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UNITED KINGDOM OF GREAT BRITAIN AND NORTHERN IRELAND

CONVERGENCE OF SCIENCE BETWEEN INTERNATIONAL TREATIES AND AGREEMENTS

1. Introduction

The Chemical Weapons Convention (hereinafter "the Convention") operates as one of many treaties and international agreements that are designed to protect people and the environment from toxic or otherwise harmful chemicals. An enhanced understanding of the decisions made in other fora on toxic chemicals through consultations, exchanges of information and documents, technical cooperation, as well as cross-representation at relevant meetings would improve the Convention's decision-making. The OPCW has extant agreements with international partners such as the United Nations, the United Nations Office for the Coordination of Humanitarian Affairs (OCHA) and the World Customs Organisation (WCO)[1]. There are other treaties and arrangements described below that are relevant to the work of the OPCW. The United Kingdom sees benefit from the OPCW Technical Secretariat (hereinafter "the Secretariat") enhancing external engagement to increase understanding of issues relevant to the Convention. This updated paper includes an issue currently under consideration by the Industry Cluster (Stockholm Convention, section 5).

2. The Biological Weapons Convention

The Biological Weapons Convention (BWC) effectively prohibits the development, production, acquisition, transfer, stockpiling and use of biological and toxin weapons. Biological science and technology has advanced exponentially since the signing of the Convention in 1972. Although the Convention is uniquely broad and bans "microbial or other biological agents, or toxins, whatever their origin or method of production," its States Parties have recognised the importance of staying informed about relevant advances in science and technology.

Advances in science and technology could pose risks that could lead to potential breaches of the Convention. On the other hand, scientific advances can benefit the Convention, for example, by improving vaccines and the diagnosis of diseases. The technology surrounding the BWC is inherently dual use, demonstrating the importance of taking into account relevant developments in science and technology.

Toxins are naturally occurring organic poisons. A toxicant is a synthetic poison. However, effective understanding of naturally occurring and artificial toxins is required to ensure international controls are effective. The Convention and the BWC should both play an

1 https://www.opcw.org/about/our-partners (Accessed: 31 October 2022).

important role ensuring that the science of toxin production and use is well researched and emerging threats captured under both conventions.

3. The Montreal Protocol on Substances that Deplete the Ozone Layer

The Montreal Protocol is the treaty that regulates the production and consumption of over 100 ozone-depleting substances. The replacement of chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) with more flammable chemicals in the production of blown foam materials has, in some cases, resulted in an increased requirement for scheduled chemicals. Several of the highest performing flame-retardants for use in blown foam materials are Schedule 2B04 chemicals, such as dimethyl propylphosphonate (DMPP). Four of the most commonly traded Schedule 2 chemicals are used as flame-retardants in the production of blown foams.

The provisions of the Montreal Protocol can be assessed to have resulted in an increased demand for Schedule 2B04 chemicals[2], but also for Schedule 3B06 phosphorus trichloride, which is the typical starting material for the synthesis of Schedule 2B04 alkylphosphonates.

4. Various national and intra-national pesticide legislation[3,4,5]

National and intra-national pesticide legislation has developed since the Convention entered into force. A step change in approach in some legislatures has seen a requirement to re-certify all chemicals used as pesticides. This has resulted in legacy pesticides being banned until they are re-approved, which, due to the cost and limited financial returns from off-patent highly regulated substances, is unlikely.

As a result, a large number of old phosphorus-based pesticides, which in some cases were the inspiration for the scheduled nerve agents, are no longer permitted for use. It is likely that a trickle-down effect of this legislation will occur as States emulate these legislative changes to meet the expectations of their own populations and to allow food exports to countries with strict legislation covering pesticide residues.

The Annex on Chemicals names two pesticides: Amiton and Fonofos.

Amiton (O,O-Diethyl S-[2-(diethylamino)ethyl] phosphorothiolate and corresponding alkylated or protonated salts) is listed under Schedule 2A01, but may now meet the guideline for Schedule 1A—a toxic chemical has little or no use for purposes not prohibited under the Convention—as a result of updated pesticide legislation.

Fonofos (O-Ethyl S-phenyl ethylphosphonothiolothionate) is specifically exempted from Schedule 2B04. However, it is no longer available for use as a pesticide in many, or possibly even any, parts of the world. Further analysis may deem the specific exemption for this chemical no longer necessary.

