OPCW

Scientific Advisory Board

Twenty-Sixth Session
16 – 20 October 2017

SAB-26/1
20 October 2017
Original: ENGLISH

REPORT OF THE SCIENTIFIC ADVISORY BOARD AT ITS TWENTY-SIXTH SESSION

1. AGENDA ITEM ONE – Opening of the session

1.1 The Scientific Advisory Board (SAB) met for its Twenty-Sixth Session from 16 to 20 October 2017 at the OPCW Headquarters in The Hague, the Netherlands. The session was chaired by Dr Christopher Timperley, with Mr Cheng Tang as Vice-Chairperson.

Executive summary

1.2 Pursuant to the deliberations of the SAB at its Twenty-Sixth Session, the following recommendations are presented to the Director-General in this report (see paragraphs 8.6 and 9.14 for further details).

(a) The SAB recognises that the emergence and practical applications of new and innovative technologies (in both research and industrial sectors), as well as the repurposing of existing technologies for unanticipated new applications, has benefited from increasingly transdisciplinary (convergent) scientific communities. As the Technical Secretariat (hereinafter "the Secretariat") and stakeholders of the OPCW 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 support robust implementation of the Chemical Weapons Convention (hereinafter "the Convention"). See paragraphs 7.1 through 7.4, 8.2 and 8.3, 9.10 and 9.11, 9.15 and 9.16, and 10.1 through 10.8; and subparagraphs 8.4(f), 8.6(b), 9.12(a) and 9.14(a).

(b) To ensure that the verification regime remains fit for purpose, the SAB encourages more extensive engagement with technical experts from industry and review of industry-focused research and development. This would keep the Secretariat usefully informed on developments in chemical industry, benefit the science review process and allow for recognition of change from previously predicted trends. See subparagraphs 8.4(a), 8.4(c), 8.4(d) and 8.6(a).

(c) In reviewing the diversity of developments across scientific communities, understanding where developments find application and recognising where these technological changes intersect with the Convention, the SAB has benefited from the practice of engaging operational staff from the Secretariat. In the view of the SAB, this practice strengthens the formulation of science advice to the OPCW. A similar approach would provide benefit in other Convention-relevant fora where proposals are drafted and considered. See subparagraphs 9.12(h) and 9.14(b).

(d) A broad set of innovative technologies are being developed that can potentially find application in the implementation of the Convention, especially for non-routine situations, enhancement of sampling and analysis capabilities, and reducing risks to personnel operating in dangerous environments. The Secretariat may wish to consider engagement with technology developers as well as outreach strategies, such as crowd source competitions, to gain access to innovative technologies and ideas that can be field tested. Benefits include raising awareness of the Convention across scientific communities, opportunities to provide feedback to technology developers on how their tools perform under field conditions, and a mechanism for the Secretariat to keep pace with technological change. In this regard, the Secretariat might consider reviewing the availability and potential capabilities of relevant innovative technologies. See paragraphs 9.5 and 9.6, 9.15 and 9.16, 10.1 through 10.8, and 11.10 and 11.11; and subparagraphs 8.4(c), 8.4(e), 9.12(a), 9.12(c) through 9.12(g), 9.14(c) and 9.14(d).

2. AGENDA ITEM TWO – Adoption of the agenda

The SAB adopted the following agenda for its Twenty-Sixth Session:

1. Opening of the session
2. Adoption of the agenda
3. *Tour de table* to introduce Scientific Advisory Board members
4. Establishment of a drafting committee
5. Welcome address by the Director-General
6. Overview of developments at the OPCW since the last session of the Scientific Advisory Board
   (a) General updates
   (b) Updates from the Open-Ended Working Group on the Future Priorities of the OPCW
   (c) Chemical security
   (d) Updates from the Sub-Working Group on Non-State Actors
   (e) Knowledge management
   (f) OPCW Fact-Finding Mission

7. Advice on chemicals

   (a) Report from the workshop on chlorine

   (b) Theoretical study of sulfur mustard

   (c) Study of the behaviour of heavy sulfur mustards against commercial decontaminants

   (d) Eliminating toxic substances and reagents from chemical synthesis

8. Chemical production

   (a) Report from the workshop on trends in chemical production

   (b) Results of the survey on biomediated processes

9. Scientific and technological elements of verification technologies, emerging technologies, and new equipment

   (a) Managing the results of on-site sampling and analysis: a methodology to resolve ambiguous identifications

   (b) Training and preparedness to address new challenges

   (c) Update from the OPCW Laboratory

   (d) Report from the workshop on innovative technologies for chemical security

   (e) Artificial intelligence and its potential application for chemical warfare agent verification

10. Developments in science and technology

   (a) Wearable sensors and nanomotor-based accelerated decontamination of chemical warfare agents

   (b) NanoContraChem: from the design to the development of nanostructured clays and oxides for the catalytic decontamination of chemical warfare agents

11. Chemical forensics and investigative technologies

   (a) Updates on formation of a temporary working group on investigative science and technology

   (b) Recent engagement with forensic science experts

   (c) Computer-aided engineering tools

12. Future work of the Scientific Advisory Board

    (a) The road to the Fourth Review Conference

    (b) Roadmap of the Scientific Advisory Board's work

    (c) The Twenty-Seventh Session of the Scientific Advisory Board

    (d) The Scientific Advisory Board's recommendations to the Fourth Review Conference[1]

    (e) Identification of key issues in science and technology

13. Inputs to the Scientific Advisory Board's report to the Fourth Review Conference

14. Any other business

15. Adoption of the report

16. Closure of the session

3. AGENDA ITEM THREE – *Tour de table* to introduce Scientific Advisory Board members

A *tour de table* was undertaken to introduce the SAB members and guests. Three new members, Dr Khaldoun Bachari (Algeria), Ms Hoe Chee Chua (Singapore), and Dr Maciej Sliwakowski (Poland) attended their first session of the SAB. A list of participants appears in the annex to this report.

4. AGENDA ITEM FOUR – Establishment of a drafting committee

The SAB established a drafting committee to prepare the draft report of its Twenty-Sixth Session.

5. AGENDA ITEM FIVE – Welcome address by the Director-General

5.1 The Director-General of the OPCW delivered the welcome address[2] thanking the Chairperson, Vice-Chairperson, and the members of the board for their contributions to the implementation of the Convention, and for their independent voice as an advisory board. The Director-General highlighted the recent milestone of completion of the chemical demilitarisation process in the Russian Federation,[3] bringing progress toward complete destruction of declared chemical weapons stockpiles to more than 96%. He then reflected on today's security environment, which continues to provide

---

1 Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

2 The full statement is available at: www.opcw.org/fileadmin/OPCW/ODG/uzumcu/DG_Remarks_SAB__161017.pdf

3 See OPCW news item: www.opcw.org/news/article/opcw-director-general-commends-major-milestone-as-russia-completes-destruction-of-chemical-weapons-stockpile-under-opcw-verification/

unanticipated situations and new challenges; with threats from chemical weapons remaining, the work of the OPCW is far from complete.

5.2 Pointing to the scientific underpinnings of the work of OPCW, the Director-General stressed that the provision of reliable scientific and technical findings is vital for verification, particularly in contingency operations, stating that findings must stand on their technical merit, and be objective, accurate, and incontrovertible. In this regard, he commented on plans to upgrade the OPCW Laboratory,[4] and spoke of the importance of the work of the temporary working group (TWG) on investigative science and technology which is set to hold its first meeting in early 2018 (see paragraphs 11.1 through 11.3).

5.3 In regard to challenges arising from the rapid advancement in science and technology, and converging scientific disciplines, the Director-General noted that our decision makers need practical advice and that many of the immediate challenges they face are not emerging new technologies. A pertinent example is the difficulty of post-event sampling and analysis to verify chlorine exposure. For this reason, he stated, we must be able to recognise opportunities from technological change.

5.4 Noting that once the report from its Twenty-Sixth Session is issued, the SAB will have produced 11 reports in an 18-month period, the Director-General reflected on the rich inputs the SAB had collected for their report to the Fourth Review Conference. He encouraged the SAB to be innovative, forward looking and bold in the drafting of the report, emphasising that the value of the report and its advice comes from the independent expert voice the SAB provides.

5.5 The Director-General closed his remarks by welcoming the new members of the Board and thanking the outgoing SAB members.

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

Subitem 6(a): General updates

6.1 The Secretariat's Science Policy Adviser and Secretary to the SAB, Dr Jonathan Forman, briefed the Board on developments at the OPCW since the SAB's Twenty-Fifth Session, briefly highlighting recent destruction milestones and several outcomes of the Eighty-Sixth Session of the Executive Council (hereinafter "the Council") (held the week preceding the Twenty-Sixth Session of the SAB),[5] most notably the decision (EC-86/DEC.10, dated 13 October 2017)[6] taken to include non-scheduled chemicals in the OPCW Central Analytical Database (OCAD).[7]

---

4 Upgrading The OPCW Chemical Laboratory to a Centre for Chemistry and Technology, S/1512/2017, dated 10 July 2017. Available at: www.opcw.org/fileadmin/OPCW/S_series/2017/en/s-1512-2017_e_.pdf

5 Documents from the session are available at: www.opcw.org/documents-reports/executive-council/documents-from-the-eighty-sixth-session-of-the-executive-council/

6 Available at: www.opcw.org/fileadmin/OPCW/EC/86/en/ec86dec10_e_.pdf

7 The OPCW Central Analytical Database; C. Nyanyira; in Chemical Weapons Convention Chemicals Analysis: Sample Collection, Preparation and Analytical Methods, M. Mesilaakso (ed); 2005, John Wiley & Sons, Ltd, Chichester, UK. DOI: 10.1002/0470012285.ch7.

Inclusion of non-scheduled chemicals in the OCAD has been a recommendation of the SAB since the Second Review Conference.[8,9] Turning to the work of the SAB, Dr Forman reviewed key messages from the Director-General's comments on the report from the Twenty-Fifth Session of the SAB.[10] He also noted that, with the conclusion of this Twenty-Sixth Session of the SAB, the scientific review for the Fourth Review Conference will have been informed by the outputs of three TWGs, seven sessions of the SAB, and four international workshops; a total of 25 meetings, with 30 reports produced. The total attendance across the review process will be 676; representing 276 individuals with a broad range of technical expertise from 56 States Parties. In total, the SAB members will have received 405 presentations from 191 individual presenters. Dr Forman explained how the outcomes of the review process will feed into the report to the Fourth Review Conference, emphasising the need to provide practical guidance on science and technology, to maintain and promote scientific literacy, to point out opportunities from new developments that may benefit the implementation of the Convention, and to promote productive discourse with the States Parties on science and technology issues.

6.2 Dr Forman continued with an overview of relevant technical expert community engagement activities since the Twenty-Fifth Session of the SAB. This included the participation in scientific conferences, updates on the OPCW's partnership with the International Union of Pure and Applied Chemistry (IUPAC),[11] reports from the Secretariat's participation at the CTBTO's[12] Science and Technology Conference in June;[13] and a briefing to the United Nations General Assembly First Committee (Disarmament and International Security).[14] Looking toward 2018, Dr Forman informed the Board of upcoming events, noting the American Chemical Society (ACS) Spring Meeting will include a symposium focused on the linkage of chemical ethics and responsible chemistry to non-proliferation, and that SAB member Professor Isel Alonso is helping to organise the 10th Congress of Chemical Sciences, Technology and Innovation in October 2018 in Havana, Cuba.[15]

6.3 The briefing concluded with a discussion on publishing the work of the SAB in peer-reviewed scientific journals as a means of raising visibility of the OPCW in scientific communities. Dr Forman noted that participants from the workshop on

---

8 Second Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

9 More specifically, riot control agents, degradation products of scheduled chemicals, and certain chemicals found in old and abandoned chemical weapons. See paragraphs 4.4 and 4.10 of: Report of the Scientific Advisory Board on Developments in Science and Technology (RC-2/DG.1, dated 28 February 2008). Available at: www.opcw.org/fileadmin/OPCW/CSP/RC-2/en/RC-2_DG.1-EN.pdf

10 The Impact of the Developments in Science and Technology in the Context of the Chemical Weapons Convention (EC-85/DG.8, dated 19 May 2017). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/ec85dg08_e_.pdf

11 For additional information on IUPAC, see https://iupac.org/

12 CTBTO = Comprehensive Nuclear-Test-Ban Treaty Organization.

13 For additional information see: https://www.ctbto.org/specials/snt2017/

14 Disarmament Machinery Must Sharpen Tools to Harness Largely Ungoverned Game-Changing New Weapons, Security Experts Tell First Committee. Available at: https://www.un.org/press/en/2017/gadis3578.doc.htm

15 For additional information see: http://www.chemistrycuba.com/

emerging technologies will be publishing their research in a special edition of *Pure and Applied Chemistry* (see paragraph 9.11) and noted the Director-General's encouragement of the SAB publishing their reports on sample storage[16] and riot control agents.[17]

Subitem 6(b): Updates from the Open-Ended Working Group on the Future Priorities of the OPCW

6.4 Dr Alexander Kelle (Senior Policy Officer in the OPCW Office of Strategy and Policy) updated the Board on the work conducted by the Open-Ended Working Group on the Future Priorities of the OPCW (OEWG-FP) since his last report at the Twenty-Fifth Session of the SAB. He recalled the mandate of the group,[18] briefly mentioned the tentative programme of work the group had given itself, and highlighted the topics and issue areas most noted during the OEWG-FP's segments on capacity development; engagement with external partners; and OPCW governance, resources and management. These three segments were held in the months after the segment on verification held in January 2017 where the SAB Vice-Chair had provided a briefing.[19]

6.5 Concerning the OEWG-FP's remaining work, Dr Kelle noted the upcoming meeting on "any other topics" that had not been addressed in the previous sessions. He noted that the OEWG-FP Co-Chairs intend to circulate an inventory of the ideas presented by States Parties, which will be discussed further in early 2018. A scarcity of inputs and unbalanced regional participation of States Parties was acknowledged, and the hope was expressed that the inventory would usefully engage greater numbers of States Parties.

6.6 In the subsequent discussion, the following points were raised:

(a) The SAB expressed interest in understanding the key issues that are raised by the States Parties in the inventory of ideas, as this may identify issues where advice from the outputs of the Board's scientific review could have relevance.

(b) There was discussion on skills management and development in the Verification Division and an acknowledgement of OPCW's efforts in knowledge management (KM) in this regard. The role of the TWG on investigative science and technology in providing links to expertise relevant to skills development was also highlighted.

---

16 See paragraph 13 of: The Impact of the Developments in Science and Technology in the Context of the Chemical Weapons Convention (EC-82/DG.13, dated 7 June 2016). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/ec82dg13_e_.pdf

17 See paragraph 18 of EC-85/DG.8.

18 Establishment of an Open-Ended Working Group on the Future Priorities of the OPCW (EC-82/DEC.2, dated 14 July 2016). Available at: www.opcw.org/fileadmin/OPCW/EC/82/en/ec82dec02_e_.pdf

19 SAB Briefing to the OEWG-FP, 31 January 2017, available at: www.opcw.org/fileadmin/OPCW/SAB/en/20170131_SAB_Briefing_to_Open_Ended_Working_Group_Future_Priorities.pdf

Subitem 6(c): Chemical security

6.7 Mr Joseph Ballard (Senior Policy Officer in the OPCW Office of Strategy and Policy) briefed the Board on how the OPCW looks at chemical security and the Organisation's response to the threat of chemical terrorism. He underlined that many of the States Parties to the Convention, as well as the Secretariat, considered these issues to be important elements of the OPCW's future priorities, in light of growing concerns around the potential of non-State actors to use toxic chemicals. Mr Ballard noted that full and effective national implementation of the Convention remained the most important contribution to counter-terrorism efforts, and that States Parties and other stakeholders may wish to reconsider what implementation of the Convention means in a counter-terrorism context. The work of the Open-Ended Working Group on Terrorism (OEWG-T) was outlined, including its focus on the legal accountability of non-State actors, in terms of prevention and response.[20]

6.8 Mr Ballard also briefed the board on the recent "Expert Workshop on International Chemical Security Coordination" held at OPCW,[21] which made some recommendations on how the OPCW could strengthen its contribution to States Parties' efforts on chemical security, in line with its mandate. Mr Ballard explained some of the approaches the Secretariat might consider to further contribute to global chemical security. These include coordination among the range of international assistance providers, and targeted capability development, which takes into account the needs of individual States Parties.

