Conference paper

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Innovative technologies for chemical security

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Abstract: Advances across the chemical and biological (life) sciences are increasingly enabled by ideas and tools from sectors outside these disciplines, with information and communication technologies playing a key role across 21st century scientific development. In the face of rapid technological change, the Organisation for the Prohibition of Chemical Weapons (OPCW), the implementing body of the Chemical Weapons Convention ("the Convention"), seeks technological opportunities to strengthen capabilities in the field of chemical disarmament. The OPCW Scientific Advisory Board (SAB) in its review of developments in science and technology examined the potential uses of emerging technologies for the implementation of the Convention at a workshop entitled "Innovative Technologies for Chemical Security", held from 3 to 5 July 2017, in Rio de Janeiro, Brazil. The event, organized in cooperation with the International Union of Pure and Applied Chemistry (IUPAC), the National Academies of Science, Engineering and Medicine of the United States of America, the Brazilian Academy of Sciences, and the Brazilian Chemical Society, was attended by 45 scientists and engineers from 22 countries. Their insights into the use of innovative technological tools and how they might benefit chemical disarmament and non-proliferation informed the SAB's report on developments in science and technology for the Fourth Review Conference of the Convention (to be held in November 2018), and are described herein, as are recommendations that the SAB submitted to the OPCW Director-General and the States Parties of the Convention. It is concluded that technologies exist or are under development that could be used for investigations, contingency, assistance and protection, reducing risks to inspectors, and enhancing sampling and analysis.

Keywords: Chemical Weapons Convention 2017; chemical weapons; emerging technologies; if plants could talk; innovation; inspector; Organisation for the Prohibition of Chemical Weapons (OPCW); precision agriculture; remote sensing; science diplomacy; sensor; unmanned aerial vehicle (UAV); unmanned ground vehicle (UGV).

Introduction

As the implementing body for the Chemical Weapons Convention (hereinafter, the "Convention") [1], The Hague based Organisation for the Prohibition of Chemical Weapons (OPCW) oversees the global effort to permanently eliminate chemical weapons [2]. The Convention entered into force in 1997. Today, with its 193 States Parties (nation states party to it), it is considered the most successful international disarmament treaty focused on eliminating an entire class of weapons of mass destruction. Over its 21 years in force, 96 % of the chemical weapon stockpiles declared by its States Parties have been destroyed under OPCW verification, and progress continues toward complete destruction of these stockpiles [2]. Recognition of the progress toward complete stockpile destruction and the extensive efforts toward eliminating chemical weapons saw the OPCW awarded the Nobel Peace Prize in 2013 [3].

The Convention is a science based treaty that has within its articles the provision for the OPCW Director-General to receive specialized advice on science and technology relevant to the implementation of the Convention through a Scientific Advisory Board (SAB). The SAB comprises 25 experts from 25 of the States Parties with term limits for members (to allow all States Parties to nominate experts to serve on the Board). The SAB functions as an independent advisory body providing advice that represents a consensus view amongst the members [4–10].

Effective implementation of the Convention requires high levels of scientific and technical expertise. Maintaining this necessitates continual engagement with scientific communities, informal or institutionalized (as exemplified by the SAB, OPCW Designated Laboratories, and the OPCW Validation Group [10]), to ensure the operation of the treaty keeps pace with scientific advances, and recognizes opportunities where relevant technological developments may prove beneficial to overcome challenges. This is especially important for verification of compliance to the treaty, for which the Convention itself (in paragraph 6 of its Article VIII) calls on the OPCW to consider measures to make use of advances in science and technology for verification activities [1]. Likewise the terms of reference of the SAB call on the Board to "assess and report on emerging technologies and new equipment which could be used on verification activities" [7]. The identification of innovative technologies that can help ensure, and enhance wherever possible, chemical security internationally, is an enduring theme toward realising a world free of chemical weapons, and preventing the re-emergence of chemical weapons [11].

As part of the science and technology review process, the SAB in cooperation with the International Union of Pure and Applied Chemistry (IUPAC) [12], The National Academies of Science, Engineering and Medicine of the United States of America (NAS) [13], the Brazilian Academy of Sciences (ABC) [14], and the Brazilian Chemical Society (SBQ) [15] held a workshop, entitled "Innovative Technologies for Chemical Security", from 3 to 5 July 2017, in Rio de Janeiro, Brazil [16–20]. This workshop was the third of a series [21–24] intended to inform the report of the SAB on developments in science and technology to the November 2018 Fourth Review Conference of the Convention [25]. The workshop, hosted generously at the ABC Headquarters, was attended by 45 scientists and engineers from 22 countries, and enabled through financial support from IUPAC, the NAS and the European Union. It explored the potential of new technologies to enhance capabilities necessary for implementation of the Convention. The inspiration for the thematic content of the workshop drew upon findings of the 2015 final report of the SAB's Temporary Working group (TWG) on Verification [26].

The emergence and practical applications of new and innovative technologies, as well as the repurposing of existing technologies for unanticipated new applications, has benefited from increasingly trans-disciplinary approaches to problem solving and technology development. A convergence[1] of scientific disciplines fuels the "rapid pace of developments in science and technology" that is often discussed within chemical and biological security communities [27–31]. New advances across the chemical and biological (life) sciences are increasingly enabled by ideas and tools originating from sectors outside these disciplines, and Convention-relevant developments in science and technology may not be easily recognised if the scientific review process is limited to chemical-specific fora. Information and communication technologies play a key role across 21st century scientific development, and the integration of these technologies with (bio)chemical, spatial, temporal and other data streams have potential applications in chemical security, including the ability to recognise unexpected or unusual (bio)chemical changes in the environment around us in real-time. Detectable changes from exposure to chemical agents might be sensed using remote monitoring and automated systems, potentially enhancing early warning and investigative capabilities.

Given the rapid pace of scientific advancements combined with readily accessible mobile technologies, and unprecedented access to and diffusion of trans-disciplinary (convergent) scientific knowledge, it is understandable that concerns about the potential for harmful uses of new science will arise. However, there is also a need for practical considerations to ensure that the science review process recognises opportunities made available through innovative technologies and applications of technology. In this regard, there is growing recognition that overcoming and responding to challenges in disarmament can benefit from seizing upon opportunities provided through technological advancement and innovation [32–34]. Emerging technologies of interest include informatics, mobile devices, robotics and remote sensing technologies.

The Rio de Janeiro workshop assembled an international trans-disciplinary group of practitioners. OPCW inspectors (Fig. 1) with field expertise set the scene by discussing their experiences in chemical weapons-related investigations, including those that had taken place in the Syrian Arab Republic. This introduction was followed by presentations from experts in sensor development, precision agriculture, mobile and wearable technologies, digital health, autonomous sample collection and analysis, satellite image analysis, and technologies that enable real-time analysis and decision making. The participants discussed capabilities,

1 The Swiss Government started a workshop series focusing on advances in chemical and biological sciences in 2014 under the title Spiez CONVERGENCE. This series is dedicated to informing participants about significant scientific developments and to serve as a forum for expert discussions. The objective of this workshop series is to identify developments in chemistry and biology which may have implications for the Biological Weapons Convention (BWC) and the Chemical Weapons Convention. Topics covered at the inaugural workshop in 2014 and follow-up workshop in 2016 included the latest advances on 'chemistry making biology' and 'biology making chemistry', and their adoption by the biotechnology and chemical industries. Participants discussed how such developments may affect production technologies for toxic chemicals, toxins and microorganisms and assessed potential implications for chemical and biological arms control. The target audience is experts from academia, industry and policy making, and experts involved with the implementation of related arms control agreements. The workshop findings are available to the Biological and Chemical Weapons Conventions communities and other interested parties [28–30].

Fig. 1: OPCW chemical weapons inspectors using hand-held chemical agent monitoring devices during training exercises. Images courtesy of OPCW (these are also available on the OPCW Flickr page).

applications and challenges in the use of new tools and technologies to detect (bio)chemical change in complex environments, and considered potential applications in support of chemical disarmament and non-proliferation.

The workshop outcomes were briefed to States Parties of the Convention by the OPCW Science Policy Adviser and SAB Chairperson [35] and discussed by full membership of the SAB at its Twenty-Sixth Session in October 2017 [36]. The output of the workshop provided the impetus for the publication of this special edition of *Pure and Applied Chemistry* [19] through the invaluable support of IUPAC, and gave those that presented their research in Rio de Janeiro an opportunity to contribute technical papers.

This paper is intended as an overview and introduction to many of the articles within this special edition. It seeks to project the work of the OPCW and its SAB to an audience of scientists that may be unfamiliar with the scientific and technological dimensions that impact on the Convention and its future. This paper is one of several articles authored by the SAB and colleagues for publication in the scientific literature [37–41] to support the Fourth Review Conference of the Convention. It is organised as a review that highlights the content of technical presentations and discussions from the original workshop report (which was issued as a working paper of the SAB in July 2017 [23]). For this *Pure and Applied Chemistry* paper, we build off the original workshop report and provide additional background material and references.