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2 Plastics, Additives and Compounding, Volume 5, Issue 6, June 2003, Pages 32-36 https://doi.org/10.1016/S1464-391X(03)00042-4.

3 https://www.hse.gov.uk/pesticides/ (Accessed: 31 October 2022).

4 https://food.ec.europa.eu/plants/pesticides/eu-pesticides-database_en (Accessed: 31 October 2022).

5 https://www.epa.gov/pesticides (Accessed: 31 October 2022).

5. The Rotterdam Convention on the prior informed consent procedure for certain hazardous chemical and pesticides in international trade

"The Rotterdam Convention" has provisions that have resulted in changes to industry with relevance to the Convention. The inclusion of tetramethyl lead and tetraethyl lead in Annex III of the Rotterdam Convention has decreased the commercial viability and therefore the availability of these chemicals. A positive knock-on effect for the Convention results, as tetramethyl and tetraethyl lead can be used to produce Schedule 2B04 chemicals from phosphorus trichloride in high yield[6].

The inclusion of organotin compounds in Article III, in particular as chemicals used in marine antifouling paints (to prevent barnacle growth) has led to the requirement for new compounds to be used. One innovation has been the development and marketing of new coatings containing medetomidine[7], a chemical that has been described as a central nervous system-acting chemical (CNSAC) or incapacitating agent[8]. This may result in a significant increase in production of this chemical.

6. Stockholm Convention on Persistent Organic Pollutants – "Stockholm Convention"

The Stockholm Convention aims to protect human health and the environment from the effects of persistent organic pollutants (POPs) by focussing on eliminating, restricting and reducing unintentional releases of POPs. Addition of chemicals to the Stockholm Convention annexes could potentially affect the Convention.

In 2009, parties agreed to add polybromodiphenyl ether (PBDE) compounds, hexabromodiphenyl ether (hexaBDE) and heptabromodiphenyl ether (heptaBDE), the main components of commercial octabromodiphenyl ether (c-octaBDE[9]), to Annex A of the Stockholm Convention, with specific exemptions[10].

The POP Review Committee, a subsidiary body established to review chemicals proposed for listing, identified Convention Schedule 2B04 organophosphonate compounds as suitable substitutes for "c-octaBDE" in synthetic textiles[11]. As such, there has been a rise in flame retardant 2B04 chemical production, use, and trade volume[12] to replace PBDEs that are

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6 Kharasch, M.S., Jensen, E.V., and Weinhouse, S., Alkylation reactions of tetraethyllead. A new synthesis of ethyldichloroarsine and related compounds, J. Org. Chem., 14, 429, 1949.

7 Lind, U. *et al*, Molecular Pharmacology August 2010, 78 (2) 237-248; DOI: https://doi.org/10.1124/mol.110.063594.

8 Black, R, CHAPTER 1:Development, Historical Use and Properties of Chemical Warfare Agents , in Chemical Warfare Toxicology: Volume 1: Fundamental Aspects, 2016, pp. 1-28 DOI: 10.1039/9781782622413-00001.

9 The term "c-OctaBDE" is determined by the organically bound bromine content, and is a complex mixture of PBDEs. It was reportedly difficult for several countries of the Stockholm Convention to enforce national regulation of "c-octaBDE". Therefore, listing PBDE chemicals within "c-octaBDE" that exhibit POP characteristics in annex A instead of "c-octaBDE" itself helped facilitate the national monitoring and control of emissions, production, and use.

10 http://chm.pops.int/TheConvention/ThePOPs/AllPOPs/tabid/2509/Default.aspx (Accessed: 16 March 2023).

11 POP Review Committee: Report of the Persistent Organic Pollutants Review Committee on the work of its fourth meeting, Stockholm Convention, UNEP/POPS/POPRC.4/15/Add.1, 30 October 2008.

12 https://www.opcw.org/sites/default/files/documents/2021/12/Most%20Traded%20Scheduled%20Chemicals%202022%20%28MTSC%29.pdf.

constrained because of decisions agreed in the Stockholm Convention. Ongoing discussions in the Industry Cluster have documented the steady increase of 2B04 organophosphonate compounds, driven by government regulations, to replace toxic halogen-based compounds, such as hexaBDE and heptaBDE, as flame retardant additives.

