OPCW

Scientific Advisory Board

Thirty-Second Session
15 – 17 June 2021

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REPORT OF THE SCIENTIFIC ADVISORY BOARD AT ITS THIRTY-SECOND SESSION

1. AGENDA ITEM ONE – Opening of the session

1.1 The Scientific Advisory Board (SAB) met virtually for its Thirty-Second Session from 15 to 17 June 2021. The session was chaired by Dr Christophe Curty, with Dr Andrea Leisewitz serving as Vice-Chairperson.

1.2 The SAB Chairperson opened the Thirty-Second Session of the SAB and welcomed SAB members, external speakers, colleagues from the Advisory Board on Education and Outreach (ABEO) and the Technical Secretariat (hereinafter "the Secretariat"), and observers. Noting that the SAB has adapted well to the current challenging circumstances, the Chairperson expressed his appreciation to all SAB members for their flexibility and dedication. He further thanked the drafting committee for its work on the previous session's report. He remarked that the reports are an important instrument for the SAB in providing advice to the Director-General and reaching all States Parties and the various divisions within the Secretariat.

1.3 The Chairperson further provided a brief overview of the response of the Director-General to the report of the Thirty-First Session of the SAB (EC-97/DG.5, dated 18 May 2021), including the Director-General's expression of appreciation to the SAB for its continued efforts during these uncertain times, and its willingness to meet virtually to discuss topics of relevance to the Secretariat. The Chairperson noted that the SAB is extremely fortunate to enjoy the full support of the Director-General and expressed special regard for his efforts to provide the Board with the tools necessary to continue to provide advice on the scientific and technological developments relevant to the Chemical Weapons Convention (hereinafter "the Convention").

Executive summary

1.4 Due to the COVID-19 pandemic, this SAB meeting was conducted in a virtual format.

1.5 This session focused on several topics, including current and upcoming SAB activities, such as the ongoing preparations for the Fifth Review Conference,[1] the newly established Temporary Working Group (TWG) on the analysis of biotoxins, and plans for upcoming workshops. Mr Günter Povoden and Dr Ahmed Saeed gave presentations to the Board on dissemination technologies and the use of artificial intelligence (AI) in

[1] The Fifth Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

chemistry. In addition, the Board heard from Dr Bartosz Grzybowski on how advances in using AI can be applied to design and predict chemical synthesis routes. Dr Rafiqul Gani addressed the SAB on the application of AI to predict the properties of chemical compounds. The Board also heard from Dr Derrick Kaseman on new approaches to using nuclear magnetic resonance (NMR) spectroscopy to detect and identify organophosphates.

1.6 Based on the deliberations at its Thirty-Second Session, the Board recommends to the Director-General through this report that:

(a) the Director-General support a SAB workshop partnering with the International Union of Pure and Applied Chemistry (IUPAC) to consider emerging technologies relevant to the SAB's preparation of its scientific report for the Fifth Review Conference;

(b) the Director-General consider convening a workshop related to the use of AI in the field of chemistry, specifically in terms of its potential in planning and performing synthetic procedures and predicting the properties of chemical compounds. Both the beneficial and potentially malicious uses of this rapidly maturing field are worth considering in terms of their impact on the Convention and the work of the OPCW; and

(c) the Secretariat consider bolstering its outreach and capacity-building events to States Parties with additional information related to dissemination technologies. The SAB notes that when seeking to prevent the use of chemical weapons, understanding dissemination approaches and technologies is critical. States Parties could therefore benefit from added information and capacity-building materials on this topic.

2. AGENDA ITEM TWO – Adoption of the agenda

The SAB adopted the following agenda for its Thirty-Second Session:[2]

1. Opening of the session
2. Adoption of the agenda
3. *Tour de table*
4. Establishment of a drafting committee
5. Welcome address by the Director of the Verification Division
6. The impact of artificial intelligence in the chemical sciences
    (a) Overview of artificial intelligence and its role in chemistry
    (b) Advanced synthesis planning by computers
    (c) Properties of organic chemicals: databases and estimation methods

[2] It should be noted that while presentations and agenda items are grouped in this report based on topic matter, they were not always presented sequentially as listed due to scheduling considerations of the presenters.

7. Overview of developments at the OPCW since the last session of the Scientific Advisory Board

8. Established and emerging technologies for the dissemination of chemical agents

9. Detecting organophosphate chemical warfare agents using low-magnetic field nuclear magnetic resonance spectroscopy

10. Current and future activities of the Scientific Advisory Board

    (a) Preparing for the Fifth Review Conference

    (b) Temporary Working Group on the analysis of biotoxins

    (c) Efforts towards a workshop in partnership with industry

11. Any other business

12. Adoption of the report

13. Closure of the session

3. AGENDA ITEM THREE – *Tour de table*

A tour de table was not done as this was not the first session of the SAB in 2021 and introductions were not deemed necessary.

4. AGENDA ITEM FOUR – Establishment of a drafting committee

The SAB Secretary asked for volunteers to contact him or the SAB Chairperson if interested in being on the drafting committee to prepare the report of the SAB's Thirty-Second Session.