Contingency operations: challenges for OPCW inspectors

Beginning with the 2013 United Nations-led mission in the Syrian Arab Republic [38, 42, 43], the OPCW has continued to undertake non-routine inspection, verification and technical assistance activities in the Syrian Arab Republic [38, 42–48], Libya [49], Iraq [50], and most recently in the United Kingdom of Great Britain and Northern Ireland [51]. These contingency operations have increasingly required investigations, analysis, and fact-finding, with collection and evaluation of oral, material, and digital evidence of the use of chemical warfare agents (CWAs). The unique and non-routine situations in which these operations have taken place are highly insightful for the consideration of new technologies with the potential to enhance capabilities available to inspectors [45, 46]. New technologies may additionally be applicable to assistance and protection missions [52]. Inspectors have faced many challenges during these non-routine missions, operating in unpredictable and dynamic environments, where improvised problem solving is frequently required.

Challenges in conducting non-routine missions have many dimensions, including non-technical issues that can impact the capabilities and resources of an inspection team. These can include customs and transportation regulations (especially regarding dangerous goods) that can delay arrival of, or prohibit access to, certain equipment, and short-notice deployment of personnel. Once inspectors are on the ground, they may have time-limited access to investigation sites, find themselves working under unfavourable environmental conditions, and any samples available to collect for analysis may be non-homogenous, degraded and/or

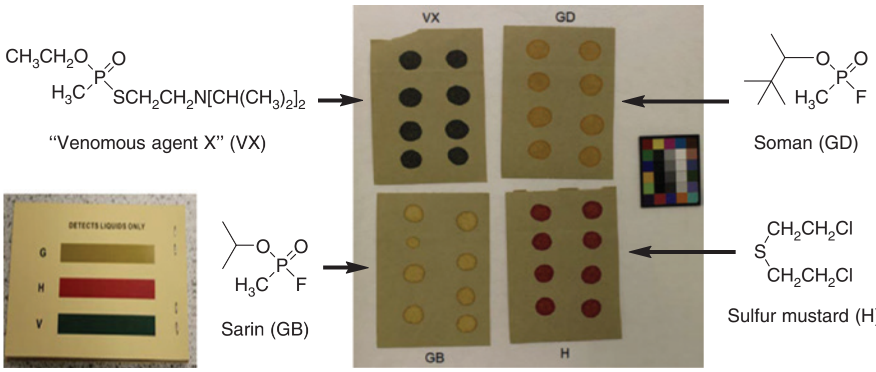

Fig. 2: CALID-3 three colour detector paper and colour reference chart [53]. The paper is designed to detect and identify V nerve agents (e.g. VX), G nerve agents (e.g. sarin GB or soman GD), and sulfur mustard (H) in the liquid state. It is beige in colour prior to reaction with liquid CWAs. The paper contains dyes which dissolve in contact with liquid CWAs producing a dark green coloration to V agents, yellow coloration to G agents, and red coloration to blister agents such as H, within 30 s (middle photo). CALID-3 comes as set of 12 sheets of adhesive-backed detector paper bound into a booklet with instructions for use printed on and inside the outer covers of the booklet (bottom left photo). Images reproduced courtesy of Dstl.

of low purity. Chain-of-custody and properly documenting evidence is required from the point of collecting/receiving a sample through its handling, transportation, storage and analysis (and beyond); requiring careful attention under potentially stressful conditions. Collected information can include videos, photos and witness statements, which must be authenticated, requiring expertise beyond chemical analysis.

There are many applications where enabling technologies might benefit inspectors. However, the adoption of any new technology must also consider the operational requirements and practical issues of the operating environment, for example: power sources for equipment, availability of consumables, set-up time, and transportation requirements (including shipping weight and possible shipment restrictions). Further complicating the use of data-driven technologies are potential restrictions on data transmission and the need for accurate, precise and secure record keeping with regard to chain of custody. Useful on-site analysis tools were suggested to be those that provide preliminary detection (indicative tests), which can help to guide where to collect samples that can be sent for more robust off-site analysis. Examples of such tools that are currently available to inspectors include CALID-3 paper (a colorimetric test) [53] and a variety of hand-held detectors [54] such as the LCD 3.3 [55] (Figs. 1 and 2).

Recognising biochemical change: “if plants could talk”

The technical sessions of the workshop began with a focus on technologies that enable recognition of (bio) chemical change. Presenters reviewed technologies for detection of observable change that can be used for the diagnosis of plant health. These technologies might allow recognition of exposure to toxic chemicals, including nerve agents [56–68] (Fig. 3). Conceptually, any observable phenotypic change in a plant would have an indicative biomolecular underpinning, and possible markers of exposure might be identified (for example, indicators of physiological stress that are not direct reaction products of the CWAs). How indicative any observable changes would be to verify exposure to a given chemical would require research and characterization.

Technologies being adopted for precision agriculture and their potential applications

Advances in the adoption of precision agriculture (farming) [59, 60] are demonstrating that plant health can be monitored and data produced that allows real-time decision making. This is enabled though the use of a

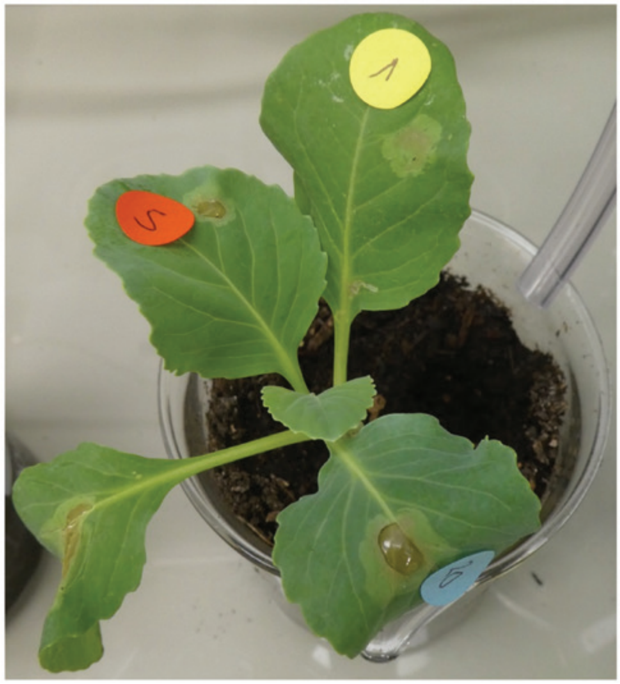

Fig. 3: Observable effects of exposure of vegetation to a chemical warfare agent. The spots seen on the leaves are the result of a 1, 5 and 20 µl drop of neat sulfur mustard (H) placed on the leaves of a pointed head cabbage plant after a 24 h period. Image reproduced courtesy of Spiez Laboratory.

variety of remote sensing, robotic and data collection technologies (Fig. 4). Dr. Ricardo Inamasu of Embrapa Labex (Brazil) provided the workshop with an overview of these technologies and methods.

Precision farming is the management of crops that takes into account spatial variability with the aim to increase economic return and reduce adverse effects on the environment. Automation and data analysis have proven to be enabling technologies for crop management. In this context, automation can be thought of as "a system in which operational processes are controlled and executed through mechanical, electronic or computational devices that multiply the capacity of human labour". The benefits provided by precision farming include improved crop yields and greater sustainability in farm management. Viable adoption of precision agriculture in large farms, demands sophisticated equipment and sensing systems (Fig. 4).

The use of hyperspectral imaging and analysis is a key aspect for the use of plants as sensors of chemical change. In particular hyperspectral and non-visible wavelength imagery that can identify sick and healthy vegetation may have value in chemical investigations (this could include satellite imagery). Areas within a field in which "sick vegetation" can be observed might indicate the release of a chemical. Comparing images showing such features with previously-collected data could help narrow down or possibly confirm the time-stamp of an incident (assuming images with appropriate temporal and other relevant metadata are available).

Many parameters can be monitored to determine plant health, including moisture levels, leaf and organ morphology, and photosensitive pigments. Even the adsorption of chemicals into a plant might produce detectable changes. Effectively understanding and recognising change from overall plant characteristics is enabled through the use of artificial intelligence (AI) based data analytics. The use of computer vision with machine learning to recognize plant diseases from digital images of individual plants is one such example [69]. Much data on crop plant health have been collected through agricultural activities. However, such data have economic value, may be proprietary, and may not be openly shared across agricultural enterprises/farms. As such, the data may not be readily accessible as part of a monitoring effort aimed at identifying potential toxic chemical exposure in areas where a toxic chemical release is suspected; yet the potential value in the use of such information for real-time chemical threat agent monitoring and for retrospective analysis is intriguing.

