OPCW

Scientific Advisory Board

SAB-V/1
1 November 2002
Original: ENGLISH

REPORT OF THE FIFTH SESSION OF THE SCIENTIFIC ADVISORY BOARD

1. Introduction

1.1 The Scientific Advisory Board (hereinafter the "Board") met for its fifth session, from 26 - 27 September 2002 in The Hague.

1.2 The proceedings of the Board were directed by its Chairman, Claude Eon of France.

1.3 The list of participants is contained in annex 1 to this report.

1.4 The Board adopted the following agenda:

(a) Opening and adoption of the agenda

(b) Welcome by the Director-General

(c) Information of the Board about the current status of the implementation of the Convention

(d) Preparation of the Report of the Scientific Advisory Board for the First Review Conference:

(i) Composition of the Schedules of chemicals
(ii) Relevant developments in the production of chemical compounds, and their impact on the Chemical Weapons Convention's verification regime
(iii) Relevant developments in chemical analysis
(iv) Chemical weapons destruction and its verification
(v) Education and outreach
(vi) The technical capabilities of the Technical Secretariat

(e) Any other business

(f) Adoption of the report and closure of the meeting

2. Report of the Board for the First Review Conference

2.1 The main objective of the Board's work at this annual meeting was to begin preparing a report for the First Review Conference of the Chemical Weapons Convention (hereinafter the "Convention"), scheduled to take place from 28 April to 9 May 2003.

2.2 To prepare this special report, the Board received and reviewed the following documents:

(a) speakers' abstracts of the International Union of Pure and Applied Chemistry's (IUPAC's) workshop, "Impact of scientific developments on the Chemical Weapons Convention", Bergen (Norway), 30 June - 3 July 2002;
(b) the penultimate draft (September 2002) of "Impact of scientific developments on the Chemical Weapons Convention – A report by the International Union of Pure and Applied Chemistry to the OPCW and its States Parties";
(c) an IUPAC technical report: "Critical evaluation of proven chemical weapons destruction technologies", prepared for publication by Graham S. Pearson and Richard S. Magee, Pure and Applied Chemistry, Volume 74, No. 4, pp. 187-316, February 2002;
(d) final or, as applicable, advanced unedited copies of the background papers issued so far by the Technical Secretariat (hereinafter the "Secretariat") for the consideration of the Working Group for the Preparation of the Review Conference; and
(e) information prepared by the OPCW Laboratory on the current capabilities of the OPCW in relation to sampling and analysis (annex 3 to this report).

2.3 The Board was also informed about the proceedings of a NATO Advance Research Workshop on "Maximising the Security Benefits from the First Review Conference of the Chemical Weapons Convention", held in Bratislava, Slovakia, from 19 to 21 September 2002.

2.4 The deliberations of the Board led to the preparation of an interim report for the First Review Conference, which is contained in annex 2. This interim report will be submitted to the Director-General, and through him, to the States Parties to the Convention. The Board will continue working on the issues raised in this report. The Board also understands that States Parties will have an opportunity to provide comments and observations on the interim report, before the Board's final report for the review conference will be prepared.

3. Other issues

3.1 The Board noted that Claude Eon of France agreed to continue to serve as Chairman for the remainder of the preparatory work for the First Review Conference, and confirmed him in this position. Will Carpenter of the USA will continue to serve as the Vice-Chairman.

3.2 The Board recalled that the issue of biomedical samples remains to be discussed in a temporary working group, in order to prepare a recommendation for the Director-General. It was understood that this temporary working group would be formed in 2003.

3.3 The Board also expressed its view that the temporary working group on chemical weapons (CW) destruction technologies should consider the verification approach to CW destruction operations as soon as possible.

3.4 The Board discussed, in the context of its interim report for the review conference, issues related to science education, outreach, and cooperation, and decided to return to these issues at its next meeting.

3.5 The Board was informed by one of its members that a symposium is planned for March 2004 to discuss the results of research related to the destruction of toxic chemicals, using a catalytic low-temperature process in aqueous solution.

4. Closure of the meeting

The meeting was closed on 27 September 2002 at 17:01 with the adoption of this report.