5. AGENDA ITEM FIVE – Welcome address by the Director of the Verification Division

5.1 The Director of the Verification Division, Dr Carolyn Browne, delivered opening remarks. She welcomed the members of the SAB and expressed appreciation for an opportunity to meet them, albeit only virtually. She then provided an update on verification activities over the last year in each of the Division's four branches, highlighting the new and ongoing developments, as well as plans for the future.

5.2 Regarding the Declarations Branch, the Director noted various upgrades to the confidential registry. She did note, however, that these upgrades may affect the compatibility of the data moving forward. She queried the SAB as to any views on how to use these aggregated data and rules regarding access to it. She further noted that the Declarations Branch is looking at some form of a proof of concept to use distributed ledger technology (also known as "blockchain technology") to help States Parties align their export records with the import records of counterparties in order to try to significantly reduce transfer discrepancies.

5.3 The Industry Verification Branch is currently in the refining stage of a three-year project to optimise the way in which the OPCW carries out Article VI inspections. The project is a collaborative effort with the Inspectorate Division and looks to optimise, streamline, and, where possible, systemise and digitise Article VI inspections. The Director noted that there are changing variables in these inspections that may result in a change to the selection and frequency criteria associated with them, but that this is a topic for States Parties to discuss and collectively provide guidance on.

5.4 The Chemical Demilitarisation Branch continues to work on the destruction activities for the possessor State's last stockpile, in addition to abandoned and old chemical weapons. One important theme, she noted, is how to capture the knowledge related to destruction activities under the Convention and apply it against the future possibility of new possessor States joining the Convention. The Branch is also exploring other elements of interest, including the possibilities, vulnerabilities, and challenges related to non-State actors. Furthermore, she noted that a member of the Chemical Demilitarisation Branch (in addition to a few staff members from the Declarations Branch) is being moved to the Laboratory ahead of the opening of the Centre for Chemistry and Technology (ChemTech Centre) in order to provide additional resources to meet the expected increase in responsibilities, operations, and work moving forward.

5.5 In terms of the OPCW Laboratory, the focus has been on maintaining its core function of authentic sample handling as the Laboratory moves from Rijswijk to the ChemTech Centre, which will enhance its capabilities. One priority will be to address the implications of the decision to schedule new chemicals (Schedule 1 chemicals), including methodologies to detect, verify the presence of, decontaminate materials from, and better understand their toxicity. Work is under way to update the OPCW Central Analytical Database (OCAD) with data on the newly scheduled chemicals.

5.6 The floor was then opened for questions from the Board. The Director of Verification was first asked whether the OPCW is looking to conduct any virtual verifications moving forward.

5.7 The Director of Verification explained that while this is possible in theory, and that there have in fact been several remote verifications conducted in the past for specific reasons, this is unlikely in the short term. She explained that relevant National Authorities would need to be willing and able to accommodate a virtual verification and that the Secretariat would also need to be sure that it can sufficiently verify declarations at a given site.

5.8 Another question centred on whether there were any trends in industry that have resulted in the increase in the number of companies that fall within the inspection and verification regime.

5.9 The Director of Verification agreed that there has been considerable growth in the chemical industry sector; nevertheless, the rules remain that a maximum of 20 inspections are permitted per State Party per year for Schedule 3 and other chemical production facility (OCPF) inspections—regardless of whatever increase in the number of facilities they have. The Head of the Industry Verification Branch, Mr Larry Denyer, further explained that the cap is different for each State Party depending on how many facilities they declare (with 20 being the limit per State Party per year). He noted that there are changes in how some scheduled chemicals are being used industrially (e.g., the

increase in the use of Schedule 2B chemicals in the pharmaceutical industry) and that this, coupled with the natural growth of the chemical industry over time, results in a small number of States Parties that declare a great number of facilities.

5.10 The Board also asked whether the OPCW now has more of a focus on Schedule 3 chemicals (commodities production). The Director of Verification noted that there is actually more focus on Schedule 1 facilities.

5.11 The issue of transfer discrepancies was then raised, with the Board asking how these will be handled moving forward. The Director of Verification noted that transfer discrepancies are an ongoing problem, as a large proportion of the transfer discrepancies that are detected are never resolved. This prompted the Verification Department to go back to basics and start the distributed ledger technology project, as it might help some States Parties, specifically those in a customs union, to tackle the issue.

6. AGENDA ITEM SIX – The impact of artificial intelligence in the chemical sciences

6.1 There has been rapid development in using AI and other automated processes in chemistry, particularly in synthesis. This emerging technology holds considerable promise for revolutionising drug design and chemical property prediction, among other fields, but may unfortunately also be misused. The SAB therefore monitors the advances in this field and periodically hears from pre-eminent experts on recent developments. At this session, the SAB heard from its own member, Dr Ahmed Saeed, who presented an overview of the field and how AI and computers have been augmenting chemistry research. The Board then heard from Dr Bartosz Grzybowski, who gave an overview of his research group's work in the field of computerised planning for chemical synthesis. Dr Rafiqul Gani also presented his team's work on predicting the properties of chemical compounds using computational chemistry approaches.