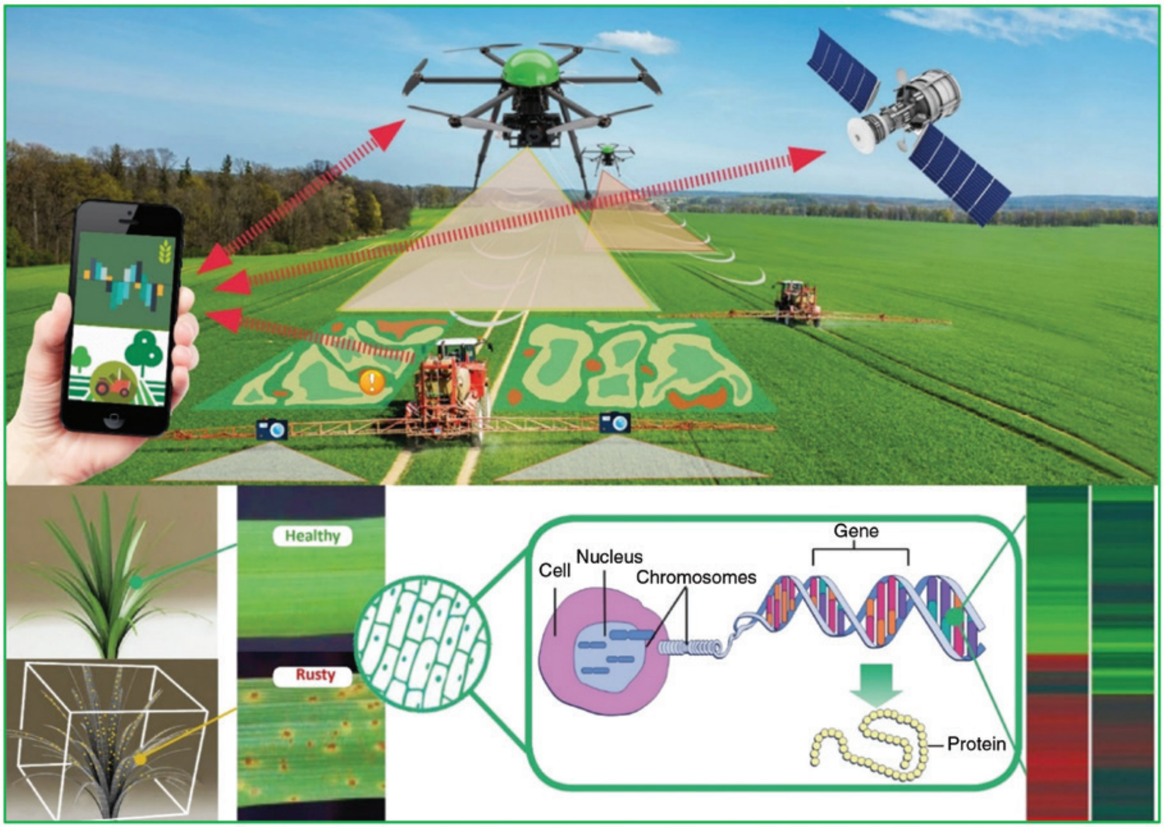

Fig. 4: "If Plants Could Talk". The methods and approaches being adopted in precision agriculture demonstrate how sensor and imaging data can be used to provide real-time indications of (bio)chemical change in vegetation. Data is collected from mobile sources (unmanned aerial and ground vehicles fitted with a range of imaging devices and sensors) as well as remote sources such as satellites (Top). Information collected can be accessed on smart phones and other mobile devices for immediate feedback (Top left). As observable phenotypic changes have an underlying biomolecular basis (Bottom right), it may be possible to correlate spectral and visual signatures with specific types of plant stress (for example: nutrient deficiency, pathogens, diseases, or exposure to specific types of chemicals). The sensor and imaging data collection represent a type of on-site analysis, which in principle can be verified using chemical and/or biomolecular analysis in a suitably equipped off-site laboratory. The figure illustrates the thematic concepts of the overall workshop: data collection through a variety of mobile and remote sensing tools (allowing inspectors to stay at safe distances from a site being assessed for potential chemical hazards or exposure), integration of data streams and real-time read-outs. The figure also illustrates how all of the different technologies would enable greater enhancement of capabilities to recognize (bio)chemical change when they are integrated into a system of data-generating devices, data analytics and communication, rather than viewed as individual technologies for use independently from one another.

Optical sensors for the detection of biophysical and biochemical changes of plants: case studies from plant-pathogen interactions

The detection and identification of plant diseases is a fundamental task in sustainable crop production. Mr. Matheus Kuska from the University of Bonn (Germany) provided a presentation on the use of optical sensors to detect biophysical and biochemical changes in plants for this application [61] (Fig. 4). An accurate estimate of disease incidence, disease severity and negative effects on yield quality and quantity is important for crop production, horticulture, plant breeding and basic and applied plant research. In this regard, remote and proximal sensing techniques have demonstrated a high potential for detecting disease and monitoring crop stands for infected plant areas. The most promising methods include thermography, chlorophyll fluorescence, and hyperspectral sensing. The variety of available sensor systems allow high-resolution imagery for crop stands or single plant organs, which can permit early detection and identification of plant diseases [62–64]. Hyperspectral imaging, in particular, of diseased plants offers insight into processes during pathogenesis. Fungal leaf pathogens can influence both structural characteristics and the chemistry within the leaf, and this is reflected in the optical properties of the plant. The combination of hyperspectral imaging and data analysis routines makes early detection, identification and quantification of a range of plant diseases possible [65–68, 70].

Expertise that includes plant pathology, engineering, and informatics is required to utilise fully the potential of plant disease recognition through optical sensors and complex data analysis. Ideally, optical sensing data should be coupled with other analysis methods (eNose technologies [71] for example) and data streams to identify a known state of plant health that would dictate any necessary action to be taken. Examples of wearable smart devices modified for use in localised plant imaging applications have also been reported [72], making handheld means of assessing plant health possible. The combination of plant imaging data and OMICS technologies[2] opens up the potential for observable physiological and phenotypic characteristics of plants to be potentially related to molecular biological mechanisms and markers. Generating and understanding the data sets for imaging tools to be able to recognise characteristics and correlate to molecular effects requires building and validating data sets. Given the wealth of information that can be inferred from observing plants (including their interaction with chemicals), Mr. Kuska explained that "plants can talk, we just need to learn their language".

Recognising biochemical change: large scale environmental monitoring

Continuing with the theme of using elements within the environment as an indicator of (bio)chemical change, the use of satellites and dispersion models was reviewed, including the potential for monitoring chemical release either in real-time or after an event.

Remote sensing of terrestrial ecosystems

Dr. Greg McCarty of the United States Department of Agriculture (USDA) – Agriculture Research Service (ARS) Hydrology and Remote Sensing Laboratory provided workshop participants with an overview of satellite imaging capabilities for environmental monitoring. Advances in space-based sensor technologies are now capable of producing datasets with high spectral, spatial, and temporal resolution, overcoming trade-offs between these domains of resolution that hampered older technologies. The older systems allowed data to be acquired at high spectral resolution with low spatial and temporal resolution; this limited the ability to acquire detailed phenology of an ecosystem and to resolve changes in leaf biochemistry in both space and time. Mature satellite systems such as those provided by the Landsat programme [73] are now being linked by cross-calibration to the Sentinel programme [74] to provide validated image datasets with approximately 3-day return frequency. The Landsat programme has built a data record that spans more than 40 years with traceable continuity between the generations of sensors used within the programme. This has allowed for the detection of long term trends within the Earth's biosphere. Continuity and enhancements in the data record by linking multiple satellite programmes adds great power to the trend analysis. Spectral enhancements include hyperspectral sensors that provide full spectral information for each pixel of an image in the context of remote sensing of vegetation [75].

Another recent development has been the deployment of miniature satellites (CubeSats) that are less expensive to build and launch: commercial ventures are deploying large swarms of CubeSats to acquire high-resolution and high-frequency data [76–78]. These advances will better enable data-intensive technologies

2 "OMICS" refers to fields of study in biology ending in -omics, such as genomics, proteomics or metabolomics [204].

such as precision agriculture. Detecting phenotypical changes in crops in fields requires availability of data collected at high spatial and temporal frequency, with additional detection of nutrient status requiring high spectral resolution.

Advances in data management and processing are required to realize fully the potential of data from advanced Earth monitoring systems. Cloud computing services are vital to this effort: Google Earth Engine (GEE) [79] is an excellent example of this rapid advance. Within GEE, various earth monitoring datasets in a consistent geospatial format are available in a multi-petabyte catalogue. Development and implementation of user derived algorithms occur within the GEE environment and algorithm output is computed in real-time using cloud-based processors. This combination of readily assessable satellite image catalogues and high throughput computing power via cloud services promises to revolutionise our ability to monitor and understand ecological processes on various scales and to detect important trends within the Earth's biosphere. In relation to localised (bio)chemical change, satellite imagery may have limitations when looking for small scale chemical release. For wider-scale dispersal of chemicals, the technologies could potentially provide indicators of biochemical change in leaves that correlate to a chemical release.

On-site data fusion – satellites and dispersion models: the 2016 Al-Mishraq sulfur plant fire

On 20 October 2016, during the battle of Mosul in Iraq, Daesh ignited the sulfur production site at Al-Mishraq. A toxic plume of sulfur dioxide and hydrogen sulfide resulted, causing casualties. The concentration of the sulfur dioxide released reached a level comparable to that of a minor volcanic eruption. The release could be observed by satellites [80]: two-dimensional data from MetOp-A and MetOp-B [81], Aura [82], Suomi-NPP [83] and Meteosat-10 [84] provided information on the dynamic concentrations and allowed the sulfur dioxide release to be modelled [85, 86]. Dr. Oscar Björnham of the Swedish Defence Research Agency (FOI) described his research on developing a dispersion model containing a source term that enabled reproduction of sulfur dioxide concentrations over the Middle East, and permitted the dynamic three-dimensional (3D) concentration field to be estimated [80].

Ground-level concentrations predicted by the simulation were compared with observations from the Turkish National Air Quality Monitoring Network [87]. The presenter showed how the simulation data could be used to estimate the human health risk area at ground level using a probit analysis. This was compared to reported accidental human cases of exposure that had required urgent medical treatment. The study demonstrated the potential for combining satellite measurements with numerical models to acquire new insight into ongoing events, by increasing the accuracy of already available data and by providing new information.