Annexes:

Annex 1: List of participants of the fifth session of the Scientific Advisory Board
Annex 2: Interim Report of the Scientific Advisory Board for the Special Session of the Conference of the States Parties to review the operations of the Chemical Weapons Convention (First CWC Review Conference)
Annex 3: Status of the OPCW's capabilities in relation to sampling and analysis

Annex 1

List of participants of the Fifth Session of the Scientific Advisory Board

1.	Will D. **Carpenter**	USA
2.	Ashok K. **Datta**	India
3.	Claude **Eon**	France
4.	Alfred **Frey**	Switzerland
5.	Tom **Inch**	United Kingdom of Great Britain and Northern Ireland
6.	Jiří **Matoušek**	Czech Republic
7.	Brahim Youcef **Meklati**	Algeria
8.	**Koichi Mizuno**	Japan
9.	Giorgio **Modena**	Italy
10.	Viktor Alekseevich **Petrunin**	Russian Federation
11.	Ernõ **Pungor**	Hungary
12.	Stanislaw **Witek**	Poland
13.	Burkhard **Seeger**	Chile
14.	Abbas **Shafiee**	Iran
15.	Theodoros **Solomon**	Ethiopia

Annex 2

Interim Report of the Scientific Advisory Board for the Special Session of the Conference of the States Parties To Review the Operations of the Chemical Weapons Convention (First CWC Review Conference)

1. Introduction and Executive Summary

1.1 Paragraph 22 of Article VIII states that "The Conference shall not later than one year after the expiry of the fifth and the tenth year after the entry into force of this Convention, and at such other times within that time period as may be decided upon, convene in special session to undertake reviews of the operation of this Convention. Such reviews shall take into account any relevant scientific and technological developments …". The first special session to review the operations of the Convention has been scheduled for 28 April to 9 May 2003.

1.2 The OPCW Scientific Advisory Board was established by the Director-General in accordance with subparagraphs 21(h) and 45 of Article VIII of the Convention to enable him to render specialised advice in areas of science and technology relevant to the Convention, to the Conference of States Parties (hereinafter the "Conference"), the Executive Council (hereinafter the "Council"), and the States Parties. In line with this mandate, and as its contribution to the preparations of the review of the operations of the Convention during the First Review Conference, the Board has prepared this special report. The report analyses relevant developments in science and technology covering the past decade. It presents to the States Parties 11 recommendations and observations that the Board feels are important for their review of the operations of the Convention, and for the future implementation of its provisions.

1.3 This report contains the following sections:

(a) the Schedules of Chemicals;

(b) chemical synthesis and the production of chemical compounds;

(c) sampling and chemical analysis on-site;

(d) chemical analysis off-site;

(e) destruction of chemical weapons and its verification;

(f) chemistry education and outreach; and

(g) the technical capabilities of the Technical Secretariat (hereinafter the "Secretariat").

1.4 The findings of the Board, which are further elaborated below, are as follows:

(a) there is no compelling need at this stage to amend the Schedules. However, scheduled chemicals are not the only route for break-out from the Convention. Furthermore, given the increasing knowledge about, and number of, toxic compounds including toxins, as well as the issues related to novel agents, there may be a need the adjust the Schedules in the future;

(b) States Parties should be encouraged to submit data on potential novel agents for further assessment. The Board stands ready to contribute to such assessment, should such data be submitted;

(c) the general purpose criterion continues to provide cover against unscheduled and new toxic compounds. However, it is not only toxicity, but the potential for weaponisation, that determines the threat. There is a need to look beyond the Schedules when developing verification procedures in the future;

(d) a small percentage of other chemical production facility (OCPF) plant sites will have the potential to be easily convertible for the production of chemical warfare agents. Of course, although there is no evidence for misuse in the chemical industry, ever-changing industrial practices and production methods do not make the problems any easier. Increasing the number of OCPF inspections would thus be prudent, but this should not, however, lead to a decrease in the effectiveness of the inspection regime for facilities involved with scheduled chemicals;

(e) to enable inspectors to be aware of new production routes and processes, suitable training must be provided, for example with the help of interested States Parties;

(f) the on-site analysis procedures based on gas chromatography, coupled with mass spectrometry (GC/MS), combined with the use of the AMDIS software and the OPCW database as target spectral library, have become a technique that meets the needs of the Convention, without being intrusive in a way that would threaten commercial confidentiality. Extension of the database is necessary to allow for the inclusion of certain unscheduled chemicals which are either related to the scheduled chemicals, or which are of concern, given their potential to be used as chemical warfare agents. States Parties should be encouraged to submit analytical data on such chemicals for validation and inclusion into the OPCW Central Analytical Database (OCAD). Such data would need to be treated as OPCW-confidential information, to minimise proliferation risks;

(g) the limitations of GC/MS for the analysis of toxins means that other techniques, such as immunoassays, need to be developed;

(h) to improve the overall verification capabilities of the OPCW, some funds should be allocated to research, to resolve problems that become apparent as a result of experience gathered in inspections. For example, there is a need to improve sample preparation on-site (improved efficiency, cost, and logistics).