6.9 The briefing concluded with a discussion on a recent decision, "Addressing the Threat Posed By the Use of Chemical Weapons by Non-State Actors", taken at the Eighty-Sixth Session of the Council (EC-86/DEC.9, dated 13 October 2017)[22] on addressing the threat posed by the use of chemical weapons by non-State actors, and the implications of the decision for the States Parties and the Secretariat.

6.10 In the subsequent discussion, the following points were raised:

(a) The SAB welcomed the approaches taken by the Secretariat and the Council decision in regard to chemical security. The Board stands ready to provide its views on relevant science and technology developments.

(b) A key message from the briefing is that the Convention already provides tools that can address chemical security issues. How to apply these tools could be usefully explored. For example, potential contributions from Article VI and

---

20 For a recent update on the work of the OEWG-T, see: (a) Report by H.E. Ms María Teresa Infante Acting Facilitator of the Open-Ended Working Group on Terrorism to the Executive Council at its Eighty-Fifth Session (EC-85/WP.2, dated 13 July 2017). Available at: www.opcw.org/fileadmin/OPCW/EC/85/en/EC-85-WP2.pdf (b) Report By H.E. Ambassador Dr Momar Diop Facilitator of the Open-Ended Working Group on Terrorism to the Executive Council at its Eighty-Sixth Session (EC-86/WP.2, dated 11 October 2017). Available at: www.opcw.org/fileadmin/OPCW/EC/86/en/ec86wp02_e_.pdf

21 See OPCW news item: www.opcw.org/news/article/experts-gather-at-opcw-to-strengthen-global-chemical-security-1/

22 Available at: www.opcw.org/fileadmin/OPCW/EC/86/en/ec86dec09_e_.pdf

associated processes, mechanisms, and information to counter-terrorism efforts have been discussed.[23]

(c) National capabilities and rosters of experts were discussed. How the OPCW could draw upon such resources was also identified as an area that could be explored further. In this regard, the TWG on investigative science and technology could potentially identify communities of experts with whom the Secretariat might wish to engage.

Subitem 6(d): Updates from the Sub-Working Group on Non-State Actors

6.11 Mr Kenneth Aoki (Senior Policy Officer in the OPCW Office of Strategy and Policy) briefed the Board on the OEWG-T's Sub-Working Group (SWG) on Non-State Actors (hereinafter the "SWG").[24] The SWG was established two years ago to help support the OEWG-T's mandate to "… examine further the OPCW's contribution to global anti-terrorist efforts, … ." (EC-XXVII/DEC.5, dated 7 December 2001). The SWG is chaired by Ambassador Maria Teresa Infante, the Permanent Representative of the Republic of Chile to the OPCW, and comprising States Parties, strives to have a well-rounded view on the issues under consideration. With this in mind, the SWG has heard from a number of national experts, international and regional inter-governmental organisations, private companies, chemical industry organisations and scholars of international law and international criminal law.

6.12 Through the SWG, States Parties have productively exchanged views on a number of issues within three topical areas: legal accountability of non-State actors, measures to prevent the hostile use of a toxic chemical by non-State actors, and ensuring an effective response to such use. Notwithstanding the recent Council decision on non-State actors (EC-86/DEC.9; see paragraph 6.9), the OEWG-T and the SWG will continue to identify issues to explore in more detail; such exploration could usefully look to science and technology for inputs. For example, at a recent SWG meeting, Singapore and Panama noted their increasing reliance on developments in science and technology to cope with the challenge of detecting illicit trade crossing their borders as the volume of global trade continues to grow each and every year. The question of what more can be done to assist States Parties that do not have the capacity or resources to use the most sophisticated or advanced technology, but that are still faced with growing volumes of trade, remains to a large extent unanswered from a technical point of view. The SWG have also recently exchanged views about the Secretariat's capacity-building efforts in African States Parties, in particular, the building of capacity in the area of national response to a chemical incident and of analytical laboratory capacity, which are both rich in science and technology considerations.

6.13 Mr Aoki noted however, that despite scientific and technological underpinnings of security issues, the SWG has yet to have a meeting specifically focused on the topic of science and technology (S&T) itself. A few States Parties have noted to the Chairs

---

23 The Contribution of Article VI to States Parties' Efforts to Counter Terrorism (S/1387/2016, dated 19 May 2016). Available at: www.opcw.org/fileadmin/OPCW/S_series/2016/en/s-1387-2016_e_.pdf

24 See also: Report by H.E Ambassador Maria Teresa Infante Facilitator of the Sub-Working Group on Non-State Actors of the Open-Ended Working Group on Terrorism - Summary of Intersessional Work (EC-86/WP.1, dated 2 October 2017). Available at: www.opcw.org/fileadmin/OPCW/EC/86/en/ec86wp01_e_.pdf

of the OEWG-T and the SWG their interest in hearing more about investigative techniques, such as chemical forensics. In closing, Mr Aoki posed questions to stimulate the SAB's thinking about scientific and technological issues: What are key S&T issues related to preventing or responding to chemical terrorism? To legal accountability? What more could the OPCW do in the area of S&T? And who else should the SWG hear from? Answers to these questions could be productive for SWG to consider, with the ultimate aim being to identify what more the OPCW could do to address the threat of chemical terrorism.

6.14 In the subsequent discussion, the following points were raised:

(a) Suggestions made in response to Mr Aoki's questions included the importance of States Parties being prepared for rapid medical response to a chemical incident; technologies that allow tracking of transfers of toxic materials (including block chain and other data-driven approaches); and the investigative aspects of holding an individual accountable for conducting activities prohibited by the Convention. The latter is a topic that will be addressed from a science and technology perspective by the TWG on investigative S&T.

(b) A wide range of science and technology elements can be found within the U.S. Chemical Facilities Anti-Terrorism Standards.[25] These include tools for risk assessment, modelling of point source releases, organisation of production processes, and responsive planning. In this regard, chemical products and production processes often use concepts of "safety by design"[26] and "quality by design"[27] to ensure quality and safety are intrinsic features of their development and design requirements; chemical security concepts could be brought into product development and production in a similar manner.[28]

(c) In quality by design, one builds quality into development (material attributes, process parameters, time, equipment, and operations).

(d) While the term "non-State actor" is used to refer to terrorists, it also covers criminal enterprises and military forces that are not State-organised.

(e) The SAB is fully supportive of the value of S&T inputs for the OEWG-T and its SWG. SAB members expressed a need for broad thinking in this regard, as the technological opportunities will come from broader areas than chemistry alone.

---

25 See: https://www.dhs.gov/chemical-facility-anti-terrorism-standards

26 Application of safety by design methodology in evaluating process safety for a Duff reaction using predictive process simulators; F. Jović, A. Sučec, I. Nekola, D. Čavužić, E. Marcelić, E. Meštrović; *Org. Process Res. Dev.*; 2015, *19(9),* 1268–1273. DOI: 10.1021/acs.oprd.5b00174.

27 (a) A review on quality by design; V. Mogal, J. Dusane; P. Borase, P. Thakare, S. Kshirsagar; *Pharmaceutical and Biological Evaluations*; 2016, *3(3),* 313–319. ISSN: 2394-0859. (b) Pharmaceutical product development: A quality by design approach; K. Pramod, M. Abu Tahir, N. A. Charoo, S. H. Ansari, J. Ali; *Int J Pharm Investig*; 2016, *6(3),* 129–138. DOI: 10.4103/2230-973X.187350.

28 The concept "secure by design" or "security by design" is used in relation to IT tools.

Subitem 6(e): Knowledge management

6.15 Mr Stephen Jones (Head, OPCW Information Services Branch) and Dr Marta Galindo (Knowledge Management Officer, OPCW Verification Division) briefed the Board on the KM activities of the Secretariat. They noted that the OPCW recognises KM as one of the enablers to ensure that the Organisation remains a global repository of knowledge and expertise with regard to disarmament of chemical weapons, verification of non-possession and non-use, and destruction.[29] This vision and the initiatives to bring it forward align with views expressed by States Parties to the Third Review Conference[30] in 2013,[31] as well as to the SAB.[32] In this regard, the Secretariat has developed a KM vision and strategy aiming to induce an organisational change during the upcoming years, looking at installing by 2021 a KM-compatible culture among the staff under the motto "ask, learn and share". Mr Jones and Dr Galindo described the OPCW's KM road map that has been developed around the elements: people, technology and processes. The Secretariat is working on local initiatives at the branch and division levels, using SharePoint as a communication tool and identifying among the entire Organisation a team of "knowledge champions" who are supporting and advocating the implementation of KM in organisational business processes. Additionally, a hiring process is under way for a KM leader, who will work cross-divisionally to manage the change process while developing and facilitating knowledge content. The efforts described are ongoing and will require continued commitment of staff members with support from management to ensure success.

6.16 In the subsequent discussion, the following points were raised:

(a) KM has many dimensions, these include processes and tools to help manage and access (data mine) knowledge, but also a critical people and soft skills aspect. Capturing all dimensions of knowledge can be difficult, making learning from the experiences of other organisations a valuable way to inform the development of KM frameworks tailored to the needs of the Secretariat. The Secretariat could usefully look to engage in KM expert forums. SAB members were encouraged to share their own experiences in KM with the Secretariat.

(b) An objective of the Secretariat's KM initiative is to form a community of practice; former members of the Secretariat as well as SAB members could usefully engage in such initiatives.

---

29 Medium-Term Plan of the Organisation for the Prohibition of Chemical Weapons 2017 – 2021 (EC-83/S/1 C-21/S/1, dated 8 April 2016). Available at: www.opcw.org/fileadmin/OPCW/EC/83/en/ec83s01_c21s01_e_.pdf

30 Third Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

31 See paragraphs 9.14 and 9.155(h) of the report of the Third Review Conference (RC-3/3*, dated 19 April 2013). Available at: www.opcw.org/fileadmin/OPCW/CSP/RC-3/en/rc303__e_.pdf

32 See for example paragraphs 20, 46, 116 and 117 of: Report of the Scientific Advisory Board on Developments in Science and Technology for the Third Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention (RC-3/DG.1, dated 29 October 2012). Available at: www.opcw.org/fileadmin/OPCW/CSP/RC-3/en/rc3dg01_e_.pdf

(c) Evaluation of the success of KM activities will be an important, but challenging, task.

Subitem 6(f): OPCW Fact-Finding Mission

6.17 Mr Aamir Shouket (Deputy Chief of Cabinet) provided the Board with an update on the work of the OPCW Fact-Finding Mission (FFM),[33] in particular regarding incidents in Ltamenah, Hama Governorate (March 2017)[34] and Khan Shaykhun, Syrian Arab Republic (April 2017),[35] where the use of sarin (or a sarin-like substance) was confirmed. Mr Shouket noted that the attribution of the use of chemical agents is outside the mandate of the FFM, and the information collected through the FFM is being further reviewed by the OPCW-UN Joint Investigative Mechanism (JIM).[36] The next JIM report is forthcoming.

6.18 In the subsequent discussion, the following points were raised:

(a) The SAB thanked Mr Shouket for his presentation and reaffirmed their concern and condemnation of the use of chemicals as weapons.

(b) The SAB noted that the TWG on investigative science and technology would benefit from hearing the experiences of inspectors involved in FFM missions to better inform their work.

7. AGENDA ITEM SEVEN – Advice on chemicals

Subitem 7(a): Report from the workshop on chlorine

7.1 Dr Stephanie Dare-Doyen (Senior Policy Officer in the OPCW Office of Strategy and Policy) briefed the SAB on recent expert consultations on chlorine that took place at the OPCW. The consultations emerged from discussions between the Secretariat and representatives of the chemical industry as a follow-up to letters[37] from ACS jointly with the American Chemical Council (ACC),[38] and the European Chemical Industry Council (Cefic)[39] in September 2016 that expressed concerns about the use of chlorine

---

33 FFM reports are available at: www.opcw.org/special-sections/syria/fact-finding-mission-reports/

34 Analysis Results of Samples Relating to the Alleged Use of Chemicals as Weapons in Ltamenah, Hama Governorate, Syrian Arab Republic, March 2017 (S/1544/2017, dated 12 October 2017).

35 (a) Report of the OPCW Fact-Finding Mission in Syria Regarding an Alleged Incident in Khan Shaykhun, Syrian Arab Republic April 2017 (S/1510/2017, dated 29 June 2017). Available at: www.opcw.org/fileadmin/OPCW/Fact_Finding_Mission/s-1510-2017_e_.pdf (b) Note by the Technical Secretariat: Further Clarifications on why the OPCW Fact-Finding Mission did not Deploy to Khan Shaykhun (S/1545/2017, dated 17 October 2017).

36 OPCW-UN Joint Investigative Mechanism Fact Sheet, available at: https://unoda-web.s3-accelerate.amazonaws.com/wp-content/uploads/2016/08/JIM-Fact-Sheet-July2016.pdf

37 See OPCW News Item: Chemical Industry Councils and Scientific Societies Condemn Use of Chlorine as Weapon; www.opcw.org/news/article/chemical-industry-councils-and-scientific-societies-condemn-use-of-chlorine-as-weapon/

38 Letter available at: www.opcw.org/fileadmin/OPCW/Industry/ACS-ACC_syrian_chlorine_letter_091516.pdf

39 Letter available at: www.opcw.org/fileadmin/OPCW/Industry/2016-09-30_Letter_from_Cefic_to_Ambassador_OPCW_DG.pdf

and other chemicals as chemical weapons. The letters included offers of cooperation with the Secretariat. In response, experts from ACS, Cefic, Euro Chlor[40], the Union des Industries Chimiques (UIC)[41] and ACC agreed to share their knowledge with the Secretariat on the following issues:

(a) Small-scale production and storage of chlorine, including in-situ production and use.

(b) Detection and identification of the effects of chlorine exposure (in animals, humans and the environment), including degradation products.

(c) The use of isotope ratios to identify the origin of the chlorine.

(d) Best practices in response to chlorine gas release (whether accidental or intentional) and protection.