Subitem 6(a): Overview of artificial intelligence and its role in chemistry

6.2 Dr Ahmed Saeed, a member of the SAB, gave a comprehensive overview of the applications of AI in science—chemistry in particular—touching on different themes and noting recent relevant literature. The themes presented include property prediction, molecule design, retrosynthesis, reaction prediction, and optimisation. He also noted some of the emerging applications, including AI for primary and secondary drug screening (predictions of physical properties and bioactivity), AI in drug design (predicting the 3D structure of a target protein and drug-protein interactions), planning chemical synthesis with AI (retrosynthesis, pathway prediction, reaction yield prediction, and insights into reaction mechanism), automation of chemical synthesis with AI digitisation and standardisation of synthesis, and automated reaction space sampling with AI.

6.3 Dr Saeed also noted that the SAB has members who conduct research in this field: Dr Ramasami and his research group have studied the underlying hydrolysis mechanism of A-234, a fourth-generation nerve agent, within a density functional theory framework[3]; and Dr Saeed's own research group has used molecular modelling approaches to study the properties of carbothioamide derivatives.[4]

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[3] H. Bhakhoa, L. Rhyman, P. Ramasami, R. Soc. Open Sci., 6, 181831. DOI: 10.1098/rsos.181831.

[4] T. T. H. Hajalsiddig, A. B. M. Osman, A. E. Saeed, ACS Omega 2020, 5, 18662−18674. DOI: 10.1021/acsomega.0c01323.

6.4 There are continuous rapid advances in AI applications in chemistry and increased interest in them as emerging technologies. Recognising the potential of using AI technologies in chemistry, and in relation to the Convention in particular, the SAB suggests continuing to follow developments in this field.

Subitem 6(b): Advanced synthesis planning by computers

6.5 Dr Bartosz Grzybowski, Professor at Ulsan National Institute of Science and Technology, gave a presentation on some of the most impactful discoveries in the area of computer-planned organic synthesis and the use of AI in reaction and drug discovery.[5] After a decade of development, in 2012 the Grzybowski group released *Chematica*, a software programme that uses algorithms and features a collective database of 250 years of synthetic organic chemistry information to predict and provide synthesis pathways for molecules. The programme can explore billions of possible syntheses in a fraction of a second and can then assist in down-selection based on user-indicated priorities, such as the cost or availability of precursors, or environmental concerns. In 2017, the software and its accompanying database were purchased by Merck KGaA and made available commercially before being rebranded as Synthia™. This retrosynthetic planning software allows chemists to select the type of retrosynthesis analysis to be performed and the target molecule from known and unknown compounds. However, as Dr Grzybowski pointed out, one of the software's limiting factors is that it does not help discover new molecules, per se.

6.6 About seven years ago, his group started working on forward synthesis, which is the process of using simple materials as substrates and further creating and navigating new chemical space and discovering new molecules. Using software they call *AllChemy*,[6] Dr Grzybowski noted that his team have been able to simulate chemical reactions that lead to life on the prebiotic Earth.[7] Starting from the six most basic and common substrates—methane, ammonia, water, hydrogen cyanide, nitrogen, and hydrogen sulphide—they were able to obtain over 1,000 chemical compounds in just five generations of calculations (consecutive reactions), including amino acids (protein components), nitrogen bases (DNA components), lipids, and enzymes. The preparation of such a complete chemical 'tree of life' and the potential to generate this large number of chemical compounds is beyond the capabilities of individual chemists. Dr Grzybowski stressed the importance of machines in driving chemical discovery.

6.7 In providing examples of other applications of forward-thinking chemistry, Dr Grzybowski concluded that programmes such as *AllChemy* will become more and more important in circular chemistry (waste management), threat reduction, and chemical forensics.

6.8 The Board asked how a programme like *AllChemy* deals with complex stereochemistry, especially in the proposed synthesis of biological natural products. Dr Grzybowski replied that in the retrosynthetic direction, stereochemistry is absolutely critical. However, in the forward direction, the premium is on the molecular skeleton, and the stereochemistry can be fine-tuned, otherwise too many potential compounds will be generated.

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5 K. Molga, S. Szymkuc, B.A. Grzybowski, Acc. Chem. Res., 54, 1094-1106 (2021).

6 Please see: https://tol.allchemy.net/.

7 B. Mikulak-Klucznik, P. Golebiowska, et. al., Nature, 588, 83-88 (2020).

6.9 The SAB also asked how AI software can be used to make other predictions, such as those concerning the physical, chemical, and hazardous properties of chemicals, or even to find pathways in the degradation of chemical warfare agents to generate useful chemicals. Dr Grzybowski confirmed that the software can predict the properties of chemical compounds. He noted a current project that his team is working on, which involves extensive calculations, including crystal packing, and indicated that he considers property prediction more straightforward than synthetic prediction. Regarding the degradation products of chemicals, he added that a computer has a distinct advantage over a human insofar as it can create degradation trees with millions of possibilities. Hence, finding potential degradation pathways to chemical weapons that result in useful industrial chemicals should be possible.