Such research could be conducted by the OPCW laboratory or by designated laboratories;

(i) procedures need to be agreed to allow for on-site analysis of samples taken during Schedule 3 and OCPF inspections, where the inspection time is limited to 24 hours;

(j) a temporary working group should be established to evaluate approaches towards the analysis of biomedical samples in investigations of alleged use;

(k) there has been insufficient urgency in addressing the problem of inspection of CW destruction operations, which currently is far too labour intensive. The Board is ready to assist in discussing this issue; and

(l) the technical capabilities of the Secretariat must be maintained by ensuring that staff receive the correct training and have fit-for-purpose equipment. On this latter point, there would be considerable merit if there was a flexible mechanism to update technical specifications of approved OPCW inspection equipment, and if responsibility were delegated to the Director-General to pursue the approval of new inspection equipment when the need arises.

2. The Schedules of Chemicals

2.1 The relationship between the CW definition and the Schedules was subject to extensive negotiations. While Article I prohibits any type of chemical weapon, as defined in paragraph 1 of Article II, not all toxic chemicals or precursors are, or in fact should be, regulated by the Convention. The Schedules of Chemicals list those (known) toxic chemicals and their precursors that were seen to pose a particular risk to the Convention.

2.2 The Convention contains a mechanism to amend the Schedules. Chemicals can be added to, or deleted from, the Schedules, or they can be moved from one Schedule to another, should the States Parties consider this beneficial for verification purposes. Threat perceptions would be important aspects of such decisions. The legal framework of the Convention, in particular, the general purpose criterion contained in the CW definition, makes it clear that the Schedules do not embrace the entire scope of the Convention. Some unscheduled chemicals could cause serious harm, if they were misused as chemical weapons. The Convention's concept of "chemical weapons" is not limited by the Schedules of Chemicals. Without that broad scope, chemical warfare agents of novel identity (including as yet undisclosed or undiscovered) would remain outside the reach of the Convention.

2.3 The Board is fully aware of the wisdom of the drafters of the Convention – international verification procedures complement the obligation of States Parties to take the necessary measures to implement the Convention, including legislation in relation to toxic and precursor chemicals, irrespective of whether they are included in the Schedules. The distinction between scheduled and unscheduled chemicals is a regulatory matter. Wherever this distinguishing line is drawn, there will always be unscheduled chemicals that, if misused, would pose a risk to the Convention.

A certain degree of "calculated risk" is unavoidable. Scientific advances will, however, have an impact on that residual risk and need, therefore, to be reviewed.

Previous observations of the Board

2.4 The Board recalled its recommendations and observations in relation to the Schedule 1 chemical ricin (subparagraph 2.2 of SAB-II/1, dated 23 April 1999), and noted that the Conference took a decision on ricin (C-V/DEC.17, dated 18 May 2000). This decision endorsed the Board's findings, but did not incorporate the understanding proposed by the Board about what constitutes "ricin". The Board had concluded that ricin should remain accountable as long as the A-S-S-B bond is not broken, irrespective of the isoform(s) present. That should also apply to toxic mutants of ricin. The Board continues to believe that this understanding would be useful for declarations related to ricin production and transfers, and resubmits to the States Parties the suggestion to apply it in their implementation work. The understanding could, for example, be incorporated into the OPCW Declarations Handbook. In this context, the Board also recognised that the role of the Chemical Abstracts Service (CAS) registry numbers used for reference in the Convention's Annex on Chemicals may require clarification. In the case of the above recommendation on ricin, the Board took the structure of the chemical compound as the governing principle, not the CAS registry number listed in the Schedule. This question is further elaborated in subparagraph 2.6 below.

2.5 The Board furthermore recalled its observations with respect to salts of scheduled chemicals. These salts are chemically distinct from the parent compounds, and have different physical and chemical properties, as well as their own CAS registry numbers. However, the dynamic equilibrium between the base and the salt is reversible, and the salt can easily be re-transformed into the base (with the exception of quaternary salts). In industry, a base is often converted to a salt if it is more convenient to handle a compound in that form. Normally, there is no essential difference between the free base and the corresponding salt from the standpoint of the end user (see subparagraph 2.10 of SAB-II/1, dated 23 April 1999). The Board noted that a group of governmental experts had disagreed with the majority view expressed in the Board's report that, consequently, there should be no differentiation in the treatment under the Convention of a free base and its corresponding salts. The Board observed, however, that even if the regulatory approach would in fact so differentiate between the salts of scheduled chemicals and their corresponding free base, certain activities related to some of these salts may still have to be declared. For example, the production of the hydrochloride of the Schedule 1 chemical HN-2 involves several interconnected chemical equilibria, with the free base essentially being an intermediate in the chemical synthesis. Consequently, there may be a need to declare this production, if the amount involved exceeded the applicable declaration threshold under Part VI-VA, even though the free base is never captured or isolated, and the final product is the salt rather than the free base.