7.2 The experts briefed the Secretariat on how chlorine is produced from salt and water as raw materials using electric energy, with three technologies available for industrial scale production: membrane,[42] mercury[43] and diaphragm.[44] They reviewed the physical and chemical properties of chlorine and its reactivity (including its impact on humans and environment). Knowledge of biomarkers specific to chlorine exposure is currently lacking; but there is ongoing research in this area. Biomarkers with potential for use in verification exposure include certain surfactant proteins,[45] Clara cell secretory proteins,[46] chlorotyrosine residues[47] and *L*-α-phosphatidylglycerol chlorohydrins.[48] The persistence of the latter biomarker allows its detection more than

---

40 For additional information on Euro Chlor, see http://www.eurochlor.org/

41 For additional information on the UIC, see: http://www.uic.fr/

42 See: http://www.eurochlor.org/the-chlorine-universe/how-is-chlorine-produced/the-membrane-cell-process.aspx

43 See: http://www.eurochlor.org/the-chlorine-universe/how-is-chlorine-produced/the-mercury-cell-process.aspx

44 See: http://www.eurochlor.org/the-chlorine-universe/how-is-chlorine-produced/the-diaphragm-cell-process.aspx

45 Acute chlorine gas exposure produces transient inflammation and a progressive alteration in surfactant composition with accompanying mechanical dysfunction; C. B. Massa, P. Scott, E. Abramova, C. Gardner, D. L. Laskin, A. J. Gow*;* *Toxicol Appl Pharmacol*; 2014*, 278(1),* 53–64. DOI: 10.1016/j.taap.2014.02.006.

46 Repair of tracheal epithelium by basal cells after chlorine-induced injury; S. Musah, J. Chen, G. W. Hoyle; *Respiratory Research*; 2012, *13*, 107. DOI: 10.1186/1465-9921-13-107.

47 (a) Sarcoendoplasmic reticulum Ca^{2+} ATPase. A critical target in chlorine inhalation–induced cardiotoxicity; S. Ahmad, A. Ahmad, B. Tara, H. Hofer, E. Joan, C. William, O. Mozziconacci, C. Schöneich, N. Reisdorph, L. R. Powell, J. D. Chandler, J. Brian, J. Day, L. A. Veress, C. W. White; *Am J Respir Cell Mol Biol*.; 2015, *52(4),* 492–502. DOI: 10.1165/rcmb.2014-0005OC. (b) Formation of chlorinated lipids post-chlorine gas exposure; D. A. Ford, J. Honavar, C. J. Albert, M. Duerr, J. Y. Oh, S. Doran, S. Matalon, R. P. Patel1; *J Lipid Res*.; 2016, *57(8),* 1529–1540. DOI: 10.1194/jlr.M069005. (c) 3-Chlorotyrosine and 3,5-dichlorotyrosine as biomarkers of respiratory tract exposure to chlorine gas; M. A. Sochaski, A. M. Jarabek, J. Murphy; *J Anal Toxicol*; 2008, *32(1),* 99-105.

48 *L*-α-phosphatidylglycerol chlorohydrins as potential biomarkers for chlorine gas exposure; P. Hemström, A. Larsson, L. Elfsmark, C. Åstot; *Anal. Chem*., 2016, *88(20)*, 9972–9979. DOI: 10.1021/acs.analchem.6b01896.

72 hours after ice had been exposed to chlorine. Finding persistent biomarkers that are not isolated to one plant or soil type[49] was identified as a challenge. With regard to possible attribution signatures for chlorine, impurities and $^{37}Cl:^{35}Cl$ isotopic ratios were discussed. These might allow the provenance of chlorine to be determined, but research would be needed to demonstrate feasibility.

7.3 Dr Dare-Doyen summarised the consultations and introduced several recommendations that came out of the workshop. These included encouraging scientific research in areas where gaps were identified, conducting a review and compendium of scientific literature, and further engaging with experts on accident investigation and medical response.

7.4 In the subsequent discussion, the following points were raised:

(a) Alternatives to chlorine were discussed, and do exist, including for water purification (see also paragraph 7.11). This area was not, however, explored in the workshop. SAB members support research into alternatives, but recognise that any such adoption would require appropriate life cycle analysis and risk assessment to determine how viable the alternatives would be, including the impacts on industry.

(b) With regard to medical response, a report by the American Thoracic Society on medical response for choking gas exposure was recently published.[50]

(c) Formation of chlorine from a precursor (reduction of chloride ion for example) was also recognised as relevant to enabling chlorine gas to be generated and released to cause harm. The chemistries deployed and the chemical markers of such processes should also be considered.

(d) The Secretariat could compile a reference guide of materials likely to react with chlorine and the products formed, to assist with identifying samples to collect during an investigation. Published information from incident response to chlorine release is also recommended for inclusion; in this regard, it may be useful to consult experts from States Parties.

Subitem 7(b): Theoretical study of sulfur mustard

7.5 Professor Ponnadurai Ramasami presented the results of a computational study of the interaction of sulfur mustard (HD) and water, explaining that hydration can influence both chemical reactions (e.g. hydrolysis[51]) and the ability to detect HD.[52] The study

---

49 Chloride in soils and its uptake and movement within the plant: a review; J. P. White, R. Martin; *Broadley Annals of Botany*; 2001, *88(6),* 967–988. DOI: 10.1006/anbo.2001.1540.

50 An Official American Thoracic Society Workshop Report: Chemical Inhalational Disasters. Biology of Lung Injury, Development of Novel Therapeutics, and Medical Preparedness; E. M. Summerhill, G. W. Hoyle, S.-E. Jordt, B. J. Jugg, J. G. Martin, S. Matalon, S. E. Patterson, D. J. Prezant , A. M. Sciuto, E. R. Svendsen, C. W. White, L. A. Veress; on behalf of the ATS Terrorism and Inhalational Disasters Section of the Environmental, Occupational, and Population Health Assembly; *Ann. Am. Thorac. Soc.*, 2017, *14(6)*, 1060–1072. DOI: 10.1513/AnnalsATS.201704-297WS.

51 Effect of adsorbed water and surface hydroxyls on the hydrolysis of VX, GD, and HD on titania materials: the development of self-decontaminating paints; G. W. Wagner. G. W. Peterson, J. Mahle; *Ind. Eng. Chem. Res.*; 2012, *51(9),* 3598–3603. DOI: 10.1021/ie202063p.

looked at microhydration[53] through adding discrete water molecules to an HD molecule and analysing changes in structural parameters,[54] energetics, vibrational frequency and dipole moment. The modelling was performed using B3LYP and M06-2X functionals, and the MP2 level of theory, using the basis set 6-311++G(2d,2p) for all atoms. Little change was observed in the geometry of HD in the hydrated clusters resulting from water molecule addition; the C–Cl bond however was found to lengthen gradually as the number of water molecules increased. The hydrated clusters were found to be energetically more stable compared to the non-hydrated HD. Such clusters might be identified by infrared spectroscopy. Hydrogen bonding, the main non-covalent interaction between HD and water molecules, was confirmed by infrared shifts of selected peaks, specifically the stretching of C–Cl, S–C and O–H bonds. The results from this microhydration study are helpful in the interpretation of infrared spectra of humid air, moist soil and water samples where HD is present. It was noted that computational studies of microhydration of nerve agents[55] and lewisite[56] have also been published.

7.6 In the subsequent discussion, the SAB members considered how modelling can be applied to the types of situations likely to be encountered. Such modelling would be complex and need to take into account bulk phase conditions (including aspects of pH and ionic strength in liquid samples, as well as phase equilibria). One such application of potential value could be in understanding the fate of mustard in degrading munitions in the Baltic Sea.

---

52 Enzyme based test stripes for the visual or photographic detection and quantitation of gaseous sulphur mustard; S. Bidmanova, M. S. Steiner, M. Stepan, K. Vymazalova, M. A. Gruber, A. Duerkop, J. Damborsky, Z. Prokop, Otto S. Wolfbeis; *Anal. Chem*; 2016, *88(11),* 6044–6049. DOI: 10.1021/acs.analchem.6b01272.

53 (a) Switching on the fluorescence of 2-aminopurine by site-selective microhydration; S. Lobsiger, S. Blaser, R. K. Sinha, H. M. Frey, S. Leutwyler; *Nature Chemistry*; 2014, *6*, 989–993. DOI:10.1038/nchem.2086. (b) Fragmentation of allylmethylsulfide by chemical ionization: dependence on humidty and inhibiting role of water; T. Maihom, E. Schuhfried, M. Probst, J. Limtrakul, T. D. Märk, F. Biasioli; *J Phys Chem A.*; 2013*, 117(24)*, 5149–51640. DOI: 10.1021/jp4015806. (c) Hydration of the bisulfate ion: atmospheric implications; E. Devon, Husar, B. Temelso, A. L. Ashworth, G. C. Shields; *J. Phys. Chem.* A; 2012, *116(21)*, 5151–5163 DOI: 10.1021/jp300717j. (d) Single solvent molecules can affect the dynamics of substitution reactions; R. Otto, J. Brox, S. Trippel, M. Stei, T. Best, R. Wester; *Nature Chemistry*; 2012*, 4*, 534–538. DOI:10.1038/nchem.1362.

54 Structural flexibility of the sulfur mustard molecule at finite temperature from car-parrinello molecular dynamics simulations; J. Lach, J. Goclon, P. Rodziewicz*; J. Hazard. Mater.*; 2016*, 306*, 269–277. DOI: 10.1016/j.jhazmat.2015.12.027.

55 (a) Infrared signature of micro-hydration in the organophosphate sarin: an ab initio study; T. M. Alam, C. J. Pearce CJ; *J. Mol. Model.*; 2015*, 21(7),* 182. DOI: 10.1007/s00894-015-2732-z. (b) Ab initio investigation of sarin micro-hydration; M. Todd, A. Charles, J. Pearce, J. E. Jenkins; 2012, *995*, 24-35. DOI: 10.1016/j.comptc. (c) Molecular modelling of organophosphorous agents and their aqueous solutions; A. Vishnyakov, G. Gor, M. T. Lee, A. V. Neimark*; The J. of Phys. Chem. A*; 2011, *115*, 5201–5209. DOI: 10.1021/jp200509u.

56 (a) Modeling the chelation of As(III) in lewisite by dithiols using density functional theory and solvent-assisted proton exchange; L. K. Harper, C. A. Bayse; *J. Inorg. Biochem.*; 2015, *153*, 60–67. DOI: 10.1016/j.jinorgbio. (b) A computational study of detoxification of lewisite warfare agents by British anti-lewisite: catalytic effects of water and ammonia on reaction mechanism and kinetics; C. Sahu, S. Pakhira, K. Sen, A. K. Das; *J. Phys. Chem, A*; 2013. *117(16),* 3496–3506. DOI: 10.1021/jp312254z.

Subitem 7(c): Study of the behaviour of heavy sulfur mustards against commercial decontaminants

7.7 Professor Roberto Martinez-Álvarez presented the results of studies conducted on the reaction of sesquimustards and oxymustards with commercially available decontaminants. He reported that the efficiency of the decontamination process is mainly dependent on the solubility of the mustards in the decontamination media.

7.8 In the subsequent discussion, the following points were raised:

(a) The decontamination chemistry that was discussed highlighted open issues in understanding the blistering mechanism of mustard agents. The blistering action of sulfur mustard itself is often invoked through the formation of an episulfonium ion, however the sulfone, which is a degradation product, is also a potent skin blistering agent, but cannot form an episulfonium ion.

(b) It was noted that very little information exists in the scientific literature on sesquimustards and oxymustards, making these studies valuable in adding to the knowledge base on vesicants. Professor Martinez-Álvarez indicated he would be publishing the results in the coming months, including information on impurities and degradation products that may be useful for verification.

Subitem 7(d): Eliminating toxic substances and reagents from chemical synthesis

7.9 Professor Ferruccio Trifirò presented an overview of his work in exploring approaches for eliminating the use of chemicals such as hydrogen cyanide (HCN), chlorine (Cl_2) and phosgene ($COCl_2$) from industrial use.[57] His motivations for this research come from a desire for a more green, or sustainable, and safe chemical industry; as well as to find ways to eliminate access to and possible misuse of toxic industrial chemicals as weapons. Professor Trifirò indicated that his research has involved collaboration with industrial scientists in effort to identify alternatives, and also to evaluate their practical and economic viability from an industry perspective.

7.10 Starting with HCN, Professor Trifirò explained that industrial uses include the manufacture of acrylonitrile (a monomer for nitrile fibres and ABS[58]), adiponitrile (the monomer for nylon-6,6),[59] methylmethacrylate (the monomer for plexiglass),[60]

---

57 (a) Acrylonitrile from biomass: still far from being a sustainable process; R. K. Grasselli, F. Trifirò*; Topics in Catalysis*; 2016, *59(17-18),* 1651–1658. (b) Ti-silicalite as catalyst for gas-phase ammoximation of cyclohexanone with molecular oxygen; D. P. Dreoni, D. Pinelli, F. Trifirò, Z. Tvaruzkova, H. Habersberger, P. Jiru; *Catalysis Letters*; 1991, *11(3-6),* 285–294. (c) Vanadium-zeolite catalysts for the ammoxidation of xylenes; F. Cavani, F. Trifirò, P. Jiru, K. Habersberger, Z. Tvaruzkova; *Zeolites*; 1988, *8*, 12–18. (d) Kinetic and Mechanistic Analysis of Toluene Ammoxidation to benzonitrile on vanadium-titanium oxides; P. Cavalli, F. Cavani, I. Manenti, M. El-Sawi, F. Trifirò; *Ind. & Eng. Chem. Research*; 1987, *26(4),* 804–810.

58 ABS = Acrylonitrile butadiene styrene, a thermoplastic polymer.

59 A review of adiponitrile industrial production processes and associated atom economies; Y. Zhu, L. Gao, Liang, L. Wen, Langyou, B. Zong, Baoning; A review of adiponitrile industrial production processes and associated atom economies; *Chinese Science Bulletin (Chinese Version)*, 2015, *60*, 1488. DOI: 10.1360/N972014-01259.

60 New developments in the production of methyl methacrylate; K. Nagai; *Applied Catalysis A: General*, 2001, *221(1-2)*, 367–377. DOI: 10.1016/S0926-860X(01)00810-9.

chelating agents such as EDTA,[61] and sodium cyanide (which is used for gold recovery and production of methionine). He noted that acrylonitrile manufacture had previously been produced from acetylene and HCN, and is now industrially produced through ammoxidation of propylene,[62] demonstrating that viable alternatives can be found. However, there is still research needed before suitable alternatives will be found for chemicals such as adiponitrile (produced by the reaction of butadiene and HCN); and methylmethacrylate (produced from acetone cyanohydrin, which is formed by reaction of acetone and HCN). Professor Trifirò discussed alternatives that have been proposed for both, indicating these were more expensive than the current methods.[63]

7.11 Turning to chlorine, Professor Trifirò provided the example of the HPPO process,[64] which produces propylene oxide from oxidation of propylene with hydrogen peroxide (H_2O_2).[65] The introduction of HPPO allowed the elimination of the use of chlorine in propylene oxide production. Chlorine is also used to produce chlorinated intermediates that are converted to fluorocarbons by reaction with hydrofluoric acid (HF). Professor Trifirò discussed the use of HF and oxygen as a fluorinating agent for olefins, which represent a possible route to eliminate chlorine from fluorocarbon production.[66] For water sterilisation applications, he noted that peroxide-based reagents and ozone have been studied.[67] Professor Trifirò also highlighted that under the Stockholm Convention[68] there are efforts to eliminate the use of a number of organochlorine compounds (primarily pesticides).

7.12 The presentation concluded with a discussion on phosgene, which is used to produce isocyanates, aromatic carbonates, and monomers for polyurethanes and polycarbonates. Professor Trifirò discussed reductive and oxidative carbonylation

---

61 EDTA = Ethylenediaminetetraacetic acid.

62 Ammonoxidation of propylene to acrylonitrile; I. Pasquon, F. Trifirò, P. Centola; *La Chimica e l'Industria*; 1967, *49(11),* 1151–1159.