7. International drug control conventions

The United Nations Single Convention on Narcotic Drugs, 1961, and the Convention on Psychotropic Substances, 1971 underpin the operational work of the United Nations Office on Drugs and Crime.

Of particular relevance to the Convention is the ongoing increase in international controls on chemicals that fall under the banner of CNSAC, and precursors to these chemicals. In response to a rapidly evolving proliferation of synthetic opioids, the regular additions to the List of Narcotic Drugs under International Control[13] of the Single Convention have enabled it to adapt to changing trends.

The International Narcotics Control Board (INCB)[14] is the independent and quasi-judicial monitoring body for the implementation of the United Nations international drug control conventions. In many respects, there are similarities with how the OPCW policy-making organs and advisory boards are constituted and act.

8. Export control regimes

The Australia Group (AG) and Wassenaar Arrangement are export control regimes that seek to enhance scrutiny of exports of Convention's Scheduled chemicals and other chemical weapons precursors, as well as items that have utility in chemical weapons programmes. Membership of the export control regimes consist of Convention's States Parties.

The AG predates the OPCW, having been formed to respond to the use of chemical weapons by Iraq under Saddam Hussein in early 1984. The AG dual-use control lists, covering chemical weapons precursors and the means to make precursors, toxic chemicals and toxins, are regularly updated to ensure cutting edge science and technology and industrial trends are reflected. A stated aim of the AG is to support the Convention as the principal instrument for addressing the threat posed by chemical weapons. AG participants' involvement in the group is fully consistent with the Convention and is an effective means of supporting implementation. For example, the AG has listed a number of Schedule 1A13 and 1A14 precursors.

The Wassenaar Arrangement addresses scheduled chemicals that are not covered by the AG, as well as agreeing to export controls on equipment that could be misused in support of an offensive programme.

The best practices of additional scrutiny over proliferation-sensitive exports improves the security of all States Parties and ensures they are not assisting anyone to engage in activity prohibited by the Convention.

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13 https://www.incb.org/documents/Narcotic-Drugs/Yellow_List/60th_edition/60_Yellow_List_EN_rev1.pdf (Accessed: 31 October 2022).

14 https://www.incb.org/ (Accessed: 31 October 2022).

9. Paris Agreement on climate change

The Paris Agreement is a legally binding international treaty on climate change. It was adopted by 196 Parties at COP 21 in Paris, on 12 December 2015, and entered into force on 4 November 2016.

Its goal is to limit global warming to well below 2, preferably to 1.5 degrees Celsius (°C), compared to pre-industrial levels.

To achieve this long-term goal, countries aim to reach global peaking of greenhouse gas emissions as soon as possible to achieve a climate-neutral world by mid-century.

In the simplest terms, anthropogenic climate change is being driven by chemical reactions conducted by humans through the burning of fossil fuels. In seeking to change this, the Paris Agreement contains many provisions, but the one most likely to affect the work of the OPCW is Article 2:

> 1 This Agreement, in enhancing the implementation of the Convention, including its objective, aims to strengthen the global response to the threat of climate change, in the context of sustainable development and efforts to eradicate poverty, including by:
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> (a) Holding the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 C above pre-industrial levels, recognizing that this would significantly reduce the risks and impacts of climate change;
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> (b) Increasing the ability to adapt to the adverse impacts of climate change and foster climate resilience and low greenhouse gas emissions development, in a manner that does not threaten food production; and
>
> (c) Making finance flows consistent with a pathway towards low greenhouse gas emissions and climate-resilient development.
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> 2 This Agreement will be implemented to reflect equity and the principle of common but differentiated responsibilities and respective capabilities, in the light of different national circumstances.

9.1 Resulting Economic Drivers for the Chemical Industry

This has the potential to be disruptive to the finance behind the chemical industry, and as a result its science and technology drivers. There will also undoubtedly be opportunities for the chemical industry, as the energy intensive sectors, which have historically been powered by fossil fuels, will become more expensive.

The need to combat anthropogenic climate change will drive the development of technologies that enable non-traditional, sustainable or waste feedstocks to be used for the production of fuels, chemicals and energy. There is a significant potential for changes to parts of the chemical industry relevant to the Verification Annex, which will play a part in identifying plant sites that are the most, and in some cases, the least relevant.