6.10 Finally, the Board noted the capabilities of the software to predict "malicious chemistry". It was then asked whether there are plans to control the software to prevent it from making calculations using controlled substances. Dr Grzybowski confirmed that the software could potentially be misused (to design or make explosives, neurotoxins, etc.) and that the group is therefore thinking about how to prevent its misuse while also exercising due caution in its collaborative activities. For example, this research group principally collaborates with the pharmaceutical industry and government agencies.

Subitem 6(c): Properties of organic chemicals: databases and estimation methods

6.11 Dr Rafiqul Gani, adjunct Professor at the Korea Advanced Institute of Science and Technology and CEO of PSE for Speed, delivered a presentation on his efforts in calculating the properties of organic chemicals.[8] Physiochemical properties of pure components serve as the basis for the design and simulation of chemical products and processes, including chemical-based weapons. The availability of accurate pure component and mixture properties has been a central objective in many engineering research efforts that seek to understand and enhance the functionality and efficiency of products and processes. Experimental observations have been the primary means of obtaining the values of the needed properties and developing hypotheses on their structure or system dependence. This, however, requires experiments to be conducted over a range of conditions, so that a knowledge base that helps to understand the underlying phenomena can be constructed. The search for desired sets of properties in literature or measured through experiments rapidly becomes prohibitive due to the number of known chemicals and their structural complexities. For example, PubChem lists 109 million chemicals in its database, but only a fraction of these have measured properties attributed to them. In addition, most of the available properties are pure component properties, not mixture properties. Given the feasibility, timescale, and costs associated with experimental measurements and mechanistic estimation methods, the development of approximate but accurate models for the estimation of pure component properties that can serve as the first step for all other property modelling is imperative in order to progress in product and process design, simulation, evaluation, among many other activities.

8 See: R. Gani, Current Opinion in Chemical Engineering 23 (2019), 184-196; A. S. Alshehri, A. K. Tula, et al., AIChE J, 2021 (submitted); and L. Zhang, H. Mao, Q. Liu, R. Gani, Current Opinion in Chemical Engineering, 27 (2020), 22-34.

6.12 Dr Gani highlighted the issues related to why properties are needed, when properties are needed, which properties are needed, and how the needed properties are obtained and used. Properties can be classified as:

(a) primary properties (those that depend only on the molecular structure, such as critical temperature, critical pressure, boiling point, LC50, etc.;

(b) secondary properties (those that depend on other properties, such as solubility parameter, octanol-water partition coefficient, heat of vaporisation, etc.);

(c) functional properties (those that are functions of temperature and/or pressure, such as vapor pressure, density, surface tension, specific heat, etc.); and

(d) mixture & phase equilibrium properties (such as vapor-liquid equilibrium, liquid-liquid equilibrium, solid-liquid equilibrium, bubble point, dew point, etc.).

6.13 Dr Gani further noted the development of the group contribution approach for predictive property modelling.[9] The reverse of the property prediction is presented as a means of designing or selecting molecules and mixtures with the desired target properties. The combination of databases, property models, and the reverse property prediction approach are presented as a means of chemical substitution where a potentially hazardous or dangerous chemical is identified and replaced with a less dangerous chemical in chemical-based products such as pharmaceutical, healthcare, household, and other goods needed to sustain modern society on planet Earth.

6.14 He concluded with the following observations:

(a) Machine learning-based models offer significant improvements (over 80% of the data can be predicted to an accuracy of less than 1%) in prediction accuracy over simple group contribution-based methods.

(b) Because of the nature of the new group contribution models, the application of these models in product design (reverse of the property prediction) requires special solution techniques, such as hybrid techniques, and it is possible to develop such model-data based systems.

(c) Chemicals and their properties need to be carefully regulated because of the many harmful effects they are likely to cause.

6.15 Dr Gani was asked if it would be possible to proceed with calculations and make estimations with a mixture of different compounds (i.e., a synergetic effect). He confirmed that his research group is developing mixture property calculations. Concerning toxicity, one challenge was determining how to measure the LD50 for a mixture if the mixture is a liquid solution. There would have to be a mixing rule that would give the final property value (linear vs. non-linear). He concluded that there is very little data related to mixtures.

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9 L. Constantinou, R. Gani, AIChE Journal, 40 (1994), 1697-1710.

6.16 It was then asked whether a safety data sheet or similar type of document could be readily generated using this programme. SAB members also asked if this approach could replace the current safety data sheet that is used, especially for new compounds that have little or no experimentally determined properties. Dr Gani confirmed that this should be possible.

7. AGENDA ITEM SEVEN – Overview of developments at the OPCW since the last session of the Scientific Advisory Board

7.1 The SAB Secretary briefed the Board on the developments that took place at the OPCW since the Thirty-First Session of the SAB. He highlighted news relevant to the SAB concerning OPCW meetings and sessions, including the resumption and conclusion of the Twenty-Fifth Session of the Conference of the States Parties (hereinafter "the Conference") and the proceedings of the Ninety-Sixth Session of the Executive Council (hereinafter "the Council").