2.6 One issue that the Board noted in the context of the previous recommendations mentioned above is the role of the CAS registry numbers indicated in the Schedules of Chemicals. There appears to be a view that these CAS registry numbers have a regulatory function. The Board would like to caution against such views. As a tool to

identify a chemical in a unique manner, CAS registry numbers appeared helpful to the drafters of the Convention. States Parties need to realise, however, that there is not necessarily a one-to-one relationship between CAS registry numbers and chemical structures, and that CAS registry numbers can be, and occasionally are, changed by the Chemical Abstracts Service. CAS registry numbers can be assigned by the Chemical Abstracts Service temporarily, and then changed. Also, different CAS registry numbers can be assigned to different forms of the same chemical compound (e.g. optical or stereo isomers, radioactively labelled, isomeric forms to be found under certain conditions of the chemical environment, even mixtures or reaction products of certain chemical compounds). The Board's view was that, while CAS registry numbers are a useful tool to clearly identify a chemical compound, that fact should not be confused with an assumption that CAS registry numbers should have any regulatory power.

Developments in chemical synthesis and screening of chemical compounds

2.7 The Board, as an international advisory body, has no access to intelligence or to classified information related to the development of novel CW agents, with the exception of information categorised as confidential under the Confidentiality Annex of the Convention, and the OPCW's confidentiality regulations. It is not in a position to speculate about the existence of new agents. It is however possible that there are such novel agents, and that they would meet the criteria for Schedule 1.

2.8 The Board stands ready to assist in the assessment of any information that States Parties might decide to submit on such chemical compounds, should they decide to do so. Furthermore, the Board is not otherwise aware of any unscheduled toxic chemicals or precursors, that were not already known when the Convention was concluded in 1992 that have actually been weaponised or used as chemical weapons.

2.9 The Board was aware of publications related to certain toxic chemicals that had not been considered when the Schedules were elaborated. This included, inter alia, a group of toxic chemicals that appear to have relevance for chemical defence, namely dialkylaminoalkyl (dialkylamido)fluorophosphonates.[1] The information available on these compounds in the public domain indicates that their toxicity is comparable to that of other nerve agents, and that they have other (physico-chemical) properties that make them relevant for CW protective purposes. In relation to the guidelines for the Schedules, the Board observed that these compounds meet some of the criteria for Schedule 1 chemicals, namely the criteria contained in subparagraphs 1(b)(ii) and 1(c) of the guidelines for Schedule 1. If a decision were to be taken to include these and similar compounds into the Schedules, Schedule 1, from a scientific perspective, would be the appropriate category to place them.

2.10 The Board reviewed the results of the IUPAC workshop held in Bergen, Norway, from 30 June to 3 July 2002, and the penultimate draft (September 2002) of "Impact of scientific developments on the Chemical Weapons Convention – A report by the International Union of Pure and Applied Chemistry to the OPCW and its States Parties". Based on this information, and based on the contributions made by the

1 J. Matoušek and I. Masek, The ASA Newsletter 94-5, Issue number 44, pages 1, and 10 – 11.

members of the Board during the meeting, the following observations were endorsed by the Board:

(a) over recent years, many new procedures have been developed to speed up the synthesis of new chemicals required, in particular, for biological evaluation by the pharmaceutical industry. Examples are combinatorial chemical techniques, together with other methods for rapid synthesis and screening;

(b) as the molecular basis of biology becomes better understood (e.g. with advances in genomics and proteomics), it is becoming easier to use that knowledge, both to design new biologically active chemicals, and to synthesise chemicals using enzymes or cell-based systems. These advances have the potential to change the nature of the way chemicals are synthesised, and to make practical the synthesis on reasonable scales of chemicals that previously were little more than curiosities;

(c) the rapid pace of developments in the bio-molecular sciences, coupled with advances in chemical synthesis, certainly increase the possibility that new toxic chemicals will be found that could be misused as chemical weapons. However, these advances do not significantly change the situation, in view of the large numbers of already known toxic compounds, many of which are not listed in the Schedules;

(d) in particular, while the time required for the early stages of agent development may have shrunk considerably as a result of these developments, the subsequent stages in the development of such a new agent into an effective weapon are not affected by these developments in science and technology; and

(e) these developments underline, on the other hand, the importance of the general purpose criterion. They also suggest the need to look beyond the Schedules in the future development of verification procedures.