63 Examples of alternative processes for production of methylmethacrylate: (a) The oxidation of isobutane to methacrylic acid: an alternative techonology for MMA production; N. Ballarini, F. Cavani, H. Degrand, E. Etienne, A. Pigamo, F. Trifirò, J. L. Dubois*; Methods and Reagents for Green chemistry;* 2007, 265–279. (b) The synthesis of methacrylic acid by isobutane oxidation: a new route of low environmental impact, alternative to the conventional industrial process; F. Cavani, E. Etienne, M. Favaro, A. Galli, G. Selleri, F. Trifirò, G. Hecquet ; *Atti*.; 1995, 43–442.

64 For further information see: http://www.chemicals-technology.com/projects/basf-hppo/

65 Catalytic behaviour of Mo-based catalysts in liquid phase epoxidation of propylene by hydroperoxides; P. Forzatti, F. Trifirò; *Reaction Kinet. Catal. Lett.*; 1974, *1(3),* 367–372.

66 Preparation of transition metal fuorides as catalysts for the environmentally sustainable HFC production; L. Forni, S. Albonetti, F. Cavani, M. Bernardi, A. Beghin, F. Trifirò; *Stud. Surf. Sci. Catal.*; 2006, *162*, 993–1000.

67 A review of imperative technologies for wastewater treatment I: oxidation technologies at ambient conditions; R. Gogate; A. B. Pandit; *Advances in Environmental Research*; 2004, *8(3-4)*, 501–551. DOI: 10.1016/S1093-0191(03)00032-7.

68 The Stockholm Convention on Persistent Organic Pollutants; for additional information see: http://chm.pops.int/TheConvention/Overview/tabid/3351/Default.aspx

processes,[69] as well as the use of dimethyl carbonate[70] as alternatives to phosgene, noting that these methods have seen industrial adoption.

7.13 In the subsequent discussion, the SAB noted that many factors must be considered when evaluating the viability of a substitution of a new chemical or process into an existing industrial product line. In addition to production and operating cost considerations, changes to established processes must undergo validation to ensure that quality, safety and regulatory design requirements are met.

8. AGENDA ITEM EIGHT – Chemical production

Subitem 8(a): Report from the workshop on trends in chemical production

8.1 The fourth and final workshop intended to inform the report to the Fourth Review Conference, covering trends in chemical production, was held from 3 to 5 October in Zagreb, Croatia.[71] The workshop was organised by the SAB in cooperation with the Institute of Medical Research and Occupational Health (IMROH).[72] The workshop was funded by the European Union[73] and organised under the auspices of the Croatian President Kolinda Grabar-Kitarović; the Ministry of Economy, Entrepreneurship and Crafts; and the City of Zagreb.

8.2 Dr Zrinka Kovarik briefed the SAB on the workshop, presenting the key findings and executive summary of the workshop report (SAB-26/WP.2, dated 19 October 2017).[74] As the OPCW transitions to a post-destruction phase, ensuring continued confidence in compliance with the obligations of the Convention will remain at the heart of its work.[75] Likewise, in the face of scientific, technological and socioeconomic change, it has been recognised by the SAB that methods and practices may need to adapt to changing realities.[76,77] The workshop was held to provide input and scientific

---

69 Away from phosgene: reductive carbonylation of nitroarenes and oxidative carbonylation of amines, understanding the mechanism to improve performance; F. Ragaini; *Dalton Trans.*, 2009, 6251–6266. DOI: 10.1039/B902425P.

70 See for example: Highly selective phosgene-free carbamoylation of aniline by dimethyl carbonate under continuous-flow conditions; S. Grego, F. Aricò, P. Tundo; *Org. Process Res. Dev.*, 2013, *17(4)*, 679–683. DOI: 10.1021/op4000048.

71 See OPCW news item: https://www.opcw.org/news/article/opcw-scientific-advisory-board-reviews-technological-developments-and-trends-in-chemical-production/

72 For additional information on IMROH, see: https://www.imi.hr/en/

73 This funding was provided through Project III (Science and Technology: Assessment of Developments in Science and Technology) of EU Council Decision (CFSP) 2015/259, dated 17 February 2015. http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv:OJ.L_.2015.043.01.0014.01.ENG

74 available at: www.opcw.org/fileadmin/OPCW/SAB/en/sab-26-wp02_e_.pdf

75 See paragraphs 9 through 11 of: Medium-Term Plan of the Organisation for the Prohibition of Chemical Weapons 2017 – 2021 (EC-83/S/1 C-21/S/1). Available at: www.opcw.org/fileadmin/OPCW/EC/83/en/ec83s01_c21s01_e_.pdf

76 See for example: Verification, Report of the Scientific Advisory Board's Temporary Working Group (SAB/REP/1/15, dated June 2015). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/Final_Report_of_SAB_TWG_on_Verification_-_as_presented_to_SAB.pdf

77 The potential for a need to change methods and practices has also been raised through OPCW's "vision paper", The OPCW in 2025: Ensuring a World Free of Chemical Weapons (S/1252/2015, dated 6 March 2015). Available at: www.opcw.org/fileadmin/OPCW/S_series/2015/en/s-1252-2015_e_.pdf

guidance on the impact to the Convention from developments and technological change that is occurring in industrial chemical production.

8.3 The workshop brought together experts from a variety of sectors across the chemical industry, experts engaged in research relevant to chemical synthesis and production technologies, and stakeholders involved in implementation of the Convention, to share experiences and to consider the short- and long-term influence of technological change on chemical production. Topics included a review of the 20 years since entry into force of the Convention[78] and the role that chemical industry has played, developments across a variety of sectors of chemical industry, chemical and biobased production methods and technologies, technical aspects and approaches to industry verification under the Convention, and insights into activities that support discovery and production of chemicals (including chemical analysis and informatics).

8.4 The SAB endorsed the report and discussed the proposals from the executive summary (paragraph 1.6 of SAB-26/WP.2), which are as follows:

(a) As technological advances related to the discovery and production of chemicals are adopted, a fit-for-purpose verification regime should maintain up-to-date operational knowledge of chemical and biological-based production methods (including aspects of synthesis and analysis). Recognising unusual processes or aspects of a laboratory or production facility that are inconsistent with allowable activities under the Convention is valuable for both prevention of re-emergence and post-event fact-finding. Training exercises could usefully take into account such considerations. (subparagraph 1.6(a) of SAB-26/WP.2)

(b) In the face of a changing global security environment, the workshop drew attention to previous advice from the SAB's TWG on verification, which considered risk-benefit approaches as a means to focus verification in areas that have greater risk to the intent and purpose of the Convention.[79] This could include consideration of relevant chemicals not on the current schedules. (subparagraph 1.6(b) of SAB-26/WP.2)

(c) The workshop recognised a number of areas with potentially transferable learnings from industrial practices. These include approaches to trace analysis and tools for chemical risk assessment. With reference to the latter, shared tools and chemical data sets have been developed to help with safer process and product design and for compliance under certain regulatory frameworks. These tools could inform risk-benefit analysis and they may also be of relevance to those involved in chemical safety and security activities. (subparagraph 1.6(c) of SAB-26/WP.2)

(d) Several significant developments in the global chemical industry observed over the past 20 years (specifically, the shifting of chemical production to Asia and the revival of the North American chemical industry due to the shale gas boom) were not recognised until they actually took shape. That is, they were unanticipated in the years just before they happened. Engagement with

---

78 For further information on the 20th Anniversary of the OPCW, see: https://20years.opcw.org/

79 See recommendations 1 through 3, 9 through 10, and 15 of SAB/REP/1/15.

technical experts from industry and more frequent review of industry-focused research and development reports[80] would benefit the science review process and help keep the Secretariat better informed. (subparagraph 1.6(d) of SAB-26/WP.2)

(e) Synthesis tools being developed for chemical discovery purposes (complemented with machine learning approaches for predicting chemistry) can potentially enable capabilities for laboratories to quickly generate large sets of analytical data, screen for reactivity and toxicity properties, and elucidate degradation pathways of a broad range of chemical classes. Such tools might be considered in the enhancement of laboratory capabilities for the implementation of the Convention. (subparagraph 1.6(e) of SAB-26/WP.2)

(f) The technical presentations and content of the workshop served as a reminder of the highly transdisciplinary (convergent) nature of technology development, with scientific disciplinary convergence going well beyond the fields of chemistry and biology. This finding further supports the view that the scientific review process must engage broad scientific communities, and look for opportunity in technological change, to support robust implementation of the Convention. Sharing of experience on science advice with other relevant disarmament communities (especially the Biological Weapons Convention stakeholders) should be encouraged. (subparagraph 1.6(f) of SAB-26/WP.2)

(g) In the discussion of changing realities and the relevance of current verification practices, it was acknowledged that greater levels of science and technology engagement, and knowledge sharing amongst States Parties, could also support the verification regime through the increased transparency such initiatives bring. (subparagraph 1.6(g) of SAB-26/WP.2)

8.5 In the subsequent discussion, the following points were raised:

(a) The SAB expressed its appreciation to the Board members and the invited speakers who participated in the Zagreb workshop, and to the IMROH, the government of the Republic of Croatia and the City of Zagreb.

(b) The workshop produced valuable inputs on chemical discovery and production methods across a range of sectors relevant to the Convention. The outcomes will inform recommendations to the Fourth Review Conference.

8.6 The following proposals derived from the report of the Zagreb workshop, specifically subparagraphs (d) and (f) from 8.4 above, are put forward as recommendations of the SAB at its Twenty-Sixth Session:

---

80 For example, to review what has and has not remained constant in global research and development (including industry contributions) from 2013 to 2016, see:
(a) *2014 Global R&D Funding Forecast*; R&D Magazine; December 2013, https://abm-website-assets.s3.amazonaws.com/rdmag.com/s3fs-public/gff-2014-5_7%20875x10_0.pdf
(b) *2016 Global R&D Funding Forecast*; A supplement to R&D Magazine; Winter 2016, https://www.iriweb.org/sites/default/files/2016GlobalR%26DFundingForecast_2.pdf
(c) *2017 Global R&D Funding Forecast*; A supplement to R&D Magazine; Winter 2017, http://digital.rdmag.com/researchanddevelopment/2017_global_r_d_funding_forecast?pg=1#pg1

(a) To ensure that the verification regime remains fit for purpose, the SAB encourages more extensive engagement with technical experts from industry and the review of industry-focused research and development. This would help to keep the Secretariat usefully informed on developments in chemical industry, benefit the science review process and allow for recognition of change from previously predicted trends.

(b) Reflecting on the findings of both the Zagreb and Rio de Janeiro workshops (see subparagraph 9.13(a)), the SAB recognises that the emergence and practical applications of new and innovative technologies (in both research and industrial sectors), as well as the repurposing of existing technologies for unanticipated new applications, has benefited from increasingly transdisciplinary (convergent) scientific communities. As the Secretariat and stakeholders of the OPCW 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. This recommendation was further informed with inputs from paragraphs 7.1 through 7.4, 8.2 and 8.3, 9.10 and 9.11, 9.15 and 9.16, and 10.1 through 10.8.

Subitem 8(b): Results of the survey on biomediated processes

8.7 Mr Larry Denyer (Head, OPCW Industry Verification Branch) discussed the issue of the meaning of the term "produced by synthesis" and briefed the SAB on the results of a recent survey[81] conducted by the OPCW to better understand how States Parties treat biomediated production processes in their implementation of the Convention, along with a consultation with States Parties on the survey outcome. He began by briefing the workshop on Part IX of the Verification Annex of the Convention (hereinafter "the Verification Annex"),[82] which uses the term "produced by synthesis" as one of the requirements that makes a chemical production facility subject to declaration. Whether the term includes biochemical and biologically mediated processes ("biomediated processes") has been an outstanding issue on the agenda of the Council since entry into force of the Convention in 1997. The SAB has made recommendations on the meaning, and are of the view that any process designed for the formation of a chemical substance should be covered by the term "produced by synthesis".[83] With additional recommendations emanating from the TWGs on the convergence of chemistry and biology[84,85] and on verification.[86]

---

81 Results of the Survey on Biomediated Processes (S/1534/2017, dated 14 September 2017). Available at: www.opcw.org/fileadmin/OPCW/S_series/2017/en/s-1534-2017_e_.pdf

82 Part IX of the Verification Annex. www.opcw.org/chemical-weapons-convention/annexes/verification-annex/part-ix/

83 See paragraph 10 of RC-3/DG.1. Available at: www.opcw.org/fileadmin/OPCW/CSP/RC-3/en/rc3dg01_e_.pdf

84 See recommendations 18 and 19 of: Convergence of Chemistry and Biology: Report of the Scientific Advisory Board's Temporary Working Group (SAB/REP/1/14, dated June 2014). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/TWG_Scientific_Advsiory_Group_Final_Report.pdf

85 A quick reference guide to the recommendations of the TWG on the convergence of chemistry and biology is available at: www.opcw.org/fileadmin/OPCW/SAB/en/Convergence_of_Chemistry_and_Biology_1-01.pdf

8.8 To assess the potential impact of the implementation of the SAB recommendation of "production by synthesis" on the verification regime, a survey on biomediated processes was conducted across the States Parties. The survey results highlighted diverse views and practices across the States Parties in regard to declarations of other chemical production facilities (OCPFs).[87] Approximately 40% of the 32 States Parties[88] that responded, do, as a general policy, declare any plant site producing discrete organic chemicals (DOCs) regardless of the type of process used in the facility (e.g. both biomediated and traditional chemical processes). Of these, nearly all allow certain exclusions from their declarations, such as those that produce alcoholic beverages and/or utilise biochemical processes within living organisms, such as fermentation. The views of the majority of delegations present during the consultation were generally consistent with the results of the survey, with several indicating they could support moving toward a decision by the Council. However, some States Parties need more time to consider the topic. It is anticipated that discussions will continue between interested delegations on possible next steps.

8.9 In the subsequent discussion, the following points were raised:

(a) It was recognised that given the number and identity of States Parties that responded to the survey, which did not include five major chemical producing countries, the results may not be fully representative. Despite this, it was noted that the States Parties themselves had requested the survey and that the results provide a better understanding of the approaches to biomediated processes.

(b) The SAB suggested that the consideration of the technical differences between biomediated versus chemical processes may be losing sight of the issue of whether or not a process or a chemical is of relevance to the intent and purpose of Convention. Risk assessment may be an approach to determining the relevance of a given type of production facility.

9. AGENDA ITEM NINE – Scientific and technological elements of verification technologies, emerging technologies, and new equipment

Subitem 9(a): Managing the results of on-site sampling and analysis: a methodology to resolve ambiguous identifications

9.1 Dr Brendan Whelan (OPCW Inspectorate Safety and Analytical Chemistry Cell) briefed the SAB on the scientific approach behind a methodology being developed to facilitate the resolution of ambiguous results obtained from on-site sampling and analysis during routine inspections, in particular suspected false positives. Dr Whelan explained that current methodologies to resolve ambiguous results are principally focused on identification of the chemicals giving rise to a false positive, which

---

86 See recommendations 9 and 10 of SAB/REP/1/15. Available at: www.opcw.org/fileadmin/OPCW/SAB/en/Final_Report_of_SAB_TWG_on_Verification_-_as_presented_to_SAB.pdf

87 OCPFs are defined in Part IX of the Verification Annex. www.opcw.org/chemical-weapons-convention/annexes/verification-annex/part-ix/

88 Additional responses have been received since the original summary of results was published; an updated summary is forthcoming.

although effective, does raise confidentiality issues relating to protection of sensitive business information.