7.2 Turning to the Ninety-Sixth Session of the Council, the SAB Secretary reported that a decision was adopted by the Council entitled "Understanding Regarding the Aerosolised Use of Central Nervous System-Acting Chemicals for Law Enforcement Purposes" (EC-96/DEC.7, dated 11 March 2021). This decision will now be considered by all States Parties at the Twenty-Sixth Session of the Conference later this year. The SAB Secretary provided an overview of the decision, including the provision requesting that the Director-General ask the SAB to continue to review relevant developments in science and technology related to central nervous system-acting (CNS-acting) chemicals and provide updates to the Conference as appropriate, and to, at a minimum, include this subject as part of its report on developments in science and technology for future Review Conferences. Further instructions, if any, will be provided after the Conference if the decision is adopted. The SAB Secretary noted that the Board is already considering CNS-acting chemicals as part of their preparations for their scientific report for the Fifth Review Conference.

7.3 In relation to Part II of the Twenty-Fifth Session of the Conference, the SAB Chairperson provided a written statement in line with the Secretariat's recommendation based on COVID-19-related measures. The modality of the Twenty-Sixth Session of the Conference has not yet been confirmed, as it will depend heavily on the status of the COVID-19 pandemic and the Dutch Government's regulations and restrictions.

7.4 The SAB Secretary then updated the Board on the Plant Biomarker Challenge, which was funded by the European Union, reporting that a total of 15 proposals were submitted (with each of the five regional groups represented). The Technical Evaluation Team has met multiple times and recommended six proposals for funding. The final confirmation of the six awardees is currently pending, but expected soon.

7.5 The SAB Secretary reiterated that both the "Call for Voluntary Contributions to the Trust Fund of the Scientific Advisory Board" (S/1923/2021, dated 14 January 2021) and the "Call for Nominations to the Scientific Advisory Board" (S/1927/2021, dated 26 January 2021) have been published. He stressed the importance of the trust fund in enabling the SAB to hold topical workshops, support SAB member representation at workshops and events, and produce outreach materials, among other things. The funds have not been utilised in the past year or so due to the pandemic.

7.6 Regarding for the call for nominations to the SAB, the SAB Secretary recalled that the deadline for nominations is 30 August 2021 and encouraged Board members to reach out to their colleagues across the globe to let them know that the Director-General is seeking nominations of experts from States Parties to be appointed to the Board starting 1 January 2022, to replace six Board members whose tenure will end at the close of this year.

7.7 Finally, the SAB Secretary clarified the procedures for the election of the SAB Chairperson and Vice-Chairperson, including the nomination and election process. The current SAB Chairperson and Vice-Chairperson are responsible for nominating the next Chairperson and Vice-Chairperson; the other 23 SAB members are responsible for agreeing with this or noting their dissent during the election process. SAB members are welcome to suggest to the current Chairperson or Vice-Chairperson other members (other than themselves) for consideration for the post of Chairperson or Vice-Chairperson in the future. There are no term limits on the Chairperson or Vice-Chairperson positions; should the Chairperson step down or no longer be able to serve (due to tenure), the Vice-Chairperson will not be automatically nominated or elected to be Chairperson. The power to nominate rests with the current Chairperson and Vice-Chairperson. The election process takes place in a closed session of the SAB and is always done by consensus.

7.8 Speaking about the dates of the next SAB session, the SAB Secretary proposed that the Thirty-Third Session be moved to 15 – 19 November 2021 to provide the highest chances of an in-person meeting in 2021.

7.9 The SAB Chairperson expressed the Board's full agreement with the points raised, including the dates for the Board's Thirty-Third Session.

8. AGENDA ITEM EIGHT – Established and emerging technologies for the dissemination of chemical agents

8.1 Mr Günter Povoden, a current SAB member, gave a presentation on established and emerging technologies for the dissemination of chemical agents. He opened his presentation with a summary of the typical means of dispersal and dissemination, as well as emerging technologies for micro-dispersal within the body. He moved on to list the types of military ammunition and containers for chemical agents, including improvised dispersal devices. He explained that another simple and reliable way of dissemination is by explosives, whilst other methods include pyrotechnic aerosolisation, pressurised canisters, and the more sophisticated option of spray tanks. He provided a survey of the various known dispersal techniques based on known attacks.

8.2 Mr Povoden then turned to unmanned aerial vehicles (UAVs), also referred to as drones, which have recently been used by terrorist groups in various types of attacks, including to deliver improvised explosive devices to a target. He provided examples of the misuse of commercially available agricultural spraying devices and discussed some of the overarching concerns regarding drones, such as the potential to use them in swarms to carry and deliver a chemical or explosive substance to a desired target.

8.3 Drones, however, also have useful counterterrorism applications (such as supporting units on the ground, reconnaissance, detection of chemical hazards and contamination, air sampling, surveillance, and documentation of sampling procedures) and support post-blast investigations (3D mapping, documentation, and chain of custody). Additional benefits might include thermal imaging (detection of heat sources) and joint robot-drone tasks.

8.4 Dr Povoden also touched upon UAVs and 3D printing. He noted that the ability of non-State actors to design and gain access to specific UAVs capable of handling and delivering hazardous or toxic chemicals and releasing them in specific environments to cause damage is something worth assessing.