2.11 The Board also was aware of concerns about the development of new riot control agents (RCAs), and other so-called “non-lethal” toxic chemicals. There are specific provisions in the Convention dealing with RCAs and other toxic chemicals which are legitimately used for law enforcement purposes. The Board noted that the science related to such agents is rapidly evolving, and that results of current programmes to develop such “non-lethal” agents should be monitored and assessed for their relevance for the Convention. It appears, however, unlikely that compounds with a sufficient safety ratio would be found, based on past experience.

2.12 The Board concluded that the rapid expansion of knowledge about new chemical compounds and their toxic and other properties could possibly lead to candidates for the development of new chemical warfare agents. The Board did not find it likely, however, that this rapid expansion of knowledge and scientific potential would actually lead to the introduction of new chemical agents given, inter alia, that many unscheduled toxic chemicals with potential as CW agents already exist, and that developing a new compound into an actual chemical weapon is not a trivial undertaking. The Board stressed, however, the importance that all such new toxic chemicals, no matter what their origin or method of synthesis, are covered by the

Convention's definition of chemical weapons, unless they were intended for purposes not prohibited under the Convention, and only as long as their types and quantities would be consistent with these purposes. The Board underlined the importance of this so-called "general purpose criterion" as a safeguard for the validity of the Convention.

2.13 In summary, the Board, at this stage, did not see any compelling reason to make recommendations aimed at amending the Schedules of Chemicals. The Board observed, however, that that may become necessary in the future because:

(a) scheduled chemicals are not the only route for break-out from the Convention's regime;

(b) there is a distinct risk associated with certain types of unscheduled chemicals, and the number of such chemicals posing a potential threat has increased, and continues to increase; and

(c) the route of unscheduled chemicals could be appealing to proliferators who would want to minimise the chances of the OPCW detecting such break-out attempts during inspections;

2.14 The verification regime of the Convention needs to be able to address the issue of those type of unscheduled chemicals that pose a direct threat to the Convention. To avoid the possibility of the OPCW being caught by surprise, emphasis needs to be placed on the general purpose criterion.

3. Chemical synthesis and the production of chemical compounds

3.1 Significant developments have taken place in the industrial production of chemicals. These developments are relevant for the functioning of the verification regime under Article VI of the Convention. Their impact is twofold. First, the relative significance for the object and purpose of the Convention of the sub-regimes under Article VI (i.e. Parts VI through IX of the Verification Annex) may have changed as a result of these developments. Second, at the same time, new technologies and equipment used for the industrial-scale production of chemicals are likely to be encountered more often by OPCW inspectors, who must be able to recognise them and draw accurate conclusions about the nature of the activities at an inspected plant site.

3.2 Changes in the chemical industry are related not only to production technology and processes, but equally to organisational and structural developments. Vertical integration of chemical manufacturing, which was typical until the 1980s, has changed. Environmental and safety regulations, liability concerns, as well as market pressures, made industry change production in a number of ways. Production was taken up in countries previously not known for their chemical production; the industry focussed on core business and outsourced synthesis to contractors, while at the same time, production volumes of bulk chemicals became global; multiple ownership has become a typical feature; principles of just-in-time production were introduced; and transfers of chemical materials increased considerably. Furthermore, the versatility of chemical manufacturing increased and chemical plants, due to environmental and safety regulations, tend to be more easily convertible to the production of toxic chemicals than they used to be in the past. This is not to say that the position of the

chemical industry vis-à-vis the Convention has changed, or that the industry's support for its implementation has diminished in any way. The industrial environment in which the Convention is being implemented has, however, become much more complex.