9.2 The new methodology is based on mass spectral analysis and does not require unscheduled chemicals to be identified. Moreover, States Parties can, under the Convention, exercise their right to protect potentially sensitive information and limit identification of chemicals to only scheduled chemicals. In such situations, the use of spectral databases such as NIST[89] is not an option. The new methodology provides for an effective and non-intrusive solution to resolving ambiguous results. Whilst the project is only partially complete, Dr Whelan presented examples where the methodology has been tested during Article VI sampling and analysis missions with very encouraging results.

9.3 In the subsequent discussion, the following points were raised:

(a) Understanding the chemistry through which impurities and unintended by-products form was recognised as a critical aspect to the methodology. Furthermore, a high level of chemistry knowledge combined with the methodology presented may also be helpful in investigative analysis of impurity profiles.

(b) The SAB noted that the methodology may have use in the identification of compounds and could be potentially automated, with the completed project serving as a training set for a computational methodology.

(c) Dr Whelan noted that the most common occurrences of false positives have occurred with organophosphorus compounds whose structures share side chains with certain pharmaceutical ingredients. He also noted that in his experience, he has not encountered false positives for mustard compounds.

(d) Several SAB members asked about the possibility to include other data streams and/or a series of analysis conditions to reduce the occurrence of molecular fragments in a mass spectrum that lead to a false positive identification. It was noted that for routine sampling and analysis inspections, time constraints, limitations of the OCAD database and the established procedures that are adhered to would be prohibitive to collecting additional data streams.

(e) The methodology is useful for on-site analysis and could be shared with the designated laboratories of the OPCW.[90] The laboratories could provide feedback that would benefit the development of the methodology.

---

89 National Institute of Standards and Technology (NIST) Mass Spectral Library, http://chemdata.nist.gov/dokuwiki/doku.php?id=start

90 The current list of designated laboratories can be found in (a) Status of Laboratories Designated for Analysis of Authentic Environmental Samples (S/1529/2017, dated 31 August 2017). Available at: www.opcw.org/fileadmin/OPCW/S_series/2017/en/s-1529-2017_e_.pdf and (b) Status of the Laboratories Designated for the Analysis of Authentic Biomedical Samples" (S/1516/2017, dated 11 July 2017), available at: www.opcw.org/fileadmin/OPCW/S_series/2017/en/s-1516-2017_e_.pdf

Subitem 9(b): Training and preparedness to address new challenges

9.4 Mr Magnus Backlund (of the OPCW Inspectorate Capacity-Building and Contingency Planning Cell) briefed the SAB on how the Inspectorate is approaching training to meet emerging challenges. He explained that the threat posed by non-State actors has been identified as a serious emerging challenge for the Convention, with the hostile use of toxic chemicals (in particular the use of toxic industrial chemicals), biothreat agents, and the potential use of radioactive materials a concern across many States Parties. Additionally, OPCW contingency operations have seen inspectors work in environments that include areas close to war zones and non-permissive environments. Mr Backlund highlighted challenges that multiple hazards present and how inspector training is being tailored to ensure inspectors are fit for mission. Key aspects are the safety and security of inspectors in non-routine situations.

9.5 In the subsequent discussion, the following points were raised:

(a) Real-world simulations for training scenarios were identified as being of greatest relevance. This would usefully include training for inspectors in investigation of clandestine laboratories and the ability to recognise improvised chemical devices and the components that would allow them to be produced.

(b) Understanding how to recognise change in chemical signatures (including through indirect measurements of chemicals present in the operating environment) might be considered. This approach may help overcome gaps in the ability of specialised detectors and equipment to recognise the presence of an unfamiliar toxic chemical.

Subitem 9(c): Update from the OPCW Laboratory

9.6 Mr Stuart Thomson (Senior Analytical Chemist at the OPCW Laboratory) updated the SAB on developments at the OPCW Laboratory. He began with an update on the preparations for the second biotoxin exercise,[91] indicating that the project is in an advanced planning stage and the Laboratory is actively testing the matrices proposed for the project. Additionally, the scoring system used for the first biotoxin exercise, has undergone some changes, now being split into three different categories: structural analysis (LC/MS[92]), biochemical analysis (ELISA) and activity testing, with points awarded to each and the use of a sliding scale of confidence of detection.

9.7 Mr Thomson also presented a primer for discussion about machine learning and pattern recognition in analytical data analysis. He noted that much of the data analysis in both GC/MS[93] and LC/MS is based on pattern

---

91 Call for Nominations for an Exercise on Analysis on Protein Biotoxins (S/1538/2017, dated 4 October 2017). Available at: www.opcw.org/fileadmin/OPCW/S_series/2017/en/s-1538-2017_e_.pdf

92 LC/MS = liquid chromatography/mass spectrometry.

93 GC/MS = gas chromatography/mass spectrometry.

recognition,[94] asking the question: can machines replace the experienced analytical chemist?

9.8 In the subsequent discussion, the SAB expressed their support for the Secretariat's consideration of the use of machine learning to help the interpretation of analytical data. The Board noted that algorithms and training would need to be developed and require confirmatory efforts to make this reliable.

Subitem 9(d): Report from the workshop on innovative technologies for chemical security

9.9 The third of a series of four workshops intended to inform the report on developments in science and technology to the Fourth Review Conference, "Innovative Technologies for Chemical Security" was held from 3 to 5 July 2017 in Rio de Janeiro, Brazil.[95] The workshop was organised by the SAB in cooperation with the IUPAC, the National Academies of Science, Engineering and Medicine of the United States of America (NAS),[96] the Brazilian Academy of Sciences (ABC),[97] and the Brazilian Chemical Society (SBQ).[98]

9.10 Mr Cheng Tang briefed the SAB on the workshop, presenting the outcomes and executive summary of the report (SAB-26/WP.1, dated 21 July 2017[99]). Mr Tang explained that the thematic content of the workshop follows the findings that arose through the report of the OPCW SAB's TWG on verification and the recognition that 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 transdisciplinary approaches to problem solving and technology development across scientific communities.[100] He noted that this convergence across traditional disciplinary boundaries fuels the "rapid pace of developments in science and technology" that is often discussed within chemical and biological security networks; and that new advances across the chemical and biological sciences are increasingly enabled by ideas and tools originating from

---

94 There are examples of this application in the scientific literature, see: (a) Artificial Neural Network for Probabilistic Feature Recognition in Liquid Chromatography Coupled to High-Resolution Mass Spectrometry; M. Woldegebriel, E. Derks; *Anal Chem.*; 2016, *89*, 1212–1221. DOI: 10.1021/acs.analchem.6b03678; and (b) Innovative methods for data analysis in analytical chemistry using Bayesian statistics and machine learning. M. T. Woldegebriel; PhD thesis 2017, University of Amsterdam, the Netherlands.

95 See also (a) Scientists review innovative technologies for chemical security, www.opcw.org/news/article/scientists-review-innovative-technologies-for-chemical-security/ and (b) Ciência para a paz, http://www.abc.org.br/centenario/?Ciencia-para-a-paz (in Portuguese).

96 The National Academies of Science, Engineering and Medicine (NAS). For additional information on NAS, see http://www.nationalacademies.org/index.html

97 Academia Brasileira de Ciências (ABC). For additional information on ABC, see: http://www.abc.org.br/rubrique.php3?id_rubrique=2

98 Sociedade Brasilia de Química (SBQ). For additional information on SBQ, see: http://www.abc.org.br/rubrique.php3?id_rubrique=2

99 Available at: www.opcw.org/fileadmin/OPCW/SAB/en/sab26wp01_SAB.pdf

100 See for example: (a) Spiez CONVERGENCE Report on the first workshop, Spiez Laboratory, 2014; available at: https://www.labor-spiez.ch/pdf/de/rue/Spiez_Convergence_2014_web.pdf and (b) Spiez CONVERGENCE Report on the second workshop, Spiez Laboratory, 2016; available at: https://www.labor-spiez.ch/pdf/en/rue/LaborSpiezConvergence2016_02_FINAL.pdf

sectors outside these disciplines. Furthermore, Convention-relevant developments in science and technology may not be easily recognised if the scientific review process is limited to chemical-specific fora.

9.11 The workshop brought together experts in areas of sensor development, precision agriculture, mobile and wearable technologies, digital health, autonomous sample collection and analysis, satellite image analysis, and other technologies that enable real time analysis and decision making. The workshop discussed capabilities, applications and challenges in the use of new tools and technologies to detect biochemical change in complex environments, and explored the potential of new technologies to enhance capabilities necessary for implementation of the Convention. The discussions and sharing of ideas across a broad range of technical expertise proved highly informative. The IUPAC journal, *Pure and Applied Chemistry*,[101] will publish a special edition in 2018 dedicated to the workshop, where workshop participants will publish peer-reviewed technical papers on the work they presented; the SAB will also contribute.[102]

9.12 The SAB endorsed the report and discussed the proposals from the executive summary (paragraph 1.6 of SAB-26/WP.1), which are as follows:

(a) The practice of bringing together international transdisciplinary groups to share and discuss ideas is vital for meeting future challenges. This practice has been a valuable part of the OPCWs science and technology review process, and the Secretariat and SAB are encouraged to continue this approach when considering scientific and technological advancements. (subparagraph 1.6(a) of SAB-26/WP.1)

(b) Through the science and technology review process, the SAB has identified a variety of innovative technologies and technology developers. The SAB could usefully facilitate engagement with these communities. (subparagraph 1.6(b) of SAB-26/WP.1)

(c) A broad set of technology exists that can potentially find application in some areas of implementation of the Convention. In general, such tools appear best suited toward non-routine (contingency) and assistance and protection operations, investigations, enhancement of laboratory capabilities, and stakeholder engagement. (subparagraph 1.6(c) of SAB-26/WP.1)

(d) 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

---

101 For additional information on *Pure and Applied Chemistry*, see: https://www.iupac.org/publications/pac/

102 Reports from workshops held for the SAB in preparation of their reports to the First, Second and Third Review Conferences had also been published in *Pure and Applied Chemistry*. See: (a) IUPAC workshop on the impact of scientific developments on the Chemical Weapons Convention, Bergen, Norway, 30 June – 3 July 2002; *Pure Appl. Chem.*; 2002, *74(12)*, 2229–2352; (b) Impact of scientific developments on the Chemical Weapons Convention; M. Balali-Mood, P. S. Steyn, L. K. Sydnes, R. Trapp; *Pure Appl. Chem.*; 2008, *80(1)*, 175–200; and (c) Impact of scientific developments on the Chemical Weapons Convention; K. Smallwood, R. Trapp, R. Mathews, B. Schmidt, L. K. Sydnes; *Pure Appl. Chem.*; 2008, *85(4)*, 851–881.

abreast of developments in these areas. (subparagraph 1.6(d) of SAB-26/WP.1)

(e) The Secretariat 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. (subparagraph 1.6(e) of SAB-26/WP.1)

(f) A number of the technologies considered during the workshop have potential for reducing risks to personnel operating in dangerous environments. Further consideration of these technologies could assist with development of recommended best practices for operating under such conditions. (subparagraph 1.6(f) of SAB-26/WP.1)

(g) Many interesting and potentially enabling technologies were discussed at the workshop. It should be emphasised that suitability for field use requires evaluation of fieldable capabilities that meet operational requirements (and fit within mission specific modalities). Opportunities to engage with technology developers and evaluate new tools should be encouraged. (subparagraph 1.6(g) of SAB-26/WP.1)

(h) The insight brought into discussions by chemical weapons inspectors regarding field and operational needs and challenges is an essential aspect of recognising opportunities where a given technology might prove valuable. The practice of engaging operational staff from the Secretariat in the scientific review process aids the formulation of practical science advice, and also allows the SAB to provide scientific guidance on operational practices. The Secretariat is encouraged to maintain this discourse with the SAB. (subparagraph 1.6(h) of SAB-26/WP.1)

9.13 In the subsequent discussion, the following points were raised:

(a) The SAB expressed its appreciation to the Board members and the invited speakers who participated in the Rio de Janeiro workshop, and to IUPAC, NAS, ABC and SBQ.

(b) The workshop produced valuable inputs on technologies with potential applications to non-routine verification, and assistance and protection activities. The outcomes will inform recommendations to the Fourth Review Conference.

(c) The outcomes of the workshop were also presented to States Parties in a "Science for Diplomats" event in the margins of the Eighty-Sixth Session of the Council.[103]

---

[103] Materials from this briefing are available at: www.opcw.org/fileadmin/OPCW/Science_Technology/Diplomats_Programme/20171010_Science_Diplomats_Emerging_Tech-Introduction.pdf (introduction) and www.opcw.org/fileadmin/OPCW/Science_Technology/Diplomats_Programme/20171010_Science_Diplomats_Emerging_Tech_Presentation.pdf (briefing).

9.14 The following proposals derived from the report of the Rio de Janeiro workshop, specifically subparagraphs (a), (b), (c), (e), (g) and (h) from 9.13 above, are put forward as recommendations of the SAB at its Twenty-Sixth Session:

(a) See subparagraph 8.6(b) that reflects common findings from across the SAB's scientific review workshop series in 2016 and 2017.

(b) In reviewing the diversity of developments across scientific communities, understanding where developments find application and recognising where these technological changes intersect with the Convention, the SAB has benefited from the practice of engaging operational staff from the Secretariat. In the view of the SAB, this practice strengthens the formulation of science advice to the OPCW. A similar approach would provide benefit in other Convention-relevant fora where proposals are drafted and considered.

(c) A broad set of innovative technologies are being developed that can potentially find application in some areas of implementation of the Convention, especially for non-routine situations, enhancement of sampling and analysis capabilities, and reducing risks to personnel operating in dangerous environments. The Secretariat may wish to consider engagement with technology developers as well as outreach strategies, such as crowd source competitions to gain access to innovative technologies and ideas that can be field tested. Benefits include raising awareness of the Convention across scientific communities, opportunities to provide feedback to technology developers on how their tools perform under field conditions, and a mechanism for the Secretariat to keep pace with technological change. This recommendation was further informed by paragraphs 9.5 and 9.6, 9.15 and 9.16, 10.1 through 10.8, and 11.10 and 11.11; and subparagraphs 8.4(c) and 8.4(d).

(d) In regard to the possibility of field testing, an inventory of available innovative tools that could be field tested would be useful for the Secretariat to consider.

Subitem 9(e): Artificial intelligence and its potential application for chemical warfare agent verification

9.15 Ms Hoe Chee Chua provided an overview of how artificial intelligence (AI)[104,105] is being used in chemistry.[106] She noted that while the use of AI in chemistry dates back

---

[104] Cold fusion TV: What is Artificial Intelligence Exactly? July 2016; https://www.youtube.com/watch?v=kWmX3pd1f10

[105] Artificial intelligence and life in 2030; Stanford University; 2016. Available at: https://ai100.stanford.edu/2016-report

[106] Holy Grails for Computational Organic Chemistry and Biochemistry; K. N. Houk, F. Liu; *Acc. Chem. Res.*, 2017, *50(3)*, 539–543. DOI: 10.1021/acs.accounts.6b00532.

to the 1950s,[107] it has been the more recent incorporation of deep convolutional neural network architecture into classical AI architecture that has enabled capabilities with potential application to chemical verification. Capabilities include exploring scientific literature,[108] assessing chemical properties and applications,[109] ADME-Tox prediction,[110] chemical discovery[111] and designing chemical synthesis routes.[112] Ms Chua described a variety of uses for AI in chemistry, and the how such capabilities can be accessed through commercially available tools such as Molgen[113] and Chematica.[114]

9.16 In the subsequent discussion, the following points were raised:

(a) AI tools and capabilities are becoming more and more accessible.[115] The hurdles to their adoption include access to adequate training datasets and their validation.