The available satellite data allowed the analysis of the sulfur dioxide generated by the fire, but not the other chemical species present. It was suggested during the workshop that analysis of particulate matter to build the dispersion model might also be explored, the premise being that the dispersion of particulates would have correlation to a broader set of harmful chemical species emitted from the fire (and be of relevance to the release of toxic chemicals by pyrotechnic means, one potential dispersal mechanism for some chemicals). Those present agreed that validation of the models is necessary for making them generally applicable and useful predictively. Dr. Björnham's work demonstrated the value of dispersion models. It was suggested that further work might focus on looking for ways to make the analysis quick and accurate enough to support risk determination and emergency response (the Al-Mishraq dataset took several weeks to develop).

Recognising biochemical change: chemical sensing

Moving from a focus on the environment itself, the next session of the workshop reviewed sensor technologies – one of the elements necessary to enable the types of monitoring already described. Presentations considered sensor and eNose related technologies in the broadest sense, and how these might be useful for the monitoring and detection of chemical releases, especially those involving CWAs or toxic industrial chemicals.

Targeted catalytic degradation of organophosphates: pursuing sensors

Many organophosphate pesticides, like organophosphorus nerve agents, are hazardous to human health. Professor Elisa Orth from the Federal University of Parana (Brazil) described her research on catalysts that can be used for degradation and/or sensing of these chemicals [88]. Her approach uses graphene and carbon nanotubes functionalised with multiple catalytic groups, for example metallic nanoparticles [89, 90]. These can be solids or thin films; the latter being more easily recycled after the organophosphate has been degraded. Thin films of catalysts can function as surface enhanced Raman Spectroscopy (SERS) sensors for organophosphates. Catalyst films have also been prepared on sustainable materials such as rice husk [91] and can be regenerated after use. With appropriate modifications, point-of-care devices for detecting organophosphate pesticides and/or nerve agents in a resource-limited setting might be possible. In regard to such a setting, the catalysts have already been used to construct low-cost colorimeters to detect and monitor the degradation of organophosphates [92]. These catalysts have been successfully used in student laboratory projects, and agricultural fields to identify high pesticide concentrations on harvested fruit. The workshop participants agreed that fundamental chemical research on catalytic means of destroying nerve agents and other toxic chemicals is important as it may offer new solutions for the destruction of chemicals under resource-limited settings and/or assist mobile destruction technologies.

Multisensor systems (eNose) for toxic gas detection and biomedical applications

Monitoring airborne chemicals can be carried out using electronic nose (eNose) and wireless communication technologies. A presentation on the use of these technologies was provided to the workshop by Professor Cristhian Manuel Durán Acevedo of the Universidad De Pamplona (Colombia). The eNose systems discussed offer advantages of low installation and maintenance costs compared to conventional wiring and chemical monitoring instrumentation [93–95]. These systems have been developed for sensing gases, especially explosive and toxic gases in mine shafts [96–98], and chemical vapours associated with volatile organic compounds [99], waste management plants [100] and food quality [101] (in some instances combined with an "eTongue" [102]).

Another application of eNose technology included in the presentation was the diagnosis of medical conditions from breath samples [103, 104]. Early detection and diagnosis of gastric cancer has been demonstrated using devices comprising a set of nanoparticle gas sensors [105, 106], a sampler device and data acquisition system. The system has been used in a clinical study, where patients were evaluated by medical tests (biopsy and endoscopy) before and after using the eNose to acquire a set of breath samples [107]. Samples were collected from gastric cancer patients, with patients having other gastric problems (e.g. gastritis and ulcers) constituting the control group. The eNose method demonstrated a classification rate of 94 %. To validate the results, another set of breath measurements of gastric cancer patients and controls were acquired by Tenax® TA tube pre-concentrators and analysed by gas chromatography-mass spectrometry (GC-MS). The methodology promises to be useful for implementation in clinical settings.

Detection limits for eNose sensors appear to be very low under certain conditions (measuring chemical species in exhaled breath). How reliable the tools are for chemical recognition depends on the datasets and algorithms used in the analysis. While an eNose is capable of detecting mixtures of exhaled biomarkers (or a specific gas), it does not recognize molecular structure (instead, it recognizes patterns of signal across the sensors that make up the eNose which correlate to specific chemical species). To use an eNose in this way, requires training of the algorithm that performs the pattern recognition. For disease detection from breath analysis, clinical studies are necessary to build datasets that can be compared to traditional methods of diagnosis for validation purposes.

Mobile and wearable technologies and point-of-care devices

Continuing to look at sensor and point-of-care technologies that could be used for wearable applications, the discussions provided insights for the concept of an 'OPCW Inspector of the Future', who may be equipped with such devices, perhaps integrated into a personal protective chemical-resistant suit, or for physiological monitoring (Fig. 5).

Fig. 5: "The Inspector of the Future". A variety of wearable technologies could be integrated into the protective ensemble worn by chemical inspectors if such devices were reliable, rugged and economical enough to use. For outward chemical sensing, chemical detection and indicators of exposure could be envisioned (left). Inward sensing wearable devices that monitor a variety of biomarkers and/or physiological indicators could also provide a constant data stream allowing real-time recognition of changes in health, including signs of chemical exposure (right). Inspiration for the devices illustrated came from references [115–128].

Flexible, foldable, and wearable paper-based electronics and electrochemical devices

Covering advances in this field, Professor Murilo Santhiago of the Brazilian Nanotechnology National Laboratory (LNNano), in the Brazilian Center for Research in Energy and Materials (CNPEM), presented his research on flexible sensor devices to the workshop. Cellulose based materials can be thin, flexible, foldable, and biocompatible, making them suitable for the fabrication of paper-based electronic and electrochemical devices [108–111]. Fabrication of electronic interconnects through these enables construction of 3D functional electronic devices [112, 113]. Through doping/de-doping processes, it is also possible to enable electrochemical detection of harmful compounds. Another approach to flexible devices involves the dry transfer of graphite onto paper, combined with an electrochemical process to create a high-performance electrochemical device. With this approach, a low-cost and flexible carbon-based platform for the construction of a reduced nicotinamide adenine dinucleotide (NADH)-based biosensor was developed [114]. Research into low-cost and foldable systems is valuable for developing components with applications in the fabrication of wearable sensor devices. Low cost, low weight and flexible devices are ideal if the sensor technology is to be made accessible on a large scale for use in the field.

Wearable technology for chemical and biological agents: existing and emerging capabilities

An overview on wearable sensors (wearables) for detecting chemical and biological threat agents was provided to the workshop by Dr. Richard Ozanich of the Pacific Northwest National Laboratory (United States of America). Wearables can be designed as inward looking (self-monitoring) or outward looking (environmental) [115]. Enablers for wearable technologies with chemical and biological security applications include miniaturisation, sensors, nanomaterials, robust flexible electrical systems, transdermal biological fluid extraction (including sweat sensors [116] and microneedles [117]), microscale power and storage, knowledge of biomarkers for disease and/or chemical exposure, and communication capabilities. Many innovative solutions to these problems are reported (using energy created by walking as a mobile device power source, for example [118]), however practicality and robustness must be taken into account. The challenges that need to be overcome [119] include obtaining stable and reversible (bio)chemical receptors, understanding relevant biomarkers in accessible body fluids (e.g. sweat), and cost. Many of the desired capabilities in wearables are likely to be at least 10 years away.

Wearables for sports (monitoring athletes) have helped to drive many advances, primarily for inward looking non-invasive health monitoring. Very few inward looking chemical monitors have been reported; yet the capability to recognise abrupt changes in vital signs from non-invasive monitors, if correlated to symptoms of exposure, could be valuable and is currently possible (as was discussed in the workshop's session on digital health that follows) [120]. Of interest to a chemical weapons inspector would be a wearable self-monitoring cholinesterase activity device for identifying nerve agent exposure at the earliest possible time point to allow immediate response. While point-of-care devices are available for other applications, continuous and real-time cholinesterase monitoring is currently a challenge [121].

A variety of outward looking wearables have been reported, including passive materials that absorb chemicals (which are then extracted and analysed) [122] and colorimetric toxic gas sensor arrays [123, 124]; the latter include examples capable of detecting explosives [125] and organophosphorus nerve agent mimics [126]. Enzymatic indicators for airborne chemical warfare agents such as sulfur mustard might also have applications as wearable early-warning indicators [127]. Reliability, sensitivity and false positive and negative rates for such devices would need to be characterised to evaluate their suitability for field use.

Common air pollutants (and particulates [128]) are routinely monitored with a variety of low-cost sensors; however environmental background concentrations are highly variable and noise levels can mask low concentrations of airborne toxic chemicals. Likewise the accuracy, precision and sensitivity of low cost devices may not be suitable for the needs of an inspector.

Wearable detection devices, even with simple colorimetric tests, could serve as valuable early detection warning systems; the ability to have skin patches or to incorporate the device into personal protective equipment offers potential advantages. Colorimetric indicators that can detect vapours rather than requiring direct contact with a liquid agent (e.g. CALID-3) are ideal for this application. These indicators would be complementary to the detection tools currently used by OPCW inspectors.