Previous observations by the Board

3.3 In relation to the production by synthesis of discrete organic chemicals, the Board concluded that, from a scientific standpoint, it is no longer possible to make a clear distinction between "chemical" and "biological and biologically mediated" processes. The emphasis should be on the product rather than on the process (see subparagraph 2.3 of SAB-II/1, dated 23 April 1999). That view was not shared by a meeting of governmental experts, but there was agreement that the issue should be kept under review. The Board came back to this issue when reviewing the impact of new developments in chemical process technology on the Convention (see below), and observed that it is indeed increasingly difficult to say whether in certain cases a process is chemical or biological, or mixed. The Board recognises that the concerns of some States Parties in relation to biological processes and the production of discrete organic chemicals (DOCs) relate to facilities in the food and drink industry, which use fermentation. The declaration and inspection provisions of the Convention should not cover these facilities. From a product point of view, the food and drink industry is not relevant to the Convention, and their products should not be considered as DOCs.

3.4 The Board also recalled its previous observations in relation to the guidelines applicable to mixtures containing Schedule 2A/A* chemicals in a low concentration. It concluded that this is a matter of regulatory intent rather than science, and had proposed possible concentration limits, depending on what the States Parties decided they wanted to regulate (see subparagraph 2.3 of SAB-IV/1, dated 6 February 2001). The Board noted that this issue was presently under discussion in the facilitation process of the Council. There was thus no need to further discuss any of the scientific aspects related to this issue.

New developments in the production of relevant chemicals

3.5 The Board reviewed the results of the IUPAC workshop on relevant scientific and technological developments, held in Bergen, Norway, from 30 June to 3 July 2002. It considered the penultimate draft (September 2002) of "Impact of scientific developments on the Chemical Weapons Convention – A report by the International Union of Pure and Applied Chemistry to the OPCW and its States Parties". Based on this information, and based on the contributions made by the members of the Board during the meeting, the observations below were recorded:

(a) many parts of the chemical industry around the world operate with multipurpose batch facilities, which can readily be switched from one product to another. The versatility of chemical manufacturing is being enhanced by technological developments (process automation, microwave chemistry, catalysis, supported chemistry, biotechnology, and microreactors). This increases versatility in the industry, and changes the appearance of chemical production plants. With the increasing globalisation of the industry,

there is a need to review the verification regime for OCPFs, to ensure that it is effective in monitoring relevant parts of the chemical industry. There would appear to be a need for conducting a larger number of inspections at OCPF facilities than in previous years. There also would appear a need to develop guidelines for the conduct of OCPF inspections; and

(b) the proposed increase of DOC inspections should, however, not lead to a decrease of effectiveness in the inspection regime of facilities involved with the production of scheduled chemicals.

3.6 In summary, the Board concluded that the developments in the production of chemicals at industrial scale over the past decade or so have increased the versatility of certain parts of the chemical industry. This relates both to processes (e.g. biological processes, biocatalysis, and supported reagents) and equipment (e.g. multi-purpose production equipment, micro-reactors, and microwave reactors). As a result, an increasing number of small-to-medium scale chemical plants with high technological relevance to the objectives of the Convention can be found in the category of "other chemical production facilities" (facilities involved with the production of discrete organic chemicals). Some of these plants look considerably different to traditional chemical plants. While the versatility of such plants is increasing, the nature of some components of the production equipment is changing and certain "traditional signatures" that in the past were associated with the handling or manufacturing of hazardous and/or volatile compounds are no longer required. It is important that OPCW inspectors are capable of recognising and assessing such novel industrial operations and equipment. Furthermore, the future development of the industry verification regime for non-proliferation purposes needs to take these trends into account, and a larger number of inspections at OCPF plant sites should be conducted.

4. Sampling and chemical analysis on-site

4.1 Sampling and analysis are inspection activities that OPCW inspection teams may employ, in accordance with the applicable provisions of the Convention, in both routine and challenge inspections, or in investigations of alleged use. Samples are, as a rule, taken by the representative of the inspected State Party or the inspected facility in the presence of OPCW inspectors. Wherever possible, the analysis of the samples is done on site. The inspection teams have the right to use their approved equipment for such on-site analysis. Alternatively, they may request the assistance of the inspected State Party to perform the analysis in the presence of the inspection team.

4.2 The Board received information on the current OPCW capabilities for sampling and on-site analysis (see annex 3). The information contained in annex 3 was provided by the OPCW Laboratory.

Current OPCW capabilities for on-site sampling and analysis

4.3 On-site sampling and analysis is required for routine inspections, challenge inspections, and investigations of alleged use of chemical weapons. For routine inspections, effective on-site analysis has the advantage over off-site analysis in that, while meeting the need of the OPCW inspection teams, it also minimises the risk of any loss of confidential information.

