sensors,” Environ. Pollut., vol. 245, pp. 932–940, Feb. 2019.

(4) K. Kaur and K. E. Kelly, “Laboratory evaluation of the Alphasense OPC-N3, and the Plantower PMS5003 and PMS6003 sensors,” J. Aerosol Sci., vol. 171, p. 106181, Jun. 2023.

(5) T. Sayahi, D. Kaufman, T. Becnel, K. Kaur, A. Butterfield, S. Collingwood, Y. Zhang, P.-E. Gaillardon, K. Kelly, “Development of a calibration chamber to evaluate the performance of low-cost particulate matter sensors,” Environ. Pollut., vol. 255, p. 113131, Dec. 2019.

(6) T. Becnel, K. Kelly, and P.-E. Gaillardon, “Tiny Time-Series Transformers: Realtime Multi-Target Sensor Inference At The Edge,” in *2022 IEEE International Conference on Omni-layer Intelligent Systems (COINS)*, Aug. 2022, pp. 1–6.