Digital health

This session of the workshop looked at the use of non-invasive physiological monitoring to provide health information with real-time feedback, building on the aforementioned 'OPCW Inspector of the Future' concept (Fig. 5).

Digital health: what you can learn from your smartwatch

A range of wearable sensors that enable frequent and continuous measurements of body functions (physiology), including heart rate, skin temperature, blood oxygen levels, and physical activity are now commercially available. These sensors can non-invasively follow physiological change occurring over the course of a day, during illness, and while engaging in physical activity [129]. Dr. Xiao Li of Stanford University (United States of America) presented research that demonstrates how data from these types of sensors can reveal personalised differences in daily patterns of activities [129], including changes in response to a change in environment. For example, while on an airplane flight, blood oxygen levels were observed to decrease, and this was associated with fatigue. The research also found that by combining sensor information with frequent medical measurements, important health-related observations could also be made. For example, wearable sensors were useful in identifying the onset of inflammation and what was later diagnosed as Lyme disease (also known as Lyme borreliosis, an infectious disease caused by *Borrelia* bacteria, spread by ticks). These observations led to the development of a computational algorithm for personalised disease detection using sensor data. It was also observed that wearable sensors could reveal physiological differences between insulin-sensitive and insulin-resistant individuals, raising the possibility that these sensors could help detect risk of mellitus type 2 diabetes (a long-term metabolic disorder characterized by high blood sugar, insulin resistance, and a relative lack of insulin). Studies such as the one presented to the workshop by Dr. Li [129] show that the information provided by wearable sensors can be physiologically meaningful and actionable.

Understanding smart data collection versus big data collection and how to focus artificial intelligence (AI) analysis

Using sensor data and other read-outs to recognise changes in health requires reliable data analytics. However, big data and active machine learning, using large data sets and requiring hundreds, or even thousands, of servers to provide analysis can be impractical for delivering solutions to remote, insecure and/or resource limited settings. The workshop was introduced to the concept of "smart data" as way to overcome these challenges by Mr. George Harris of Basil Leaf Technologies (United States of America). Smart data is a methodology that uses AI systems to create solution sets that can be packaged into smaller, transportable systems (such as smart phones, tablets or watches). This can eliminate the need for access to uplink feeds during use, and still provide accurate data analysis at the point of collection. Data and analyses can then be shared at a later time, taking the information directly off the device on which it is stored.

An example of a system that uses smart data in the diagnosis of health is the DxTER™ [130], which Basil Leaf Technologies developed as a solution to the Qualcomm Tricorder XPRIZE challenge [131–133]. DxTER™ embodies the use of the tools and techniques described in the previous paragraph to create a medical device. The XPRIZE challenge required that the device be usable by a layperson in a remote/disconnected setting to diagnose, with at least 70 % accuracy, if they did or did not have any one of 13 diseases and conditions, monitor five vital signs, and maintain a high user-friendly interface and experience [134].

Wearable devices that can track health-related information have many potential applications in monitoring individuals working in remote and dangerous environments and/or under other stressful conditions (extended hours on airplanes for example). It is important to keep abreast of further developments in the field to better understand practical use and clinical potential. It may also be possible to find correlations between monitored signals and the health status of an individual. While observable changes in the monitored health indicators may not diagnose the specific health condition responsible for the onset of the change, they could serve as a trigger to seek medical attention.

One area of application could be real-time health and safety monitoring in environments where workers are at risk from chemical exposure. In this respect, the technologies allow individuals to be monitored for significant changes in vital signs, rather than or in addition to, monitoring dosage of exposure over given time periods, which is common practice for minimising worker risk in certain hazardous environments. Digital health technologies offer potential benefits to first responders and those working in contaminated areas.

In technical publications within the field, digital health technologies are seen as enabling technologies to help medical doctors make better decisions and diagnoses. For consumer use, about 200 disease indicators would need to be available to allow routine diagnostic use. This requires expanding molecule/phenotypic detection algorithms and ideally finding the minimum number of observations required to aid identification of a given clinical condition. A significant challenge for digital health technologies is to be as non-invasive as possible, avoiding the use of blood draw. The placement of monitors on fingers can provide good quality vital sign data; however such placements are not user friendly for extended data collection times. The potential use of digital health technologies for clinical decision making is still in an exploratory phase. Development of appropriate processes for bringing these devices into clinical use, and the regulatory oversight that would govern their use, is required.

Collecting data in remote and dangerous environments

This session of the workshop reviewed current capabilities of unmanned equipment that might be used by inspectors in future to make autonomous *in situ* chemical measurements under harsh conditions, collect and process samples in remote and dangerous locations, and operate robotic systems on land, sea or air. Such automated systems are desirable as they would enable inspectors to perform reconnaissance and sample collection remotely for non-routine situations where inspectors are at risk of harm. The examples that will be discussed next – the remote sampling and identification of volcanic gases, the collection and analysis of marine samples, the versatility of robotic tools for chemical sampling, and the design of unmanned vehicles (UVs) for making chemical measurements – could be used to augment the capabilities of the ‘OPCW Inspector of the Future’.

Aerial platforms for reconnaissance, sample planning and basic detection

Applications for aerial UVs (UAVs) in support of chemical emergency response include area reconnaissance, scene assessment and documentation, monitoring inspectors in hazardous environments and chemical detection. These applications could enable the development of chemical forensics and evidence management capabilities, and are topics of discussion in the SAB’s Temporary Working Group on Investigative

Science and Technology[3] [135–137] and the Chemical Forensics International Technical Working Group (CFITWG)[4] [138].

UAV technologies with an imaging capability can be used to verify and record information to help prove chain of custody. Linking detection information to a UAV's global positioning system (GPS) was identified as a desirable feature; this capability could allow chemical presence and contamination to be indicated on maps and geospatial images. UAV-enabled remote sensing and detection capabilities have clear value. Advances (especially miniaturization) in sensors and robotic platforms have made possible a number of cost effective and accessible UAV based solutions (Fig. 6) with potential applications for responding to chemical threats.

Unmanned airborne mass spectrometer (UAS-MS) for autonomous *in situ* chemical measurements under harsh environment conditions

UAVs capable of taking chemical and physical measurements are already used to make measurements in hazardous environments. Dr. Jorge Andrés Díaz of the University of Costa Rica addressed this topic, describing his work studying volcanic gases [139]. The integration of small UAVs with increasing payload capacity to carry a variety of chemical and physical sensor packages and instrument technologies is enabling the development of completely autonomous unmanned aerial systems (UAS) for *in situ* chemical analysis that can be used under harsh environmental conditions. This development has strongly impacted the way researchers and civil authorities can explore locations that were previously unreachable, due to unavoidable exposure to hazardous environments when collecting real-time chemical or geophysical information near the source. With UAS, *in situ* and proximal remote sensing measurements of volcanic plumes are now possible, without risking human lives. This has enabled the collection of *in situ* data very close to an eruption (something that had previously not been possible). This *in situ* measurement and validation capability improves the monitoring of pre-eruptive and eruptive volcanic emissions, allowing the acquisition of data to enhance trajectory models and provide better forecasting of volcanic plume impact on nearby population centres and aircraft. If this is possible around active volcanoes, the same technology should also be capable of assessing chemical weapons release, and chemical warfare agent presence, as well as providing a means to assess a potentially contaminated area without requiring personnel on the ground.

Dr. Diaz described two commercially available mass spectrometer systems with UAS application: the miniGAS [140] and the miniMS. The miniGAS has a 1.2 kg payload that includes four chemical sensors;

3 The objective of the SAB's Temporary Working Group on Investigative Science and Technology is to "review the science and technology relevant to investigations such as those mandated under Articles IX and X of the Chemical Weapons Convention" [135–137]. This would include science and technology for the validation and provenancing (i.e. determining the chronology of ownership, custody, or location) of evidence, and the integration of multiple and diverse inputs to reconstruct a past event. The first meeting was held at OPCW Headquarters in The Hague, from 12 to 14 February 2018 [137], and provided an opportunity to engage with the OPCW, particularly with individuals experienced in contingency operations, in order to highlight the operational capabilities, requirements and challenges for inspectors, as well as the OPCW Laboratory and designated laboratories. Forensic experts shared their experience in investigative and laboratory practices suitable for jurisdictional legal environments, with the aim of highlighting forensic capabilities and potential resources that are important for the review of relevant methods and capabilities. The Temporary Working Group will convene next from 14 to 16 November in The Hague. Its Chairperson is Dr. Veronica Borrett (of the SAB) and its Vice-Chairperson is Dr. Ed van Zalen (the current director of the Netherlands Forensic Institute).

4 The Chemical Forensics International Technical Working Group (CFITWG) was established as an informal and voluntary association of practitioners of chemical forensics in 2017. Its objectives are to collaborate with different analytical (chemistry) forensic communities to share commonalities and lessons learned, to identify general gaps and needs that can be addressed by one community, and to devise ways to organize, share and collaborate on: (a) research efforts to address gaps in chemical forensics capability, (b) access to chemicals, data and information to strengthen chemical forensic communities, and (c) standardization of forensics approaches across communities [138]. The group's efforts support the work of the OPCW SAB, specifically the SAB's Temporary Working Group on Investigative Science and Technology, to strengthen the OPCW's investigative options in future. The CFITWG met from 3 to 5 April 2017, and from 21 to 22 August 2018, during the American Chemical Society meetings in San Francisco and Boston, respectively. The CFITWG is coordinated by Dr. Carlos Fraga of the Pacific Northwest National Laboratory (PNNL) of the United States of America.