This paper now describes several examples of technologies that are in development or already deployed in pursuit of the aims and objectives of the Paris Agreement. The relevance of the chemistry and chemicals involved to the aim and purpose of the Convention will vary by sector and task, and ultimately have a bearing on its verification regime:

(i) Carbon capture

A significant effort to develop technologies to remove carbon dioxide (CO_2) from waste streams and atmospheric air is being undertaken by academia and industry. Existing technology used to scrub CO_2 and other unwanted chemicals from natural gas are available and used in optimised formulations for this task. Work on further optimising formulations to remove CO_2 from waste streams from industry outside of fossil fuel production within the research sector are creating potential solutions.

A promising chemical investigated for Direct Air Carbon Capture (DACC), and already used within natural gas scrubbing formulations, is methyldiethanolamine (Schedule 3B16)[15]. The potential for widespread use of these formulations beyond the current well-understood geographical distribution is something the Secretariat should seek to understand. Methyldiethanolamine is a scheduled chemical because it is a direct precursor to the Schedule 1A06 blister agent, HN2: bis(2-chloroethyl)methylamine.

The August 2015 edition of The OPCW Science & Technology Monitor suggested pinacolyl alcohol (Schedule 2B14) as having potential for use in CO_2 sequestration (injection of CO_2 into underground storage facilities). To date, there is little further information beyond the quoted paper, and the likelihood of non-scheduled alternatives means serious consideration for use is unlikely.

Other methods do not involve scheduled chemicals[16] and therefore pose less of a risk to the Convention, but there are many which rely on the use of amine chemistry[17]. Other than the sarin family (Schedule 1A01), all scheduled nerve agents contain an amino group. Developments involving the potentially disruptive changes such as these to the chemical industry may be a suitable topic for periodic review by the Scientific Advisory Board (SAB).

(ii) Carbon dioxide as a feedstock

A further significant effort to investigate the possibility of using CO_2 to synthesise new chemicals will result in plant sites that are diverse in location and design. The location for such plants will be near a source of the waste CO_2 (if the focus is on preventing the emission of CO_2, but could feasibly be located anywhere near a source of low carbon energy for a DACC plant).

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15 Antonini, C, Pérez-Calvo, J-F, van der Spek, M, Mazzotti, M, Optimal design of an MDEA CO_2 capture plant for low-carbon hydrogen production — 'A rigorous process optimization approach, Separation and Purification Technology', Volume 279, 2021, 119715, https://doi.org/10.1016/j.seppur.2021.119715.

16 Raktim Sen, R, Goeppert, A, Sayan Kar, A, Surya Prakash. G.K, Hydroxide Based Integrated CO_2 Capture from Air and Conversion to Methanol, Journal of the American Chemical Society 2020 *142* (10), 4544-4549 DOI: 10.1021/jacs.9b12711.

17 Kikkawa, S, Amamoto, K, Fujiki, Y, Hirayama, J, Kato, G, Miura, H, Shishido, T, Yamazoe, S, Direct Air Capture of CO_2 Using a Liquid Amine–Solid Carbamic Acid Phase-Separation System Using Diamines Bearing an Aminocyclohexyl Group, ACS Environmental Au 2022 2 (4), 354-362 DOI: 10.1021/acsenvironau.1c00065.

Multiple Discrete Organic Chemical (DOC) products, which are widely traded chemicals, have the potential to be produced from CO_2. While this is not a new area of research, and many extant chemical plants use CO_2 (e.g. to produce urea), it is an area of increasing interest. The point at which economic viability for waste-stream carbon capture use will depend on further technological developments, and economic drivers in the form of increased financial costs imposed on emissions via Emissions Training Schemes (ETS).

The George Olah plant in Iceland[18] is a shining example of an operating DOC plant that utilises CO_2 as a feedstock. The plant takes this from a geothermal energy waste stream and treats it with hydrogen (produced by hydrolysis) to produce around 4600 tonnes of methanol per year.

This plant is currently unique as an operational site, but other larger scale sites are being developed. Before the next Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention (Review Conference), there are plans to open three separate 100,000 tonne scale carbon dioxide-to-methanol plants[19].

According to the methanol institute, the global demand for methanol in 2015 was 75 million tonnes[20]. This will potentially increase substantially as methanol is a clean-burning fuel that can be used in fuel cells that are an alternative to batteries. As methanol is classed as a DOC, methanol plants are subject to declaration and verification inspections. Due to the scale of the industry, the plant sites are amongst the largest in the wider chemical industry subject to declaration. Changes to this sector, in particular using technology to capture and convert CO_2 waste streams to methanol, will potentially significantly increase the number of declarable and inspectable plant sites. The location of the sites might also affect the site selection methodology, as sites will likely be situated close to plants that emit significant quantities of CO_2, therefore disproportionately affecting countries with large industries.