8.5 He noted that there are various international projects and associated reports on emerging technologies incorporating drones, including the European Union Permanent Structured Cooperation project (PESCO) entitled "CBRN[10] Surveillance as a Service", and the European Defence Agency's "Improvised Explosive Device Detection Programme". Mr Povoden also noted a possible link with the OPCW's plant biomarker challenge in the event that a developed detection system can be mounted on a UAV.

8.6 Dr Povoden concluded by recalling the ongoing worldwide efforts to develop appropriate capabilities to combat the malicious use of drones, to include the modelling and simulation of drones carrying hazardous payloads.

8.7 The SAB Secretary asked how different international non-proliferation or disarmament treaties and conventions, or the bodies thereof, are handling drones, and what the general consensus is in terms of their regulation and prevention of their misuse going forward. Mr Povoden replied that in the case of small-scale drones, he is not aware of any activities related to proliferation control. As for medium- and larger-sized drones, the situation is different, primarily because of the hazard they pose to urban areas and airports due to their size; as such, these tend to garner most of the attention.

8.8 The Board asked about the possibility of using specific enzymes to bring a toxic chemical directly into a specific part of the body. In response, Mr Povoden said this might be possible, and brought up the example of so-called 'DNA origami technology', where DNA parts are folded like pockets encapsulating a substance that can then be carried along to targeted areas of the body. However, this technology is still in its infancy.

8.9 The Board also asked how easily aerial drones can be controlled when filled with liquids, in light of the problems of weight movement (ballast-type issues). Mr Povoden confirmed that such drones are used more and more in agriculture, and that they can be pre-programmed or steered manually, but there are no issues with instability during use.

9. AGENDA ITEM NINE – Detecting organophosphate chemical warfare agents using low-magnetic field nuclear magnetic resonance spectroscopy

9.1 Dr Derrick Kaseman from the Los Alamos National Laboratory (LANL) gave a presentation to the Board on the use of low-magnetic field NMR spectroscopy to detect organophosphate nerve agents. The presentation highlighted two low-magnetic field NMR spectroscopy systems—SpEctroscopic Detection Of Nerve Agents (SEDONA) and Earth's field Resonance and Evaluation (ERDE)—that were developed at LANL.[11] NMR is a powerful non-destructive and quantitative analytical technique that is routinely used to deduce the chemical structure of organic compounds. However, traditional superconducting NMR systems are not portable due to their size, weight,

10 CBRN = chemical, biological, radiological, and nuclear.

11 See: S. J. Widgeon Paisner, M.T. Janicke, et al, J. Anal. Chem., 92 (10) (2020); D. C. Kaseman, M. T. Janicke, et al, Appl. Phys., 10 (11) (2020); and D. C. Kaseman, P. E. Magnelind, et al, Rev. Sci. Instr., 91 (5) (2020).

and requirement of liquid cryogens. One approach to increasing portability is to use permanent magnet systems, which mitigates the need for cryogens and reduces the size and weight of the NMR system. However, the magnetic fields that are obtainable with permanent magnets (1.5 T) are ~10 times lower than conventional superconducting NMR systems, resulting in considerable overlap between the spectral resonances, and thereby reducing the amount of obtainable chemical information. Thus, there is usually a trade-off between portability and the resolution achievable with commercial NMR systems; the LANL team thinks they have bridged this gap between portability and resolution.

9.2 The first system, SEDONA, was developed as a portable 100 ml bottle scanner in collaboration with the United States Department of Homeland Security. This system uses a 250 mT Halbach magnet to measure the NMR signatures of ^{1}H, ^{19}F, and ^{31}P; from these signatures, it deduces the H:F:P ratio, the molecule specific relaxation time constants, and the presence of a P-F bond. As the P-F bond is a unique signature to many organophosphate nerve agents and manifests as a unique signature in the NMR spectroscopy, SEDONA can quickly deduce the presence of these organophosphate chemical warfare agents in a bottle with both low false positive and false negative rates. SEDONA may further be developed to detect a broader range of nefarious materials, including other chemical warfare agents, opioids, and explosives.

9.3 ERDE is the second system that LANL researchers have developed. ERDE uses Earth's magnetic field (~50 μT) for NMR spectroscopy, in which a unique high-resolution spectral regime emerges, providing additional molecular information that is not available at higher magnetic fields. ERDE was specifically designed for fieldable NMR spectroscopy, as Earth's magnetic field solves portability issues, and the high-resolution nature of the technique mitigates the trade-off between portability and resolution. ERDE is fully quantitative and simultaneously measures all NMR-active nuclei in a single experiment—a feat that cannot be accomplished at high magnetic fields. Furthermore, ERDE is insensitive to background signatures from contaminates such as soil, making it an ideal fieldable detector requiring small sample volumes (200 μL). ERDE provides a fieldable solution for high-resolution spectroscopic fingerprints of chemical warfare agents.

9.4 The Board had several questions, the first being whether the research team has identified compounds that may give false positive results with SEDONA, or if results thus far have only been from using surrogates. Dr Kaseman confirmed that only surrogate compounds have been tested with SEDONA so far. He noted, however, that it is unlikely a false positive would be seen using a 250 μT field because the chemical shifts you typically get will be much smaller than the J-coupling between the phosphorus and fluorine atoms. Additionally, the phosphorus-fluorine J-coupling signature is fairly distinct. He noted that with ERDE, the research team has tried over 50 different items so far, and ERDE has been able to distinguish all of these from hazardous surrogates.