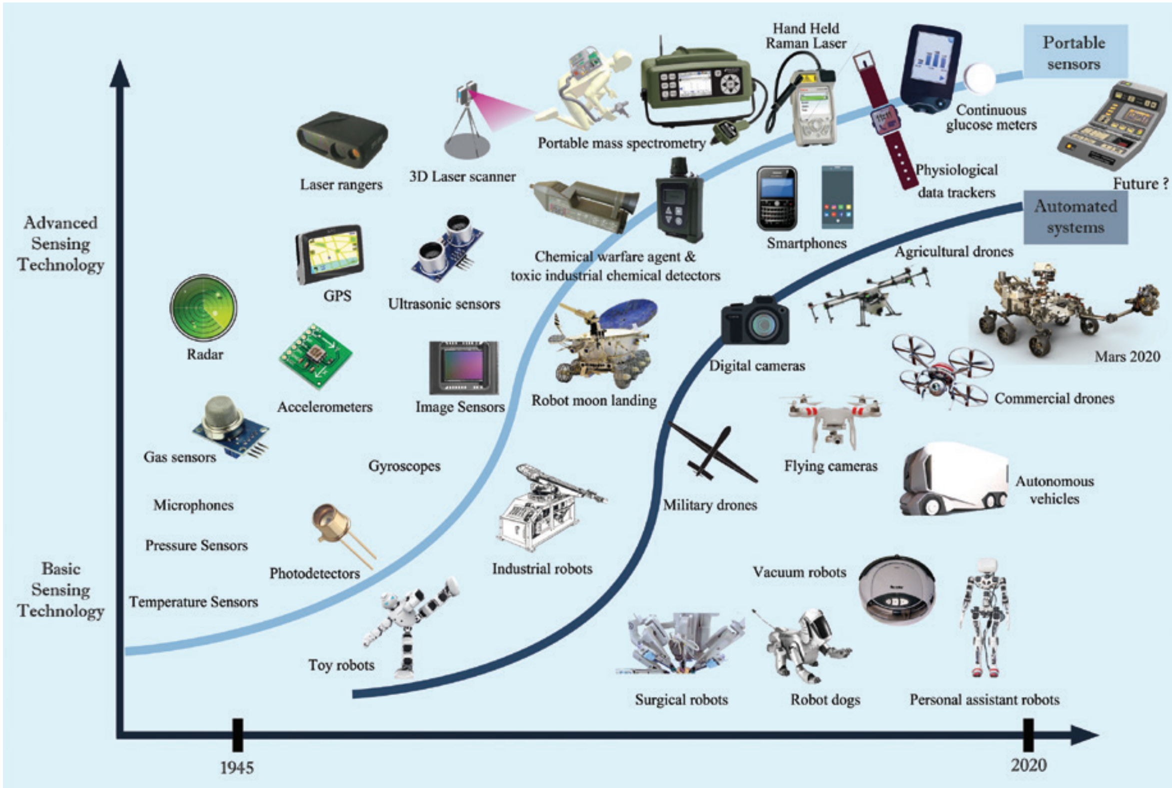

Fig. 6: Advances in sensing technologies and robotic platforms. The figure illustrates off-the-shelf, emerging and one-off devices and robotic platforms that are now, or soon will be available. There are a multitude of possible combinations of devices and platforms that can be integrated into mobile systems with capabilities for remote detection, monitoring, decontamination, identification, and/or sampling of chemical warfare agents, or other toxic chemicals, ultimately reducing the risk to an operator, who might control such a system remotely to avoid entering a hazardous environment. The timeline of the figure is intended to be illustrative not exact or comprehensive. The figure is indicative of how miniaturization and advances in robotics are making accessible greater numbers of enabling technologies that can be engineered for use across a broad range of applications.

pressure, temperature and relative humidity sensors; a global positioning system (GPS), on-board data storage, and video camera. Data is transmitted by telemetry in real time, which can generate 3D gas concentration maps of the active volcanic plumes. The miniMS has a 10 kg payload system that incorporates a miniature mass spectrometer (MS) with mass range of 1–200 atomic mass units (amu), together with a small turbo molecular pump, embedded computer and telemetry for real-time chemical analysis of the target area. Both systems have been successfully integrated into different unmanned aerial platforms and field tested, targeting *in situ* volcanic emissions and plume analysis, for calibration and validation of the US National Aeronautics and Space Administration (NASA) satellite-based remote sensing data from volcanoes in Costa Rica (Turrialba, Miravalles and Poas) [141, 142], Italy (Solfatara [143] and Vulcano Island), Nicaragua (Masaya) and the United States of America (Kilauea). These systems might also be used in chemical security applications and situations [144].

In studies of the chemical emissions of volcanos, UAVs are lost periodically, but the transmitted data are more valuable than the machine (this is also a driver to build cost-effective equipment). Of relevance to non-proliferation activities with a MS-equipped UAV, a system for chemical agent analysis would have similar logistical requirements to equipment used for volcanology: a UAV with 12 kg payload, 1 h flight time, 3–5 km range, and automatic take off/landing capability to allow sampling capabilities. The mass spectrometers used in volcanology can make measurements in the 100–200 amu mass range, and would be able to detect sulfur mustard, organophosphorus nerve agents, and their degradation products (if these were sufficiently volatile).

Collection and processing of biological samples in remote and dangerous places: the Environmental Sample Processor as a case study

Dr. Jim Birch of the Monterey Bay Aquarium Research Institute (MBARI) (United States of America) introduced the workshop to the marine unmanned systems for sample collection and processing developed at his institute [145, 146]. Oceans have proven problematic to study, in part because persistent access can be difficult and costly. MBARI design, test, and deploy instruments that address the issue of access. The analytical sides of these instruments are modelled after the tools and techniques derived from the biomedical diagnostics and research industries. Coupling these analytical techniques with traditional oceanographic sensors that characterise the physical, chemical and optical properties of ocean waters has led to the concept of the 'ecogenomic sensor', a device that can apply biomolecular analytical techniques *in situ*.

The Environmental Sample Processor (ESP) serves as a case study [146]. The ESP employs low-density DNA probe and protein arrays to assess in near real-time the presence and abundance of specific organisms, their genes and/or metabolites. In addition, a two-channel real-time polymerase chain reaction (PCR) module supports deployment of a variety of user-defined master mixes, primer/probe combinations and control templates. The ESP can also be used to preserve samples for a variety of laboratory tests once the instrument is recovered, including metatranscriptomic analyses of natural microbial populations. The ESP was originally designed as a mooring, and has been further developed to fit within an Autonomous Underwater Vehicle, adding mobility for ecogenomic sensing.

Sample collection and processing is a key aspect of marine ecosystem monitoring. In addition to the ability to recognise oceanic toxin blooms, the genomic analysis of environmental DNA (eDNA) in seawater provides opportunities to look at changes in communities of marine animals (and especially microbes) as indicators of change. These systems could have application in studying the ecosystem around sea- or fresh water-dumped chemical munitions [147–152].

Modular robotic toolbox for counter-CBRN support

Unmanned ground vehicles (UGVs) are also seeing interest as systems for countering Chemical, Biological, Radiological and Nuclear (CBRN) risks [153]. Mr. Grzegorz Kowalski of the Industrial Research Institute for Automation and Measurements (PIAP) (Poland) [154] discussed the design and construction of modular robotic platforms for this purpose [155]. The knowledge base of mobile robots for countering improvised explosive device and disposal of ordinance has enabled robotic security applications to expand into other specialised fields. Robots can be constructed for specific environments and applications (e.g. for operating in nuclear power plants) and equipped with dedicated tools, so that only modular changes to a base platform are required to fit the robots for any specific application. These modular components can include sensors and other data collecting devices, forensic and counter-CBRN robotic accessories, offering high configurability and interoperability.

The concept of a modular robotic toolbox relies on interoperability/configurability, handheld wireless controls, ease of maintenance, remote measurement capability, platform independence, and maintaining an internal power source. This requires that a family of accessories can work independently from the host platform and can be controlled using a user selected interface. The toolbox employs software interfaces to allow the user to adjust the set of accessories and their means of control to specific needs of a mission, permitting on demand reconfiguration. The toolbox devices use similar electronic subsystems for the realization of the interfaces, and standardized mechanical attachments, such as NATO weapon rails. There is additional flexibility when sampling and analysis systems to be integrated into the robot are sourced from manufacturers as ready-to-use components (this expands the capabilities the robot can have based on what is available from others off-the-shelf, see also Fig. 6).

Unmanned aerial vehicle equipped with CBRN – detection, identification and monitoring (DIM) capability to enhance chemical awareness

Dr. Marcel van der Schans of TNO (The Netherlands Organisation for Applied Scientific Research) [156] discussed the development of a CBRN Detection, Identification, and Monitoring (DIM) UAS. Detection of toxic chemicals at and around secured areas and other critical infrastructure is crucial and normally monitored by point detectors; requiring large numbers of detectors (organised in a network) for large areas. The mobility of an unmanned system with DIM capability could help overcome this limitation and also allow measurements to be taken in areas that may be dangerous or problematic for inspectors to access. Passive stand-off detectors can be placed on the border of a secured or contaminated area and used to monitor the surroundings. These systems can determine the presence of chemicals based on spectroscopy (infrared for example). However, the detectors can suffer from interference by weather conditions and various airborne chemicals, and there may be limitations for detection at longer distances. A UAV equipped with DIM capabilities could fill this gap.