---

107 For examples from the 1970s and 1980s, see: (a) Dendral and meta-dendral-the myth and the reality; N. A. B. Gray; *Chem. Intell. Lab. Sys*; 1988, *5*, 11–32; (b) Further development of structure generation in the automated structure elucidation system chemicals, K. Funatsu, N. Miyabayaski, S. Sasaki*; J. Chem, Inf. Comput. Sci*.; 1988, *28*, 18–28; (c) A computer program for generation of constitutionally isomeric structural formulas; H. Abe, T. Okuyama, I. Fujiwara, S. Sasaki; *J. Chem. Inf. Comput. Sci*; 1984, *24*, 220–229; (d) GENOA: A computer program for structure elucidation utilizing overlapping and alternative substructures; R. E. Carhart, D. H. Smith, N. A. Gray, J. G. Nourse, C. Djerassi; *J. Org. Chem*; 1981, *4*, 1708-1718; (e) Chemics-UBE, A Modified System of Chemica; T. Oshima, Y. shida, K. Saito, S, Sasaki; *Anal. Chim. Acta*; 1980, *122*, 95–102; (f) Application of artificial intelligence for chemical inference. XVII. an approach to computer-assisted elucidation of molecular structure; R. E. Carhart, D. H. Smith, H. Brown, C. Djerassi; *J. Am. Chem. Soc*; 1975, *97*, 5755–5762; and (g) Applications of artificial intelligence of chemical inference. XII. Exhaustive generation of cyclic and acyclic isomers; L. M. Masinter, N. S. Scridharan, J. Lederberg, D. H. Smith; *J. Am. Chem. Soc.*; 1974, *96*, 7702–7714.

108 See for example: (a) The Arxiv Sanity Preserver, http://www.arxiv-sanity.com/ and (b) Iris.AI, https://the.iris.ai/

109 The architecture and evolution of organic chemistry; M. Fialkowski, K. J. M. Bishop, V. Chubukov, C. J. Campbell, B. A. Grzybowski; *Chematica*; 2005, *44*, 7263. DOI: 10.1002/anie.200502272.

110 ADME-Tox: absorption, distribution, metabolism, excretion and toxicity of xenobiotics. See for example: Applying machine learning techniques for ADME-Tox prediction: a review; V. G. Maltarollo, J. C. Gertrudes, P. R. Oliveira, K. M. Honorio; *Expert Opinion on Drug Metabolism Toxicology*; 2015, *11*, 259–271. DOI: 10.1517/17425255.2015.980814.

111 The drug-maker's guide to the galaxy: How machine learning and big data are helping chemists search the vast chemical universe for better medicines; A. Mullard; *Nature*, 2017, *549*, 445–447. DOI: 10.1038/549445a.

112 Learning to plan chemical syntheses; M. H. S. Segler, M. Preuss, M. P. Waller; available as a pre-print, 2017, arXiv:1708.04202v1.

113 Molgen 5.0, a molecular structure generator; G. Ralf, K. Adalbert, K. Axel, L. Reinhard, M, Markus, R. Christoph, R. W. Alfred; *Advances in Mathematical Chemistry and Applications*; 2014, 113–138. DOI: 10.2174/9781608059287114010010.

114 Chematica: computer aided solutions for your synthetic challenges; Merck KGaA, http://chematica.net/#/

115 Developers providing access to their AI tools include: Amazon Web Services, https://aws.amazon.com/amazon-ai/ Facebook Open Source, https://code.facebook.com/projects/ Google.ai, https://ai.google/tools/ IBM Analytics, https://www.ibm.com/analytics/us/en/technology/open-source/ and Microsoft AI, https://www.microsoft.com/en-us/ai/ai-platform

(b) Noting that the development of reliable AI tools is non-trivial, it was suggested to look to university partners, designated laboratories, or commercial providers to enable the development of useful capabilities.

(c) AI technologies have potential for automating workflows and helping recognise unusual features in the information. Developments in the area for chemical applications should continue to be monitored in the Secretariat's science review activities.

(d) The dual-use potential of AI analysis and design for providing access to chemical synthesis routes for toxic chemicals was noted.

(e) Capabilities of AI tools versus those of a well-trained organic chemist in retrosynthetic analysis was discussed. Developments in this area would usefully be monitored.

10. AGENDA ITEM TEN – Developments in science and technology

Subitem 10(a): Wearable sensors and nanomotor-based accelerated decontamination of chemical warfare agents

10.1 Professor Joseph Wang (guest speaker, University of California San Diego, United States of America) provided the Board with a review of recent advances in synthetic micro/nanomachines[116] that have opened new horizons for addressing environmental[117] and security problems.[118] Professor Wang highlighted the opportunities and challenges in translating this remarkable progress in nanomotor technology toward practical applications, covering various environmental and defence areas that would benefit from such developments, with a focus on nanomachine-based accelerated degradation and 'on-the-fly' detoxification of chemical warfare agents[119] and removal of major contaminants. This accelerated remediation was illustrated in connection to a variety of self-propelled reactive materials, involving a variety of purification processes. The examples included new mobile reactive materials based on

---

116 *Nanomachines: Fundamentals and Applications*; J. Wang; Wiley-VCH; 2013, ISBN: 978-3-527-33120-8.

117 (a) The environmental impact of micro/nanomachines: a review; W. Gao, J. Wang; *ACS Nano*; 2017, *8(4),* 3170–3180. DOI: 10.1021/nn500077a. (b) Efficient biocatalytic degradation of pollutants by enzyme-releasing self-propelled motors; J. Orozco, D. Vilela, G. V. Ramírez, Y. Fedorak, A. Escarpa, R. V. Duhalt, J. Wang; *ChemPubSoc Europe*; 2014, *20(10),* 2866–2871. DOI: 10.1002/chem.201304179. (c) Superhydrophobic alkanethiol-coated microsubmarines for effective removal of oil; M. Guix, J. Orozco, M. García, W. Gao, S. Sattayasamitsathit, A. Merkoçi, A. Escarpa, J. Wang; *ACS Nano*; 2012, *6(5)*, 4445–4451. DOI: 10.1021/nn301175b.

118 Nano/micromotors for security/defense applications: a review; V. V. Singh, J. Wang; *Nanoscale*; 2015, *7(46)*, 19377-19389. DOI: 10.1039/c5nr06254c.

119 (a) Water-driven micromotors for rapid photocatalytic degradation of biological and chemical warfare agents; J. Li, V. V. Singh, S. Sattayasamitsathit, J. Orozco, K. Kaufmann, R. Dong, W. Gao, B. J. Sanchez, Y. Fedorak, J. Wang; *ACS Nano*; 2014, *8(11),* 11118–11125. DOI: 10.1021/nn505029k; and (b) Micromotor-based high-yielding fast oxidative detoxification of chemical threats; Orozco, Jahir, Cheng, Guanzhi, Vilela, Sattayasamitsathit, Sirilak, V. Duhalt, Rafael, V. Ramírez, Gabriela, S. Pak, On, Escarpa, Alberto, Kan, Chengyou, Wang, Joseph; *Angewandte Chemie*; 2013, *52*. DOI: 10.1002/anie.201308072.

zeolite[120] or activated carbon.[121] Professor Wang explained that the propulsion of micromotors and their corresponding bubble tails impart significant mixing that greatly accelerate the detoxification processes reflecting the continuous motion of micro/nanoscale reactive remediation platforms and the corresponding fluid transport.[122] He also discussed future operations of autonomous intelligent multi-functional nanomachines, monitoring and responding to hazardous chemicals (in a 'sense and destroy' mode') and using bio-inspired chemotactic search strategies to trace chemical plumes to their source.[123] Drug delivery applications have also been demonstrated.[124] Professor Wang suggested that with continuous innovations we could expect that man-made nano/microscale motors will have profound impact upon detoxification of chemical weapon agents, and defence applications, in general. Dr Wang also introduced wearable devices that can detect certain types of chemicals and are integrated with mobile devices to provide real time readouts;[125] including wearable sensors that can detect organophosphorus compounds (specifically pesticides and, potentially, nerve agents).[126]

---

120 Multifunctional silver-exchanged zeolite micromotors for catalytic detoxification of chemical and biological threats; V. V. Singh, B. J. Sánchez, S. Sattayasamitsathit, J. Orozco, J. Li, M. Galarnyk, Y. Fedorak, J. Wang; *Advanced Functional Materials*; 2015, *25(14),* 2147–2155. DOI: 10.1002/adfm.201500033.

121 Self-propelled activated carbon Janus micromotors for efficient water purification; J. Sánchez, S. Sattayasamitsathit, W. Gao, L. Santos, Y. Fedorak, V. V. Singh, J. Orozco, M. Galarnyk, J. Wang; *Small*; 2015, *11(4)*, 499–506. DOI:10.1002/smll.201402215.

122 (a) Bubble-propelled micromotors for enhanced transport of passive tracers; J. Orozco, B. J. Sánchez, G. Wagner, W. Gao, R. V. Duhalt, S. Sattayasamitsathit, M. Galarnyk, A. Cortés, D. Saintillan, J. Wang; *Langmuir*; 2014, *30(18),* 5082–5087. DOI: 10.1021/la500819r. (b) Efficient bubble propulsion of polymer-based microengines in real-life environments; W. Gao, S. Sattayasamitsathit, J. Orozco, J. Wang; *Nanoscale*; 2013, *5*, 8909-8914. DOI: 10.1039/C3NR03254J.

123 (a) Aptamer-modified graphene-based catalytic micromotors: off-on fluorescent detection of ricin; B. E. F. Ávila, M. A. Lopez-Ramirez, D. F. Báez, A. Jodra, V. V. Singh, K. Kaufmann, J. Wang; *ACS Sens*.; 2016, *1(3),* 217–221. DOI: 10.1021/acssensors.5b00300. (b) Lysozyme-based antibacterial nanomotors; M. Kiristi, V. V. Singh, B. E. F. Ávila, M. Uygun, F. Soto, D. A. Uygun, J. Wang; *ACS Nano*; 2015, *9(9),* 9252–9259 DOI: 10.1021/acsnano.5b04142. (c) Dual-enzyme natural motors incorporating decontamination and propulsion capabilities; S. Sattayasamitsathit, K. Kaufmann, M. Galarnyk, R. V. Duhaltb, J. Wang; *RSC Adv*.; 2014, *4*, 27565-27570. DOI: 10.1039/C4RA04341C. (d) Artificial enzyme-powered microfish for water-quality testing; J. Orozco, V. G. Gradilla, M. D'Agostino, W. Gao, A. Cortés, J. Wang; *ACS Nano*; 2013, *7(1),* 818–824. DOI: 10.1021/nn305372n.

124 Micromotor-enabled active drug delivery for in vivo treatment of stomach infection; B. E. F. Ávila, P. Angsantikul, J. Li, M. A. L. Ramirez, D. E. R. Herrera, S. Thamphiwatana, C. Chen, J. Delezuk, R. Samakapiruk, V. Ramez, L. Zhang, Jo. Wang; *Nature Communications*; 2017, *8,* 272. DOI: 10.1038/s41467-017-00309-w.

125 (a) Eyeglasses based wireless electrolyte and metabolite sensor platform; J. R. Sempionatto, T. Nakagawa, A. Pavinatto, S. T. Mensah, S. Imani, P. Merciera, J. Wang; *Lab Chip*; 2017, *17,* 1834-1842. DOI: 10.1039/C7LC00192D. (b) Wearable chemical sensors: present challenges and future prospects; A. J. Bandodkar, I. Jeerapan, J. Wang; *ACS Sens*.; 2016, *1*, 464−482. 2016, 7, DOI: 10.1021/acssensors.6b00250.

126 (a) Wearable ring-based sensing platform for detecting chemical threats; J. R. Sempionatto, R. K. Mishra, A. Martín, G. Tang, T. Nakagawa, X. Lu, A. S. Campbell, K. M. Lyu, J. Wang; *ACS Sens*.; 2017. DOI: 10.1021/acssensors.7b00603. (b) Wearable flexible and stretchable glove biosensor for on-site detection of organophosphorus chemical threats; R. K. Mishra, L. J. Hubble, A. Martín, R. Kumar, A. Barfidokht, J. Kim, Mu. M. Musameh, I. L. Kyratzis, J. Wang; *ACS Sens*.; 2017, *2(4)*, 553-561. DOI: 10.1021/acssensors.7b00051.

10.2 In the subsequent discussion, the following points were raised:

(a) The SAB expressed its appreciation to Professor Wang for his inspiring presentation. There are many applications in detoxification advances on the horizon.

(b) In regard to detoxification of large biological molecules, it was noted that microscale molecular motors are more efficient than nanoscale motors.

(c) The use of zinc and magnesium in the self-propelled motor systems allows for materials that self-decompose after detoxification. The metals ultimately dissolve in media such as ocean water in environmental clean-up applications or the gastrointestinal tract for drug delivery applications, and the degradation products do not pose a risk to either environmental or human health respectively.

(d) Availability of the technologies described by Professor Wang was discussed. Wearable technologies already exist. For such devices, biomarker recognition and chemical specificity beyond ion-specific electrode technologies have limitations, yet the ability to collect data streams and recognise unusual signals can be powerful in monitoring health.[127] Micromotors, however, are an area of research and there are no current commercial products.

Subitem 10(b): NanoContraChem: from the design to the development of nanostructured clays and oxides for the catalytic decontamination of chemical warfare agents

10.3 Professor Matteo Guidotti (guest speaker, Institute of Molecular Sciences and Technologies, ISTM-CNR, Milan, Italy and Academy of Sciences of the Institute of Bologna, Italy) provided an overview of the "NanoContraChem",[128] a project supported by the NATO Science for Peace and Security Programme.[129]

10.4 Professor Guidotti noted that the degradation of highly hazardous chemical and biological warfare agents typically relies on the use of strong oxidants with high environmental impact or on thermal abatement under harsh conditions.[130] He described the developments of two new classes of chlorine-free catalytically active sorbent solids which can promote the oxidative sorption and degradation of toxic organosulfur and organophosphorus chemical warfare agents into non-toxic products. These materials can also destroy biological warfare agents.

---

127 Digital health: tracking physiomes and activity using wearable biosensors reveals useful health-related information; X. Li, J. Dunn, D. Salins, G. Zhou, W. Zhou, M. S. Rose, D. Perelman, E. Colbert, R. Runge, S. Rego, R. Sonecha, S. Datta, T. McLaughlin, M. P. Snyder; *PLoS Biol.*; 2017, *15(1)*: e2001402. DOI: 10.1371/journal.pbio.2001402.

128 NanoContraChem: Nanostructured Materials for the Catalytic Decontamination of Chemical Warfare Agents, Project 984481. For additional information see: http://www.spsnanocontrachem.org/

129 For additional information on the NATO Science for Peace and Security Programme, see: http://www.nato.int/cps/en/natolive/78209.htm

130 Destruction and detection of chemical warfare agents; K. Kim, O. G. Tsay, D. A. Atwood, D. G. Churchill; *Chem. Rev.*; 2011, *111(9),* 5345–5403. DOI: 10.1021/cr100193y.