The burden of declaration and verification of plant sites where such activities have a negligible impact on proliferation risk for the Secretariat and the plant site will work against the aims of the Convention and the Paris Agreement. Discussions on this issue within the Industry Cluster will help form a future pathway to meet this challenge.

9.2 Chemical forensics

It is very difficult—and almost impossible—to produce a chemical so pure that it cannot be distinguished from other samples produced at different times and places, by different methods, at different temperatures etc. There will always be some impurities present, because of such factors as the purities of the precursors themselves, the chemical reactions involved in their production, and the production equipment itself. The complete picture of all the chemicals and impurities present in any given sample can provide a unique "fingerprint" that can be specific to one route of production.

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18 https://www.carbonrecycling.is/project-goplant (Accessed: 31 October 2022).

19 https://www.carbonrecycling.is/projects (Accessed: 31 October 2022).

20 https://www.methanol.org/the-methanol-industry/ (Accessed: 31 October 2022).

Chemical forensics aims to attribute this "fingerprint" to its source—how and where it originated (and also to determine whether two samples of the same chemical are from the same batch of material)—through chemical analytical methods (including those used in OPCW designated laboratories) to answer investigative, legal or intelligence questions. Combining the results with other scene-related evidence can increase confidence in determining the origin of a chemical agent, and can provide the OPCW with a forensic level of certainty in its findings.

The SAB[21,22,23] and Chemical Forensics International Technical Working Group (CFITWG)[24] recognise the value of this approach. Real-life environmental samples have shown a diversity of analytes and complexity not replicated in historic laboratory work; there will probably always be some puzzling features involving new science that will require careful consideration, especially with regard to novel analytes and their relevance. Understanding these requires expert knowledge of synthetic chemistry and advanced analytical chemistry techniques and knowledge.

The knowledge base of production routes and challenges obtained from historical programmes that produced scheduled chemicals is preserved through archives and documents. For example, the reports of the OPCW Fact-Finding Mission for Syria regarding alleged incidents in Ltamenah, Syrian Arab Republic in March 2017[25][26] described the identification of di-isopropyl phosphorofluoridate (DIFP) and hexafluorophosphate (HFP) alongside sarin in soil and other samples. Such information is clearly indicative of the production route due to the known side reactions that resulted in DIFP and HFP impurities in the sarin. If a previously unknown chemical is used as a weapon in the future, identifying production routes may be more challenging. This underlines the importance of efforts to develop the analytical techniques and technical understanding required for future challenges before they are needed.

The science of chemical forensics is still at an early stage and full development of the capability might take at least 10 years. Given the requirement for the OPCW to be able to investigate any alleged use of non-scheduled toxic chemicals, the capability to detect and identify traces of such chemicals, and associated degradation and reaction products, should continue to be strengthened wherever possible.

Since the original version of this paper was circulated, the United Kingdom has co-sponsored with Finland the working paper entitled "Strengthening verification through the promotion of chemical forensics at the OPCW". This working paper makes a number of highly relevant recommendations on how to advance the field of chemical forensics in respect to the Convention.

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21 SAB: Report of the Scientific Advisory Board's Workshop on Chemical Forensics, OPCW, SAB-24/WP.1, 14 July 2016.

22 SAB: Report on Developments in Science and Technology to the Fourth Review Conference, OPCW, RC-4/DG.1, 30 April 2018.

23 SAB: Report of the Scientific Advisory Board's Temporary Working Group on Investigative Science and Technology, OPCW, SAB/REP/1/19, December 2019.

24 Chemical Forensics International Technical Working Group - United States Department of State.

25 Technical Secretariat: Report of the OPCW Fact-Finding Mission in Syria Regarding Alleged Incidents in Ltamenah, The Syrian Arab Republic 24 and 25 March 2017, OPCW, S/1636/2018, June 2018.

26 Technical Secretariat: Report of the OPCW Fact-Finding Mission in Syria Regarding an Alleged Incident in Ltamenah, The Syrian Arab Republic, 30 March 2017, OPCW, S/1548/2017, November 2017.