In a National Technology Project, the Dutch Ministry of Defence sponsored a joint project between Delft Dynamics, a manufacturer of UAV's, and TNO, to develop a prototype of a CBRN-drone with integrated sensors and sampling systems. The resultant UAV was equipped with a 'smart sampling' system, consisting of a vacuum canister or helium diffusion sampler, which can be manually activated or triggered by an on-board detection system. The system requires that location of sampling and detection systems must be designed to avoid the interference by downwash caused by the rotor blades of the UAV. There are some disadvantages with small UAVs, as they often have limited payload capacity (typically 1–2 kg) and limited battery life, restricting their utility to a directed use, rather than a monitoring mode. Battery powered UAVs do however, avoid interference with detection of specific CWAs that can result from chemicals present in the exhaust from a gasoline powered UAV engine. The TNO design discussed at the workshop was based on a scenario of small chemical plumes where a UAV could have the capability to fly to the source, identify the chemical and take a sample. In this regard, UAV systems that collect air/vapour samples are commercially available [157].

All the mobile systems discussed at the workshop were capable of streaming data as it was being collected, raising the issue of data security. For sensor arrays, the data generated would be comprised of electronic signals (patterns) of the sensor component response. The data might then be difficult to decipher without the algorithm and training data required for analysis. Theft of data from a mass spectrometer based system however, would provide spectral data that can be interpreted without purpose-specific data analytics.

International monitoring networks

The session on monitoring networks discussed how the various technologies reviewed in the previous sessions of the workshop might serve as components of an integrated data collection and analysis capability (Fig. 4) for a larger (international) monitoring system. Tracking biogeochemical change through remote sensing may have applications for non-proliferation research.

Monitoring networks tracking biogeochemical changes in coastal and maritime environments

An example of an international monitoring system was provided to the workshop by Dr. Andrés Arias from the Instituto Argentino de Oceanografia (Argentina). Dr. Arias discussed the Global Argentine Basin Array [158], which serves as one of the stations of the Ocean Observations Initiative (OOI) [159] (Fig. 7). Various scientific networks are currently working in Argentine urban, coastal and maritime environments, performing

Fig. 7: Ocean Observatory Initiative (OOI) Station Map [159]. The stations comprise an integrated system of platforms and sensors that collect physical, chemical, geological and biological information about the ocean. Data is collected continuously from each station and made available to scientists involved with the initiative. Large-scale monitoring networks such as the OOI offer examples of how data can be collected on an international scale and serve as a means to facilitate scientific collaboration. The data streams generated by these monitoring systems may offer opportunities that could potentially be used to benefit non-proliferation. In this regard, the CTBTO and its International Monitoring System (made up of seismic, infrasound, hydro-acoustic and radionuclide monitoring stations) provides an example of how this concept has been applied to nuclear non-proliferation [162]. The image is reproduced under a creative commons license, credited to OOI Regional Scale Nodes program, and the Center for Environmental Visualization, University of Washington, USA.

both classical and novel remote sampling, including the tracking of persistent pollutants using passive monitoring (such as passive air- and XAD samplers[5]), classical bio-indicators, and autonomous maritime buoys [160] and boats. In addition to furthering international scientific collaboration, the data generated by these

5 XAD refers to highly-absorbent resins that are used for continuous sampling of organic materials.

monitoring networks have provided input to policymakers to inform strategies for land management, and have helped in the assessment of environmental vulnerabilities.

Monitoring networks such as OOI bring together a large number of scientists from the region where the system operates (and connects them with scientists associated with other stations of the OOI, Fig. 7). This kind of scientific collaboration across international borders is recognised for its value for science diplomacy. Additionally, the data sets generated by these monitoring systems are used to inform policymakers, thus serving to facilitate scientist-policymaker engagement. International monitoring networks also offer opportunities in outreach and awareness-raising, as they can serve to bring scientific experts from across disciplinary boundaries together, as well as facilitate citizen science initiatives to engage the general public (this in turn might facilitate crowd sourcing of new ideas and innovative technologies). In the disarmament community, the international monitoring system (IMS) [161] of the Preparatory Commission for the Comprehensive Nuclear Test Ban Treaty Organisation (CTBTO) [162] plays a similar role.[6]

Remote sensing and open-source research for non-proliferation analysis

The applications of remote sensing capabilities, particularly satellite and aerial imagery, for security and non-proliferation topics are vast, with researchers exploring their applicability to nuclear, chemical and biological security. Ms. Catherine Beatrice Dill addressed this topic, presenting work ongoing at the Middlebury Institute of International Studies (MIIS), James Martin Center for Non-proliferation Studies (United States of America) [163]. Non-proliferation researchers have used optical satellite imagery to map, geo-locate and monitor facilities of interest and/or concern [164, 165]. In addition to natural colour imagery, satellite imagery collected using non-visible wavelength light (for example thermal infrared and short-wave infrared) can be used to better understand the nature and operating status of facilities of interest and their surrounding environments. Combinations of satellite and ground imagery have been used to assess activities taking place at several facilities in the Democratic People's Republic of Korea. For chemical security applications, the use of hyperspectral and short-wave infrared satellite imagery, combined with other forms of remote sensing was suggested to be well suited. Satellite image analysis for non-proliferation research requires access to a broad range of experts. In addition to the data analysis and image analysis capabilities, those with knowledge of the types of infrastructure and chemical change that the imagery is capturing are necessary in order to draw meaningful conclusions.

Crowd sourcing to annotate image data has been used successfully by agencies like NASA [166] and non-proliferation researchers have also used this approach [167]. These annotations combined with other training data can help to optimise machine learning tools that aid image analysis. With the increase in CubeSat companies and the complete Earth observation these can provide, there are more opportunities to access images and information (including through public outreach initiatives from satellite imagery providers). Other satellite imagery, from the Landsat programme for example, is available as open access data. Landsat satellite images have been used to estimate the levels of certain chemical elements in soil [168] and identify toxic algae blooms [169]. An advantage of using open-source information includes the ease and speed of accessing data, and the ability to readily share analysis results.

6 The Comprehensive Nuclear-Test-Ban Treaty (CTBT) bans nuclear explosions by everyone, everywhere: on the Earth's surface, in the atmosphere, underwater and underground. Since the Treaty is not yet in force, the organization is called the Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO). It was founded in 1996, has over 260 staff from over 70 countries, and is based in Vienna, Austria [162]. The CTBTO's main tasks are the promotion of the Treaty and the development of the verification regime so that it is operational should the Treaty enter into force. To build and strengthen its relationship with the broader science community in support of the CTBT, the CTBTO invites the international scientific community to conferences held every 2 years. These multidisciplinary scientific conferences attract scientists and experts from the broad range of the CTBT's verification technologies. The next CTBT Science and Technology Conference will be held at the Hofburg Palace, Vienna, from 24 to 28 June 2019 [162].

Computer aided engineering tools applied to Chemical Weapons Convention implementation

The previously described workshop sessions looked at a variety of technologies that make measurements, yet it should be appreciated that all the examples relied on having access to data analytics to process information and integrate it with other data streams. As computational tools become more powerful, they provide opportunities to use modelling tools and simulations to more effectively complement experimental studies. Simulations can also provide useful information for a variety of applications relevant to chemical disarmament and non-proliferation. Dr. Evandro de Souza Nogueria (of the SAB) provided a presentation on the use of Computer Aided Engineering Tools (CAE) to explore potential applications.

CAE have been finding use across a variety of applications, including innovation [170], chemical engineering education [171], product development and improvement [172, 173], chemical emergency response scenarios [174], chemical reactor design [175–179], blast explosion studies [180, 181], and the interaction of CWAs with enzymes [182, 183]. Freely available [184–187] and commercial [188, 189] software packages can be used to perform calculations and to study dispersion modelling of toxic chemical releases (which allows such studies to be carried out without having to actually handle any toxic chemicals).