10.5 Transition metal-containing phyllosilicate clays have been identified as catalysts for the oxidative abatement of chemical and biological warfare agents in the presence of in situ produced hydrogen peroxide (H_2O_2), as an oxidant. These materials can be developed into bifunctional catalytic-sorbent solids, able to enhance the oxidising capability of H_2O_2 and to show a marked acid character.[131] Analogously, metal oxide materials with different chemical compositions, textural morphology and porosity can be prepared and Professor Guidotti described their testing under mild decontamination conditions.[132,133]

10.6 The performance of clay materials (Nb-saponite and Fe-montmorillonite) and inorganic oxides (Nb_2O_5, TiO_2, γ-Al_2O_3 and WO_3)[134] were evaluated at room temperature in the oxidative degradation of (2-chloroethyl)ethyl sulfide (CEES)[135] and dimethyl methylphosphonate (DMMP), simulants for sulfur mustard and nerve agents, respectively, with solid oxidants able to release H_2O_2 in situ. The impact on living microorganisms was also evaluated through biotoxicity testing on bioluminescent bacteria (*Photobacterium leiognathi Sh1*).[136] The toxicological effect on the environment was assessed with specific tests on vegetation.[137]

10.7 Fe-montmorillonite, Nb-saponite, Nb_2O_5 and WO_3, in the presence of H_2O_2, sodium perborate or sodium percarbonate displayed interesting results in terms of decontamination activity and selectivity to non-noxious degradation products. The most promising and innovative formulations were compared with a conventional decontamination powder (Italian Armed Forces M75) and tested on samples of genuine sulfur mustard agents. The powder formulations have been loaded in prototypal on-field portable spraying devices and incorporated into a glove for immediate personal decontamination. These decontamination tools were developed for professionals who may be operating in high-risk emergency contaminated scenarios (e.g. first responders, armed forces, and police).

---

131 Niobium(V) saponite clay for the catalytic oxidative abatement of chemical warfare agents; F. Carniato, C. Bisio, R. Psaro, L. Marchese, M. Guidotti; *Angew. Chem.*, 2014, *53*, 10095–10098. DOI: 10.1002/anie.201405134.

132 Nanosized inorganic metal oxides as heterogeneous catalysts for the degradation of chemical warfare agents; C. Bisio, F. Carniato, C. Palumbo, S. L. Safronyuk, M. Starodub, A. Katsev, L. Marchese, M. Guidotti; *Catal. Today*; 2016, *277*, 192–199. DOI: 10.1016/j.cattod.2015.12.023.

133 Tungsten oxide: a catalyst worth studying for the abatement and decontamination of chemical warfare agents; D. Costenaro, C. Bisio, F. Carniato, A. M. Katsev, S. L. Safronyuk, N. Starodub, C. Tiozzo, M. Guidotti; *Global Security: Health, Sci. Policy*; 2017, 1–14. DOI: 10.1080/23779497.2017.1330662.

134 Nanosized inorganic metal oxides as heterogeneous catalysts for the degradation of chemical warfare agents; C. Bisio, F. Carniato, C. Palumbo, S. L. Safronyuk, M. F. Starodub, A. M. Katsev, L. Marchese, M. Guidotti; *Catalysis Today*; 2016, *277(1),* 192–199. DOI: 10.1016/j.cattod.2015.12.023.

135 Catalytic aerobic oxidation of 2-chloroethyl ethylsulfide, a mustard simulant, under ambient conditions: effect of solvents, ligands, and transition metals on reactivity; E. Boring, V. Yurii, Geletii, C. L. Hill; *J. Mol. Catal. A: Chem.*; 2001, *176*, 49. DOI: 10.1016/S1381-1169(01)00246-1.

136 Nanomaterials: biological effects and some aspects of applications in ecology and agriculture; N. F. Starodub, K. E. Shavanova, M. V. Taran, A. M. Katsev, R. V. Son'ko, C. Bisio, M. Guidotti; *Proc. SPIE*; 2014, *9421*, 942106-1 - 942106-14. DOI: 10.1117/12.2081468.

137 Physico-chemical properties, biological and environmental impact of Nb-saponite catalysts for the oxidative degradation of chemical warfare agents; D. Costenaro, C. Bisio, F. Carniato, S. L. Safronyuk, T. V. Kramar, M. V. Taran, M. F. Starodub, A. M. Katsev, M. Guidotti; *Global Security: Health, Sci. Policy*; 2017. DOI: 10.1080/23779497.2017.1330662.

10.8 In the subsequent discussion, the following points were raised:

(a) The SAB expressed its appreciation to Professor Guidotti for his presentation, pointing out that it presented a view of technology development and field testing that nicely complemented Professor Wang's work on researching new types of systems for detoxification.

(b) Decontaminants for use by first responders should, ideally, be easy to deploy, versatile, cost effective and environmentally benign after neutralisation of toxic materials. In this regard catalytic methods are important to consider.

(c) The NanoContraChem products are envisioned for direct use on contaminated protective suits and materials.

11. AGENDA ITEM ELEVEN – Chemical forensics and investigative technologies

Subitem 11(a): Updates on formation of a temporary working group on investigative science and technology

11.1 Veronica Borrett (Chairperson of the TWG on investigative science and technology) briefed the Board on the formation of the TWG. Dr Borrett recalled that lessons learned from contingency operations, such as the OPCW Fact-Finding Mission in the Syrian Arab Republic,[138] highlighted the need for continued broad engagement and evaluation of technologies and methods (both current and emerging) relevant to the verification regime. In response, the SAB co-organised the first of its science review workshop series together with VERIFIN. The workshop "Chemical Forensics: Capabilities across the Field and the Potential Applications in CWC Implementation" was held in Helsinki from 20 to 22 June 2016.[139] In the workshop report (SAB-24/WP.1, dated 14 July 2016[140]), the SAB recommended that additional workshops or a TWG be considered to strengthen the understanding of technologies, procedures and capabilities that forensics can bring to investigations. The SAB also highlighted the importance of engagement with forensic experts, forensic practitioners and OPCW inspectors and laboratories, to explore methods and capabilities relevant to the verification of the Convention. The Director-General, in his response to the Report of the Twenty-Fourth Session of the Scientific Advisory Board (EC-84/DG.9,

---

138 (a) R. Trapp. Lessons Learned from the OPCW Mission in Syria, 2015. www.opcw.org/fileadmin/OPCW/PDF/Lessons_learned_from_the_OPCW_Mission_in_Syria.pdf (b) The Secretary-General's Mechanism for Investigation of Alleged Use of Chemical, Bacteriological (Biological) or Toxin Weapons: a lessons-learned exercise for the United Nations Mission in the Syrian Arab Republic; United Nations Office of Disarmament Affairs, May 2015. https://www.un.org/disarmament/publications/more/syrian-ll-report/ (c) Workshop on the Lessons Learned from the International Maritime Operation to Remove and Transport the Syrian Chemical Materials in Furtherance of Security Council Resolution 2118 (2013) and Relevant OPCW Executive Council Decisions; United Nations office of Disarmament Affairs, March 2015. https://unoda-web.s3-accelerate.amazonaws.com/wp-content/uploads/2015/05/proceedings-maritime-public.pdf

139 See also: www.opcw.org/news/article/scientists-review-the-science-of-chemical-forensics-and-potential-applications-in-chemical-weapons-investigations/

140 Report of the Scientific Advisory Board's Workshop on Chemical Forensics (SAB-24/WP.1). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/sab24wp01_e_.pdf

dated 18 January 2017[141]) requested that the SAB establish a TWG on investigative science and technology.

11.2 Dr Borrett updated the Board on the TWG membership and discussed the programme of work of the TWG. The TWG has an objective “to review the science and technology relevant to investigative work, especially for the validation and provenancing (determining the chronology of ownership, custody and/or location) of evidence, and the integration of multiple and diverse inputs to reconstruct a past event”.[142] The terms of reference contains eleven questions related to this objective for the TWG to address.[143] Dr Borrett suggested that these questions be grouped under related themes that may include forensic methods and capabilities; data collection and management; sampling, detection and analysis; integrity of scene and evidence collection; and provenance to assist with the work of the TWG. The first meeting will be held from 12 to 14 February 2018.

11.3 In the subsequent discussion, the following points were raised:

(a) The SAB recognised forensic science as an example of a highly transdisciplinary area. Noting that the methods used go beyond chemistry, with chemical forensics being one source of data that in a forensic context must be linked with other inputs for provenancing.

(b) It was recognised that investigative science and technology provides useful opportunities to identify new tools and capabilities relevant to verification. In particular, technologies for authentication of documents and digital media may be important.

(c) The SAB noted the importance of bringing operational members of both the Secretariat and forensic community to brief the TWG at its first meeting.

Subitem 11(b): Recent engagement with forensic science experts

11.4 Dr Borrett reported on a two-day symposium on chemical forensics,[144] followed by a workshop to establish the Chemical Forensics International Technical Working Group (CFITWG) held in San Francisco, California, at the 253rd National Meeting of the ACS in April 2017. The events were organised by the Pacific Northwest National Laboratory (PNNL)[145] with support from the ACS, the United States Department of State, and the ACC.[146] Several SAB members and staff from the Secretariat participated and provided presentations. The objectives of the workshop were to: collaborate with different analytical (chemistry) forensic communities to share

---

141 Available at: www.opcw.org/fileadmin/OPCW/EC/84/en/ec84dg09_e_.pdf

142 The terms of reference can be found in Annex 2 of: The Report of: the Scientific Advisory Board at its Twenty-Fifth Session (SAB-25/1*, dated 31 March 2017). Available at: https://www.opcw.org/fileadmin/OPCW/SAB/en/sab2501_e_.pdf

143 A summary of the questions from the TWG’s terms of reference is available at: www.opcw.org/fileadmin/OPCW/SAB/en/TWG_Investigative_Science_Tech_Questions.pdf

144 See https://cbrnecentral.com/pnnl-spotlights-chemical-forensics-cw-counternarcotics/10651/

145 For more information on PNNL, see: https://www.pnnl.gov/

146 For more information on ACC, see: https://www.americanchemistry.com/

commonalities and lessons learned; identify general gaps and needs that can be addressed as a whole or those that need to be addressed by one community; explore ways to organise, share and collaborate in research efforts to address gaps in chemical forensics capability, access to chemicals, data and information to strengthen chemical forensics outcomes; and to discuss standardisation of chemical forensics approaches across communities. The workshop was attended by 49 experts from seven States Parties, representing a wide range of expertise. The outcome of the workshop was the establishment of the CFITWG[147] which was modelled on the Nuclear Forensics International Technical Working Group (ITWG).[148] The CFITWG intends to hold its second meeting at an ACS National Meeting in August 2018.

11.5 Dr Christopher Timperley described his engagement with the Scientific Advisory Board of the Office of the Prosecutor (the OTP SAB) of the International Criminal Court (ICC). He reported on their fourth annual meeting held on 22 and 23 June, where as an observer to the meeting, he briefed the OTP SAB on the role and scientific accomplishments of the OPCW's SAB.

11.6 The OTP SAB was established in 2014, to provide recommendation to the ICC Prosecutor on the most recent developments in new and emerging technologies and scientific methods and procedures that can reinforce the capabilities of the Office in the collection, management and analysis of scientific evidence relating to the investigation and prosecution of genocide, crimes against humanity and war crimes. Adapting the Office's investigative and prosecutorial capabilities and networks to the rapidly changing scientific and technological environment in which it operates is a strategic goal set by the Prosecutor. The contribution of the OTP SAB is crucial to the work of the Office in honing scientific standards governing operations and to the Office's duty to guaranteeing that the evidence presented to the Court's judges is credible and reliable.

11.7 To date, the OTP-SAB has reviewed and certified five standard operating procedures (SOPs) of the Office relating to, amongst others, human remains recovery, autopsies, forensic clinical examinations, as well as crime scene examination. During this year's meeting of the OTP SAB, two additional procedures for the handling of medical information and the use of remote sensing evidence were reviewed and another four SOPs are currently under examination by this Board. At the June meeting, the OTP SAB concluded that it should continue to promote the forensic work already done through its respective organisations and networks; it intends to publish its SOPs in international scientific journals in the near future.

11.8 Eighteen forensics organisations are currently represented on the OTP SAB: the Academia Ibero-americana de Criminalística y Estudios Forenses: the African Society of Forensic Medicine; the Australian and New Zealand Forensic Science Society;[149] the European Council of Legal Medicine;[150] the European Network of Forensic

---

147 Chemical Forensics International Working Group, Inaugural Workshop Report, 5 April 2017.

148 For additional information on the ITWG, see: http://www.nf-itwg.org/

149 For additional information on the Australian and New Zealand Forensic Science Society, see: http://anzfss.org/

150 For additional information on the European Council of Legal Medicine, see: http://www.eclm.info/

Science Institutes;[151] the Ibero-american Network of Forensic Medicine and Forensic Science Institutions; the International Association of Forensic Sciences; [152] EUROPOL/European Cybercrime Centre;[153] the International Academy of Legal Medicine;[154] International Forensic Strategy Alliance;[155] INTERPOL/Global Complex for Innovation;[156] INTERPOL/International Forensic Science Managers Symposium;[157] the Indo-Pacific Association of Law, Medicine and Science;[158] the New Mediterranean Academy of Forensic Sciences; the Arab Union of Forensics and Toxicology;[159] the Southern Africa Regional Forensic Science Network; the United Nations Institute for Training and Research (UNITAR/UNOSAT);[160] and the World Association for Medical Law.[161]

11.9 In the subsequent discussion, the following points were raised:

(a) The OPCW SAB and the OPCW TWG on investigative science and technology will benefit from continued engagement with the CFITWG and forensic organisations such as those represented within the OTP SAB. These networks represent international cooperative groups of experts who share best practices.

(b) Within the forensic science networks, there is recognition of the value of independent peer-reviewed scientific publications. The acceptance by scientific communities of the validity of methods helps to establish credibility of methodologies applied in legal settings. A collection of papers from CFITWG members who presented in the San Francisco symposia will be published in a special edition of the peer-reviewed scientific journal *Talanta*,[162] as a means to share methodologies and experiences. The SAB

---

151 For additional information on the European Network of Forensic Science Institutes, see: http://enfsi.eu/

152 For additional information on the International Association of Forensic Sciences, see: http://ialfs.org/

153 For additional information on EUROPOL/European Cybercrime Centre, see: https://www.europol.europa.eu/about-europol/european-cybercrime-centre-ec3

154 For additional information on the International Academy of Legal Medicine, see: http://www.ialm.info/

155 For additional information on the International Forensic Strategy Alliance, see: http://www.ifsa-forensics.org/

156 For additional information on INTERPOL/Global Complex for Innovation, see: https://www.interpol.int/About-INTERPOL/The-INTERPOL-Global-Complex-for-Innovation

157 For additional information on INTERPOL/International Forensic Science Managers Symposium, see: https://www.interpol.int/INTERPOL-expertise/Forensics/Forensic-Symposium

158 For additional information on the Indo-Pacific Association of Law, Medicine and Science, see: http://inpalms.tripod.com/

159 For additional information on the Arab Union of Forensics and Toxicology, see: http://auft-arab.org/

160 For additional information on UNITAR/UNOSAT, see: https://unitar.org/unosat/

161 For additional information on the World Association for Medical Law, see: http://wafml.memberlodge.org/

162 *Talanta*, the International Journal of Pure and Applied Analytical Chemistry. For additional information see: https://www.journals.elsevier.com/talanta

could usefully take this as an opportunity to publish its sample storage[163] and chemical forensic workshop reports (see also paragraph 6.3).