4.4 The main equipment currently available to the OPCW for on-site analysis is gas chromatography, coupled with mass spectrometry (GC/MS)[2], with associated databases and software, as well as sample preparation methods. The mode of operations is that, following appropriate sample preparation, the chromatography and mass spectroscopy data of the sample run through the equipment is compared with data contained in an instrument database. If this instrument database was extracted on-site from the OCAD, it would only contain validated data pertaining to some 600 scheduled chemicals, including toxic chemicals, precursors, and degradation products. This allows for a convenient check for the presence (or absence) of scheduled chemicals.

4.5 The sensitivity of the equipment is sufficient to allow detection of scheduled chemicals at levels likely to be present in production and storage facilities (i.e. chemicals in bulk, materials contained in mixtures at concentration levels regulated by the decision of the Conference on low concentration guidelines, and scheduled chemicals and their degradation products in environmental samples collected in close proximity to the production or storage equipment), and therefore is most suitable for use in routine inspections. The software was specifically designed for this purpose, and also allows information to be purged from the hard disk of the instrument's computer after the instrument has been used by the inspectors. To all intents and purposes, as operated and designed, this is a very non-intrusive method of analysis, which is very well suited to the purpose of avoiding compromising confidential information contained in the sample.

4.6 The Board concluded that the OPCW has established an adequate, state-of-the-art sampling and on-site analysis capability. There are, however, factors that limit the utility of this capability. These factors are primarily in the area of logistics and the cost of inspections. In this context, the Board recalled some of its previous observations on sampling and analysis that may be useful in addressing these limitations. Furthermore, the current GC/MS equipment for on-site analysis needs to be replaced, as it is getting to the end of its servicable life span.

Past recommendations by the Board in relation to on-site analysis

4.7 The Board observed that in routine inspections, simple methods such as infrared spectroscopy would suffice for the identification of declared chemicals in bulk. The Board was told, however, that infrared spectroscopy is no longer in use by the OPCW. Alternatively, the Board pointed out that analytical equipment belonging to the inspected State Party could be used when this has been regulated in a facility agreement, and when conditions are fulfilled to ensure the independence of the analytical results (see subparagraph 2.10 of SAB-III/1, dated 27 April 2000).

4.8 The Board also observed that simple screening techniques will not be sufficient if, in a routine inspection, sampling and analysis become necessary to demonstrate the absence of scheduled chemicals (in particular the absence of Schedule 1 chemicals in industry inspections). At the same time, the removal from the inspection site of a

2 The Board discussed that the use of liquid chromatography coupled with mass spectrometry should also be considered in the future, in particular in relation to the detection of larger molecules. Other options that should be explored related to chemical sensors and biochemical analysis.

large number of samples for analysis at designated laboratories would be impractical and expensive. The best approach, in cases when immediate on-site analysis is not feasible, would be to collect for subsequent analysis an appropriate number of samples, and leave them on site under secured conditions, and under conditions aimed at minimising sample degradation (see subparagraph 2.11 of SAB-III/1, dated 27 April 2000). An analytical team could then be sent to the site, with the agreement of the inspected State Party, and the analysis could be undertaken at a later stage. The Board continues to believe that concepts such as this, or the use of analytical equipment belonging to the inspected State Party under conditions that demonstrate the independence and reliability of the analytical results, could help resolve problems associated with logistics, and the cost of sampling and analysis in routine inspections.

4.9 In relation to the OCAD, the Board continues to believe that data relating to characteristic degradation products (whether scheduled or unscheduled), chemicals found in old and abandoned CW, salts of scheduled chemicals, non-scheduled precursors and byproducts of the synthesis of scheduled chemicals, and standard riot control agents should be incorporated, and that priorities must be set for the inclusion of additional spectra (see subparagraphs 2.14 of SAB-III/1, dated 27 April 2000 and 2.5 of SAB-IV/1, dated 6 February 2001). The Board noted the inclusion of the retention indices and mass spectra of additional compounds, and concluded that the database is rapidly becoming a reliable reference point for on-site analysis. This is important when on-site instruments use the OCAD database as the instrument's target database and the AMDIS software is being used, because the scope of the on-site database extracted from the OCAD sets the limits for which scheduled chemicals can be identified, and which can not.

New developments

4.10 The Board then reviewed developments in chemical analysis relevant to on-site sampling and analysis, taking into account the issues presented at the IUPAC workshop in Bergen (Norway) 2002, and the penultimate draft (September 2002) of "Impact of scientific developments on the Chemical Weapons Convention – A report by the International Union of Pure and Applied Chemistry to the OPCW and its States Parties".