9.5 The Board asked Dr Kaseman about the sensitivity of the system used in terms of the amount of sample needed and how it handles mixtures, given the potential for overlapping peaks. Dr Kaseman replied that the SEDONA system requires samples of ~100 mL and that the research group has not yet looked extensively into mixtures. However, he expects that even in a mixture, the phosphorus-fluorine coupling is

sufficiently unique to indicate whether a compound containing a P-F bond is present. As for ERDE, there is presently a trade-off between sample size and measurement time. He noted that this system would likely benefit from a machine-learning approach to drive down measurement times.

9.6 The Board then asked about the portability, set-up time, and operability of these two systems. Dr Kaseman confirmed that the group is working to demonstrate portability by taking the instruments into the field. Both ERDE and SEDONA have been transported to several locations within the Los Alamos Lab; however, they are looking to demonstrate greater portability with both, to include testing live agents. He also noted that ERDE can detect samples on solid matrices. In terms of set-up time, he indicated that both systems can be set up and calibrated in about 15 minutes.

9.7 The Board then asked whether either or both systems could be modified to look for other toxic compounds. Dr Kaseman confirmed that both ERDE and SEDONA could be modified to look for other kinds of agents. This could be done by adding more channels to allow for the detection of different elements. The research group is also looking at how to increase the signals of different atomic couplings to allow for greater detection possibilities.

9.8 Finally, it was asked if there were any benefits from utilising multiple magnetic fields for an orthogonal approach to detection and identification. Dr Kaseman confirmed that there are indeed ways to do this. One benefit of using NMR spectroscopy is that the technique is non-destructive, allowing for multiple analyses, such as with different magnetic fields. The data collected could then be used in an orthogonal way to enhance the analysis.

10. AGENDA ITEM TEN – Current and future activities of the Scientific Advisory Board

10.1 The SAB Secretary reminded the Board of its near-term objectives and commitments. The SAB devoted a substantial amount of time at its Thirty-Second Session to working and reporting internally on the preparation of its scientific report for the Fifth Review Conference. In addition, the Board heard updates on the first meeting of the recently established TWG on the analysis of biotoxins and the ongoing planning for a workshop on partnership with industry.

Subitem 10(a): Preparing for the Fifth Review Conference

10.2 The SAB split into seven groups for breakout sessions during the second day of its Thirty-Second Session. Each group discussed progress to date on collecting information, as well as the first steps in structuring advice on their specific themes in preparation for the Fifth Review Conference. They also prepared summaries of their work to date and the expected next steps to share with the Board, which they did during the last day of the session. The Board had fruitful discussions during these updates from group leads, noted some synergies in approaches and areas for internal collaboration. The SAB also identified some external experts who should be invited to present to the Board on different areas of expertise relevant to the Convention.

Subitem 10(b): Temporary Working Group on the analysis of biotoxins

10.3 Dr Noort, Chairperson of the TWG, updated the SAB on the progress of the TWG. He started by giving an overview of the objective and composition of the TWG, as well as the definition, use, and application of biotoxins that the Group had been considering. He reported that the TWG recently held its first meeting on 3 and 6 May 2021. The questions in the TWG's terms of reference were divided up and are being considered by five subgroups within the TWG. Individual subgroups held initial deliberations during the meeting in breakout sessions, with the idea that they would continue to meet virtually in between TWG meetings. He noted that the official report of the first TWG meeting is in its final stage. Dr Noort then turned to the questions considered by the group leads and related discussions, the issues identified by individual subgroups, and the output generated so far.

10.4 In terms of plans for the near future, Dr Noort noted that there are ongoing deliberations within individual subgroups, organised by subgroup leads, ahead of the second meeting of the TWG, which is scheduled for 21 and 23 June. The meeting will discuss the agreed approaches by subgroup, the knowledge that is still lacking within the group, and which external speakers to invite to future meetings. Dr Noort then reported that the TWG plans to have an in-person meeting in November 2021, at the OPCW headquarters in The Hague.

Subitem 10(c): Efforts towards a workshop in partnership with industry

10.5 Dr Becker-Arnold and Dr Syeda Razia provided an update on the SAB's planned workshop in partnership with chemical industry. During the intersessional period, contacts were made with the OPCW Chemical Industry Coordination Group (CICG). An initial virtual meeting was held in May with the CICG noting its interest and suggesting several speakers from the United Nations Environment Programme, among others.

10.6 Dr Becker-Arnold further reported that a second meeting with the CICG and the European Chemical Industry Council (CEFIC) was held a few weeks later, with a brief follow-up with the CEFIC one week after that. There was a productive brainstorming session on how to contribute to the planned industry workshops (one virtual and another in-person meeting hopefully next year) at both meetings. The suggested topics mainly revolved around trends in the chemical industry, efforts to highlight the life cycle assessment, and sustainable approaches along the value chain. Additional speakers were identified and have been contacted regarding their willingness to participate.