(c) The SOPs being developed by the OTP SAB are relevant to the work of the OPCW TWG on investigative science and technology, especially in allegations-of-use fact-finding and contingency operations involving non-routine implementation of the Convention.

Subitem 11(c): Computer-aided engineering tools

11.10 Dr Evandro Nogueira discussed the potential applications of computer-aided engineering (CAE) tools for the implementation of the Convention, discussing relevant applications for assistance and protection, international cooperation and verification. Dr Nogueira discussed the use of CAE simulations for predictive value, noting how the geometry, meshing, numerical settings, turbulence models and previous modelling of physical and chemical phenomena can influence the outcomes. He further described limitations to the use of models and their interpretation. He noted that in recent years, these tools have been finding use across in a variety of sectors, including innovation,[164] chemical engineering education,[165] product development and improvement,[166] chemical emergency response,[167] chemical reactor design,[168] and

---

163 Response to the Director-General's Request to the Scientific Advisory Board to Provide Further Advice on Chemical Weapons Sample Stability and Storage (SAB-23/WP.2, dated 25 May 2016). Available at: www.opcw.org/fileadmin/OPCW/SAB/en/sab-23-wp02_e_.pdf

164 Open computer aided innovation to promote innovation in process engineering; R. L. Floresa, J. P. Belaud, S. Negnya, J. M. L. Lanna, *Chemical Engineering Research and Design*; 2015, *103,* 90–107. DOI: 10.1016/j.cherd.2015.08.015.

165 Towards outcomes-based education of computer-aided chemical engineering; Z. N. Pintarič, Z. Kravanja; *Journal of Food Engineering;* 2016, *38*, 2367–2372. DOI: 10.1016/B978-0-444-63428-3.50399-4.

166 (a) Toward computer-aided food engineering: mechanistic frameworks for evolution of product, quality and safety during processing; A. K. Datta; *Computer Aided Chemical Engineering*; 2016, *176*, 09–27. DOI: 10.1016/j.jfoodeng.2015.10.010. (b) Challenges and opportunities in computer-aided molecular design; L. Y. Ng, F. K. Chong, G. Nishanth; *Computers and Chemical Engineering*; 2015, *81*, 115-129, DOI: 10.1016/j.compchemeng.2015.03.009.

167 (a) Multiphase computational fluid dynamics simulation as a tool for planning emergencies with chemical agents; I. V. M. Barbosa, J. C. C. Pinto, E. S. Nogueira*; Revista Virtual de Química*; 2014, 6, 795-814. DOI: 10.5935/1984-6835.20140048. (b) CFD dispersion modelling for emergency preparadness; M. Kisˇa, L. Jelemensky; *Journal of Loss Prevention in the Process Industries*; 2009, 97–104. DOI: 10.1016/j.jlp.2008.09.013 (c) Quantitative risk analysis of toxic gas release caused poisoning—A CFD and dose–response model combined approach; B. Zhang , G. M. Chen, *Process Safety and Environmental Protection*; 2010, *88*, 253–262. DOI: 10.1016/j.psep.2010.03.003.

168 (a) Particle responses to flow field oscillations in heterogeneous polymerizations performed in tank reactors; W. M. Poubel; C. E. F. C. Silva, E. N. Souza, J. C. Pinto; *Macromolecular Reaction Engineering,* 2013, *8*, 374–391. DOI: 10.1002/mren.201300142. (b) Analysis of energy dissipation in stirred suspension polymerisation reactors using computational fluid dynamics; E. S. Nogueira, J. C. Pinto, A. S. Vianna. *Canadian Journal of Chemical Engineering*; 2012, *90*, 983–995. DOI: 10.1002/cjce.20611. (c) An experimental and CFD study of liquid jet injection into a partially baffled mixing vessel: a contribution to process safety by improving the quenching; J. P. Torré, D. F. Fletcherb, T. Lasuyec, C. Xuereba; *Chemical Engineering Science*; 2008, *63*, 924–942. DOI: 10.1016/j.psep.2010.03.003.

medical countermeasure design.[169] Two cases studies were presented as examples relevant to non-routine verification activities related to the alleged use of toxic chemicals. The first example used computational fluid dynamics (CFD) to model a large scale chlorine release with validation by experimental data;[170] this example demonstrated the predictive value of CFD models. In the second example, Dr Nogueira looked at the influence of meshing size and two-dimensional approaches for a CAE study that used meteorological forecasting models and data to determine the influence of atmospheric factors on the dispersion of a chemical plume.[171] Both of the studies presented by Dr Nogueira were performed using free open access CAE tools.[172]

11.11 In the subsequent discussion, it was noted that CAE tools can provide valuable information in evaluation of the impact of a toxic chemicals release, having the ability to develop models that can reproduce experimental data. However, the use of such methods requires deep knowledge of chemical and physical behaviour, and numerical methods. Oversimplifying or overfitting models can limit their utility. In this regard, the limitations of the models should always be considered.

12. AGENDA ITEM TWELVE – Future work of the Scientific Advisory Board

Subitem 12(a): The road to the Fourth Review Conference

12.1 Mr Szymon Bochenski (Senior Policy Officer in the OPCW Office of Strategy and Policy) briefed the Board on the preparations for the Fourth Review Conference. He emphasised the strategic significance of the review process and pointed to paragraph 22 of Article VIII of the Convention, which stipulates that the review process should take into account developments in science and technology, underscoring the important contribution of the SAB report. Mr Bochenski also noted that in support of the preparatory work to the Fourth Review Conference, the Secretariat intends to submit a Note containing an overview of implementation of the Convention since the last review conference.

12.2 In the subsequent discussion, it was agreed that the SAB would be kept abreast of the modalities of holding the Fourth Review Conference as further information arises. The SAB Chairperson also intends to brief States Parties on the developments in science and technology report during the review conference.

---

169 (a) Structure of HI-6* sarin-acetylcholinesterase determined by X-ray crystallography and molecular dynamics simulation: reactivator mechanism and design; F. Ekström, A. Hörnberg, E. Artursson, L.-G. Hammarström, G. Schneider, Y.-P. Pang; *PLoS ONE*, 2009, *4(6)*, e5957. DOI: 10.1371/journal.pone.0005957. (b) Crystal structure of human butyrylcholinesterase and of its complexes with substrate and products; Y. Nicolet, O. Lockridge, P. Masson, J. C. Fontecilla-Camps, F. Nachon; *J. Biol. Chem.*; 2003, *278(42)*, 41141–41147. DOI: 10.1074/jbc.M210241200.

170 The Jack Rabbit chlorine release experiments: Implications of dense gas removal from a depression and downwind concentrations; S. Hannaa, R. Britter, E. Argenta, J. Chang; *Journal of Hazardous Materials*; 2012, *213–214*, 406–412. DOI: 10.1016/j.jhazmat.2012.02.013.

171 Assessment of the plume dispersion due to chemical attack on April 4, 2017, in Syria; K. Bhaganagar, S. R. Bhimireddy; *Nat. Hazards*; 2017, *88(3)*, 1893–1901. DOI: 10.1007/s11069-017-2936-x.

172 ANSYS® Student, http://www.ansys.com/nl-nl/academic/free-student-products

Subitem 12(b): Roadmap of the Scientific Advisory Board's work; Subitem 12(c): The Twenty-Seventh Session of the Scientific Advisory Board; and Subitem 12(d): The Scientific Advisory Board's recommendations to the Fourth Review Conference

12.3 The SAB discussed its future work. The Board will hold its Twenty-Seventh Session from 19 to 23 March 2018, ahead of the December 2018 Fourth Review Conference, and intends to hold a single session again in 2019, its Twenty-Eighth.

12.4 The SAB continued its discussion of the thematic topics for which individual members will provide content for the report to the Fourth Review Conference as described under agenda item 13 below.

12.5 The report on developments in science and technology would usefully be submitted to the Director-General at the Twenty-Seventh Session of the SAB, so that:

(a) States Parties will be able to take the SAB's advice into account when formulating national positions;

(b) States Parties will be able to discuss scientific and technological developments in preparation for the Fourth Review Conference; and

(c) The Secretariat will be able to take scientific and technological advice into account when making substantive proposals to the Fourth Review Conference.

12.6 Additionally, to encourage discourse on scientific and technological issues, the SAB will continue to hold briefings for States Parties and review its findings from the scientific review process in "Science for Diplomats" side events.[173] The SAB Chairperson will also consider briefing the Twenty-Second Session of the Conference of the States Parties in November of 2017.[174]

Subitem 12(e): Identification of key issues in science and technology

12.7 Dr Jonathan Forman updated the SAB on preparations being made for future work of the SAB, including proposals for crowd-sourcing challenge projects to collect useful scientific information and discussed horizon scanning and technology approaches that might also be considered (the latter, following on from the discussion at the SAB's Twenty-Fifth[175] Session). Projects based on these proposals would be considered after completion of the report to the Fourth Review Conference in mid-2018.

12.8 In the subsequent discussion, it was noted that the report to the Fourth Review Conference could usefully include in its introductory sections indications of trends and predictions identified in the SAB's report to the Third Review Conference that are no longer relevant or have continued along as forecast.

---

173 For information on the "Science for Diplomats" Initiative, see: www.opcw.org/special-sections/science-technology/science-for-diplomats/

174 For more information, visit: https://csp22.opcw.org/. Documents from the session will be available at: https://www.opcw.org/?id=2659

175 See paragraphs 13.5 through 13.7 of SAB-25/1. Available at: www.opcw.org/fileadmin/OPCW/SAB/en/sab2501_e_.pdf

13. AGENDA ITEM THIRTEEN – Inputs to the Scientific Advisory Board's report to the Fourth Review Conference

The members of the SAB met in subgroups to consider inputs for the report to the Fourth Review Conference. They reviewed materials already submitted by members of the SAB, and discussed key points that might be usefully captured in the executive summary. The SAB members will continue to work intersessionally in correspondence groups to complete the draft and prepare it for finalisation and adoption at the Twenty-Seventh Session of the SAB (see also paragraph 12.4).

14. AGENDA ITEM FOURTEEN – Any other business

14.1 The SAB Chairperson bade farewell to Dr Augustin Baulig, Professor Roberto Martínez Álvarez, Dr Koji Takeuchi and Professor Ferruccio Trifirò, whose terms of office on the SAB will come to a close before the next session of the Board. He thanked all of them for their commitment to the norms of the Conventions, and their distinguished service and substantive contributions to the SAB.

14.2 In the margins of the SAB's Twenty-Sixth Session, the SAB Chairperson and Vice-Chairperson briefed States Parties on 19 October,[176] presenting an overview of the activities of the SAB to representatives of the following States Parties: Australia, Austria, Bangladesh, Canada, Finland, France, Germany, India, Islamic Republic of Iran, Iraq, Italy, Japan, Jordan, Morocco, the Netherlands, Norway, Pakistan, Portugal, the Republic of Korea, Romania, Serbia, Singapore, Sri Lanka, Saudi Arabia, Sweden, Switzerland, Ukraine, the United Kingdom of Great Britain and Northern Ireland, the United States of America and Yemen.

14.3 In a closed session, the members of the Board re-elected Dr Christopher Timperley as Chairperson and Mr Cheng Tang as Vice-Chairperson for 2018.

Acknowledgement

14.4 The SAB acknowledges Ms Nadezda Malyutina, Ms Marlene Payva, Ms Siqing Sun and Ms Pei Yang of the OPCW Office of Strategy and Policy, for their support of and contributions to the session and its preparations, and for sourcing many of the references provided herein.

15. AGENDA ITEM FIFTEEN – Adoption of the report

The SAB considered and adopted the report of its Twenty-Sixth Session.

16. AGENDA ITEM SIXTEEN – Closure of the session

The Chairperson closed the session at 12:35 on 20 October 2017.

Annex: List of Participants in the Twenty-Sixth Session of the Scientific Advisory Board

---

176 The Chairperson's briefing is available at: www.opcw.org/fileadmin/OPCW/SAB/en/SAB26_Chair_Briefing_to_States_Parties.pdf

Annex

LIST OF PARTICIPANTS IN THE TWENTY-SIXTH SESSION OF THE SCIENTIFIC ADVISORY BOARD[177]

	Participant	Institution
1.	Dr Pål Aas	Norwegian Defence Research Establishment (FFI), Kjeller, Norway
2.	Professor Mohammad Abdollahi	Tehran University of Medical Sciences, the Islamic Republic of Iran
3.	Professor Isel Pascual Alonso	University of Havana, Cuba
4.	Dr Khaldoun Bachari	Algerian Public Scientific and Technical Research Centre in the Physico-Chemical-CRAPC, Algiers, Algeria
5.	Dr Augustin Baulig	Secrétariat général de la défense et de la sécurité nationale, Paris, France
6.	Dr Renate Becker-Arnold	BASF, Ludwigshafen, Germany
7.	Dr Veronica Borrett	BAI Scientific and Honorary Fellow, University of Melbourne, Australia
8.	Ms Hoe Chee Chua	DSO National Laboratories, Singapore
9.	Dr Christophe Curty	Spiez Laboratory, Switzerland
10.	Professor David Gonzalez	Department of Chemistry, University of the Republic of Uruguay and Ministry of Education, Montevideo, Uruguay
11.	Dr Zrinka Kovarik	Institute for Medical Research and Occupational Health, Zagreb, Croatia
12.	Professor Roberto Martínez Álvarez	Complutense University, Madrid, Spain
13.	Dr Robert Mikulak	U.S. Department of State, Washington, DC, the United States of America
14.	Dr Evandro De Souza Nogueira	Brazilian Ministry of Science, Technology, Innovation and Communications (MCTIC), Brasilia, Brazil
15.	Professor Ponnadurai Ramasami	University of Mauritius
16.	Dr Syed K. Raza	Institute of Pesticide Formulation Technology (IPFT), India
17.	Professor Ahmed E. M. Saeed	Sudan University of Science and Technology, Khartoum, Sudan
18.	Dr Maciej Sliwakowski	Institute of Industrial Organic Chemistry, Warsaw, Poland
19.	Dr Koji Takeuchi	National Institute of Advanced Industrial Science and Technology (AIST), Japan
20.	Mr Cheng Tang[178]	Office for the Disposal of Japanese Abandoned Chemical Weapons, Ministry of National Defence, China
21.	Dr Christopher Timperley[179]	Defence Science and Technology Laboratory (Dstl), Porton Down, the United Kingdom of Great Britain and Northern Ireland

177 Mr Valentin Rubaylo, having sent his apologies, was unable to attend the Twenty-Sixth Session of the SAB.

178 Vice-Chairperson of the SAB.

	Participant	Institution
22.	Professor Ferruccio Trifirò	Department of Industrial Chemistry, University of Bologna, Italy
23.	Mr Francois Mauritz van Straten	Chemical Weapons Working Committee, South Africa
24.	Ms Farhat Waqar	Pakistan Atomic Energy Commission
25.	Professor Matteo Guidotti (guest speaker)	Institute of Molecular Sciences and Technology Institute (ISTM), Italian National Research Council (CNR), Milano, Italy; and Academy of Sciences of the Institute of Bologna, Italy
26.	Professor Joseph Wang (guest speaker)	University of California San Diego, United States of America
27.	Dr Jonathan Forman	Secretary to the Scientific Advisory Board, Organisation for the Prohibition of Chemical Weapons, The Hague, the Netherlands

- - - o - - -

179 Chairperson of the SAB.