There are several CAE methodologies that can be applied to the preparedness for response, or investigation of chemicals dispersed into urban environments and infrastructure. In regard to applications

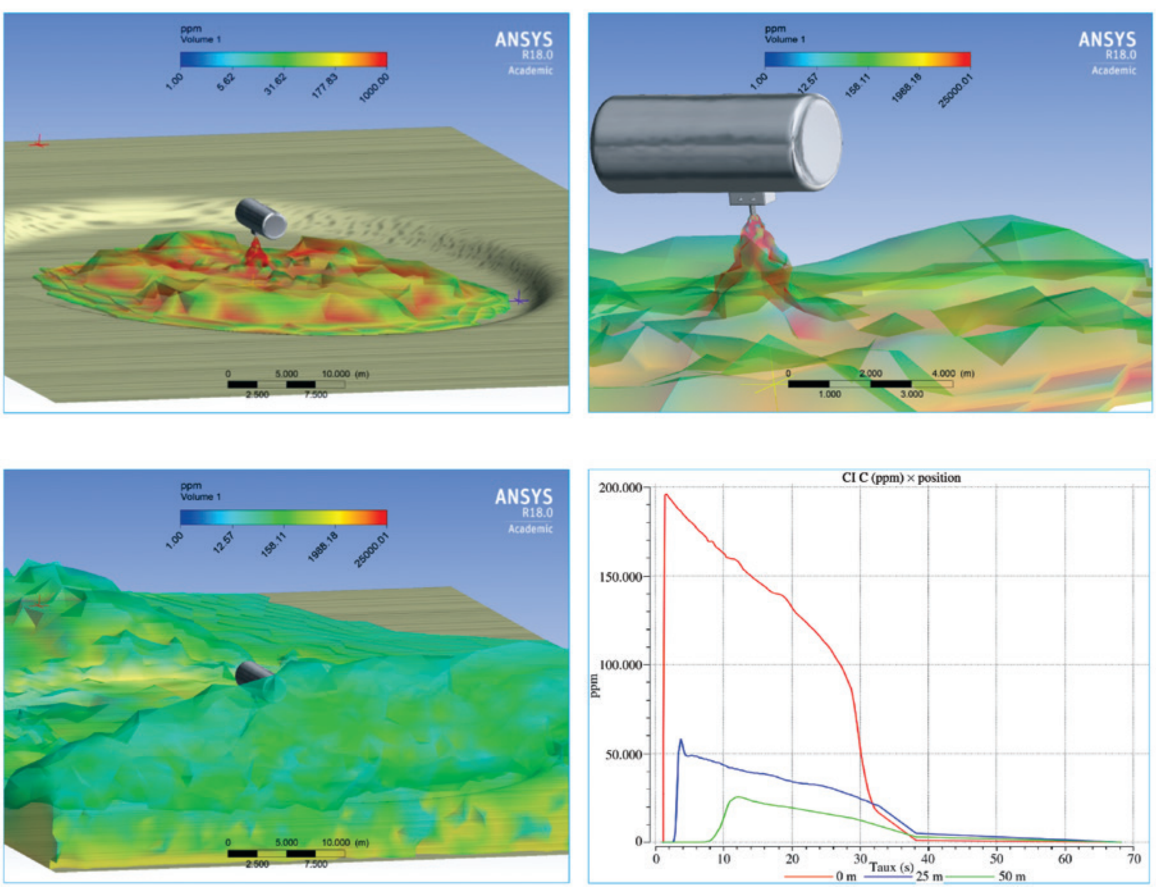

Fig. 8: CFD predictions for chlorine concentration (ppm) from an intentional release from a two ton container in the Jack Rabbit Chlorine Release Experiment [195]. Initial release (Upper left). Container detail (Upper right). High concentration chlorine cloud (Bottom left). Concentration profiles at selected time points (Bottom right). The simulation was performed using the ANSYS® 18 CFD software package, Ansys Inc., Canonsburg, PA, USA [189].

relevant to the Convention, an example of dispersion modelling related to events in the Syrian Arab Republic, using open source information (including weather reports and satellite imagery) to inform the model, was recently published [190]. It is also possible to model industrial accidents for response planning and risk mitigation [191] and indoor dispersion of chemicals.

Computational Fluid Dynamics (CFD) is a useful approach for the analysis of systems involving fluid flow, heat transfer and other related phenomena such as chemical reactions, adsorption, blast explosion and fluid-structure interaction (FSI) [192–194]. The technique is very powerful and spans a wide range of industrial and non-industrial application areas. Figure 8 illustrates the use of CFD for evaluating the dispersion of a chemical release, using chlorine gas, and data and observations from the Jack Rabbit Chlorine Release Experiment [195]. The simulation prediction suggests that a lethal contaminant concentration [over 1000 parts per million (ppm)] is established in a few minutes over a 50 m radius zone.

While much can be done with CAE, models have limitations. As seen with the research presented from FOI Sweden, it is important to have accurate source terms, preferably derived from experimental studies to provide confidence in the predictions. Information on chemical concentrations, atmospheric data, urban topology, blast effects, chemical reactivity and adsorption processes can all impact the dispersion of a chemical cloud or plume. Other sources of information such as witness statements and imagery or video might help inform the modelling by challenging assumptions made in defining input parameters.

Conclusions

The presentations and discussions at the Rio de Janeiro workshop served as inputs for some of the recommendations in the SAB's report the Fourth Review Conference, which was published in April 2018 [196–198]. In closing this paper, the insights and recommendations submitted in that report are discussed.

A broad set of innovative technologies exist, with many more in development, that could find application in the implementation of the Convention, especially for investigations and other non-routine (contingency) and assistance and protection operations. The benefits that could be realised include reducing risks to personnel operating in dangerous environments, enhancing sampling and analysis capabilities, and stakeholder engagement. The insight brought to discussions by inspectors regarding fieldable and operational needs and challenges is essential for recognizing opportunities where new technologies (or new ways to deploy existing technologies) might prove valuable [36].

For technologies with potential to reduce risk for personnel operating in dangerous environments, further consideration could assist with development of recommended best practices for operating under such conditions. Suitability for field use requires evaluation of fieldable capabilities that meet operational requirements (and fit within mission-specific modalities). In regard to the possibility of field testing, an inventory of available innovative tools that could be tested would be useful for the OPCW to consider. Opportunities to engage with technology developers and evaluate new tools should be encouraged.

The practice of bringing together international trans-disciplinary groups to share and discuss ideas is vital for overcoming current and future challenges. The convergent science and technology review by the SAB for the Fourth Review Conference [196] has been conducted across scientific and international borders. In the lead up to the report submitted for the Review Conference, 27 meetings and workshops were organized by the SAB or its Temporary Working Groups. These had a combined participation of 747 people (comprising 289 individuals from 58 Nations [196]). This wide reach ensured that a diversity of scientific views and technical expertise underpinned the advice and recommendations.

Engaging operational staff from the OPCW in the review process has aided the formulation of practical science advice and allowed the SAB to provide scientific guidance on operational practices. The SAB encourages the OPCW to continue this approach when considering scientific and technological advancements. Technologies that integrate informatics tools, mobile devices and remote sensing with an expanding range of capabilities are becoming increasingly accessible. The Convention's science review process should continue to keep abreast of developments in these areas.

The OPCW might consider outreach strategies, such as crowd source competitions to engage and gain access to innovative technologies and ideas. Engaging relevant innovators to participate in Convention-related training and familiarisation would provide an additional avenue to reach out to innovation communities. As the OPCW and its stakeholders consider technological change, it is imperative to maintain high levels of scientific literacy, to engage with broad scientific communities, and to consider technological opportunities that enable robust implementation of the Convention.

The OPCW Director-General was supportive of these outcomes, addressing them and how they might be taken forward within OPCW, in his response to the report of the SAB's Twenty-Sixth Session [199].

Recommendations and response

Recommendations that were included in the report for the Review Conference [196, 197], stemming from contributions of participants in the Rio de Janeiro workshop, include the following:

– The SAB notes that satellite imagery has proven useful in planning contingency operations and recommends that the Secretariat consider cooperating with other international organisations and experts to enhance its capability to interpret and apply satellite information to non-routine operations. The use of hyperspectral, thermal, and near-infrared imagery can provide information related to chemical changes in the imaged area [196].
– In order to enable inspection teams to operate in dangerous or remote areas, the Secretariat should review remote and automated monitoring technologies to identify where their capabilities could be beneficial. Corresponding equipment should be added to the list of approved inspection equipment [196].
– In view of the increasingly interdisciplinary nature of advances in science and technology relevant to the Convention, the SAB should continue to build close working relationships with relevant professional societies and science advisory bodies of other relevant international organizations to enable it to identify and assess developments that may impact the Convention or the OPCW. Such relationships should also be utilized to raise awareness of the Convention and to promote its norms [196].

The OPCW Director-General in his June 2018 response to the SAB's report [198] highlighted aspects of all these recommendations, giving them support and pointing out their value to the States Parties.

The States Parties had also taken notice of the Rio de Janeiro workshop. The joint Statement of the European Union members at the 2017 Conference of States Parties [200] called for the OPCW to keep pace with advances in science and technology, such as those discussed in the workshop. Additionally, a working group of States Parties (co-chaired by Ambassadors from Canada and South Africa) on future priorities of the OPCW stated that "The Secretariat's capabilities of conducting both inspections and fact-finding missions should be further strengthened, including by enhancing capabilities for assessment of declarations and sampling and analysis, and by adopting new or emerging technologies as identified by the Scientific Advisory Board (SAB) and the Secretariat" [201]. In this statement, "Secretariat" refers to the OPCW (the staff of the OPCW comprise a "Technical Secretariat" [202]), and "emerging technologies" was in the title used for the SAB working paper that came from the workshop [23].

The SAB is encouraged to see statements such as those pointed out in the paragraph above. These are an indication that the work of the Board has been considered by some of the States Parties for their deliberations in November 2018.

Closing remarks

In view of the many interesting and potentially enabling technologies that are described in this report, the OPCW is encouraged to consider ways in which such technologies may prove valuable in enhancing its capability to verify compliance with the Convention and to assist States Parties in improving their own capabilities. This should be informed by capability requirements, not the technology itself. The SAB is of the view that technological change is best considered from a practical perspective, focusing on capabilities relevant to the Convention, irrespective of scientific discipline [196]. It hopes that the information contained in this article, and the rest of this special issue of *Pure and Applied Chemistry* describing the OPCW-IUPAC Workshop on Innovative Technologies for Chemical Security, serves as a springboard for further scientific progress in the service of peace.

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