10.7 Dr Razia concluded the presentation by reminding everyone that the goal of the proposed workshops is not to duplicate previous efforts. That being said, and after discussions with members of the chemical industry, it is clear that this can be avoided. Both Dr Razia and Dr Becker-Arnold thanked the CICG for their efforts and work to connect the SAB with the appropriate stakeholders and partners.

10.8 The SAB Chairperson commended the work undertaken and supported the need for OPCW partners to understand the SAB's role in the process. The Board then discussed the related timeline and the dates of planned workshops, and the option to hold the first iteration virtually before holding a more in-depth workshop in person in the first half of 2022. It was also recommended that the organisers include the use of AI and computing power in the chemical industry as one of the workshop topics.

11. AGENDA ITEM ELEVEN – Any other business

The SAB expressed its appreciation to the Director of the Verification Division, Dr Carolyn Browne, for her welcoming remarks, Ms Virginie Poujade of the Language Services Branch, and Ms Ernesa Ademagić of the Office of Strategy and Policy, for their support of and contributions to the SAB's Thirty-Second Session and its preparations. A special thanks went to the interpretation teams, who made the meeting possible by allowing everyone to participate. The SAB is grateful for the voluntary contributions made to support its work, as well as the European Union for its April 2019 Council decision, which provides funding for TWGs.

12. AGENDA ITEM TWELVE – Adoption of the report

The SAB considered and agreed upon a process for the preparation of the report for its Thirty-Second Session, with a view to adopting it via correspondence after the session.

13. AGENDA ITEM THIRTEEN – Closure of the session

The Chairperson made concluding remarks on the session, and the SAB Secretary closed the virtual session at 15:41 CET on 17 June 2021.

Annex: List of Participants in the Thirty-Second Session of the Scientific Advisory Board

Annex

LIST OF PARTICIPANTS IN THE THIRTY-SECOND SESSION OF THE SCIENTIFIC ADVISORY BOARD

	Participant	Institution
Members of the Scientific Advisory Board		
1.	Prof Isel Pascual Alonso	University of Havana, Cuba
2.	Dr Khaldoun Bachari	Algerian Public Scientific and Technical Research Centre in the Physico-Chemical-CRAPC, Algeria
3.	Dr Renate Becker-Arnold	BASF, Germany
4.	Dr Elma Biscotti	Scientific and Technical Research Institute for Defense, Argentina
5.	Dr Anne Bossée	DGA CBRN Défense, France
6.	Dr Christophe Curty (Chairperson)	Spiez Laboratory, Switzerland
7.	Prof Vladimir Dimitrov	Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Bulgaria
8.	Dr Mostafa Ghanei, MD	Baqiyatallah University of Medical Sciences, Islamic Republic of Iran
9.	Dr Norman Govan	Defence Science and Technology Laboratory, United Kingdom of Great Britain and Northern Ireland
10.	Mr Wilford Zungkat Jwalshik	Institute of Chartered Chemists of Nigeria, Nigeria
11.	Prof Victor Kholstov	Ministry of Industry and Trade, "GosNIIOKhT", Russian Federation
12.	Dr Zrinka Kovarik	Institute for Medical Research and Occupational Health, Croatia
13.	Dr Andrea Leisewitz (Vice-Chairperson)	Universidad San Sebastián, Chile
14.	Prof Imee Su Martinez	University of the Philippines-Diliman, Philippines
15.	Dr Robert Mikulak	United States Department of State, United States of America
16.	Dr Daan Noort	TNO, Rijswijk, Netherlands
17.	Prof Ponnadurai Ramasami	University of Mauritius, Mauritius
18.	Mr Günter Povoden	EU CBRN Centres of Excellence Initiative, Ministry of Defence, Austria
19.	Dr Syeda Sultana Razia	Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh
20.	Prof Ahmed E. M. Saeed	Sudan University of Science and Technology, Sudan
21.	Dr Yasuo Seto	RIKEN SPring-8 Center, Japan
22.	Dr Maciej Sliwakowski	Lukasiewicz Research Network – Institute of Industrial Organic Chemistry, Poland
23.	Prof Fengxia Sun	Hebei University of Science and Technology, China
24.	Dr Nomandla Magnificent Vela	Protechnik Laboratories, South Africa
25.	Ms Farhat Waqar	Pakistan Atomic Energy Commission, Islamabad, Pakistan

Invited Participants		
26.	Dr Carolyn Browne	Director of the Verification Division, OPCW, Netherlands
27.	Dr Craig Cormick (Member of the ABEO)	Independent Consultant, Australia
28.	Dr Bartosz Grzybowski	Ulsan National Institute of Science and Technology, Republic of Korea
29.	Dr Rafiqul Gani	PSE for SPEED, Denmark
30.	Dr Alastair Hay (Member of the ABEO)	University of Leeds, United Kingdom of Great Britain and Northern Ireland
31.	Dr Derrick Kaseman	Los Alamos National Laboratory, United States of America
Secretary to the Scientific Advisory Board		
32.	Dr Peter Hotchkiss	Organisation for the Prohibition of Chemical Weapons, Netherlands

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