4.11 In future, the analytical capability should be increased by continuing to expand the validated OCAD by:

(a) including data on chemicals likely to be confused with scheduled chemicals, as well as well-known degradation products of scheduled chemicals; and

(b) adding data on certain non-scheduled toxic chemicals which have the potential to be used in chemical warfare.

4.12 This latter procedure could be done in a manner that would keep the data confidential within the domain of the OPCW (i.e. transparent to States Parties, but otherwise confidential), and would allow the OPCW to have and to use data on potential threat agents without changing the Schedules, and without alerting terrorist organisations or non-signatory States to their existence. In other words, this approach would be an

important step in implementing the general purpose criterion of the Convention, with minimum inconvenience to the chemical industry.

4.13 Thus, what is being developed is an analytical system that could fully meet the requirement of not being too intrusive, while meeting most requirements for inspections at Schedule 2 and 3 facilities, as well as at OCPFs.

4.14 In future, as further development of GC/MS occurs, it will become more effective, easier to transport, and easier to use, so it will be necessary for the OPCW to keep up to date with commercially available equipment.

4.15 The rate-determining step for on-site analysis is the time and effort necessary for sample preparation. For Schedule 2 facilities, the 96 hours allocated for inspection conduct provide ample time for analysis, if required. For Schedule 3 and OCPF inspections, where only 24 hours are available for the inspection, there may be problems, depending on the number of samples to be analysed. Thus, alternative procedures may need to be agreed, such as those previously suggested by the Board, i.e. storage of samples and subsequent analysis on site by a separate analytical team.

4.16 The above discussion relates generally to small molecules and not to toxins, including ricin and saxitoxin, for which generic GC/MS procedures currently being used are inappropriate. It is suggested that for toxins, consideration should be given to obtaining and validating a range of specific immunoassays. If these were available, the OPCW would have a battery of techniques very suitable for the purpose of on-site inspections, and which would also be of considerable value for challenge inspections and investigations of alleged use. The Board observed that, at the moment, the OPCW has no on-site capability for the analysis of toxins.

4.17 The OPCW, furthermore, should devote more research efforts to addressing the problems related to sample preparation. This would not only reduce the time needed for analysis on-site, but would also reduce the amount of auxiliary equipment to be transported. The Board noted that it is important for the OPCW to understand that it needs to invest an adequate amount of resources into research aimed at the development of analytical and sampling techniques. Such research could be done at the OPCW laboratory or by designated laboratories.

5. Chemical analysis off-site

5.1 For the performance of off-site analysis of samples acquired by OPCW inspection teams during on-site inspections, the Convention assigns the primary responsibility for the security, integrity, and preservation of those samples, and for the protection of confidentiality of samples transferred off-site to the Director-General. The Director-General is required to do this in accordance with procedures which the Conference was to adopt at its First Session. The States Parties continue to negotiate these procedures, and no decision has yet been taken by the Conference.

5.2 The Convention requires the Director-General to establish a stringent regime for the entire chain, from sample collection to sample transportation for off-site analysis. The Director-General must certify the laboratories designated to perform different types of analysis; oversee the standardisation of equipment and procedures for both

on-site and off-site activities related to sampling and analysis, including the monitoring of quality control; and select from among the designated laboratories those which shall perform analytical or other functions in relation to specific investigations.

5.3 Although the Conference has yet to adopt the procedures for sampling and analysis, the OPCW has developed and tested technical procedures for sampling and analysis as part of its quality assurance policy, and has designated laboratories for the analysis of authentic samples. The Board reviewed the current capabilities of the OPCW in this respect. They are briefly described in annex 3 of this paper. This information was provided to the Board by the OPCW Laboratory.

Current capabilities of the OPCW for off-site analysis

5.4 The current situation in relation to off-site analysis is described in annex 3.

5.5 The proficiency testing for the designated laboratories organised by the OPCW has been targeted primarily on the analysis of scheduled chemicals and related compounds (in particular, degradation products) in environmental samples. Good progress has been made in developing techniques and protocols, and in ensuring that the staff of designated laboratories are well trained and well practised. Some of the lessons learned, particularly in regard to sample preparation, are also applicable to on-site analysis.

5.6 If, however, on-site analysis becomes the normal approach, particularly in routine inspections, it will become necessary to redefine the main anticipated role of the designated laboratories, and to ensure that they are experienced in terms of responding to likely scenarios.

5.7 For example, perhaps the main role of designated laboratories will be to analyse environmental samples in instances of alleged use or for challenge inspection, in situations where the levels of concentration are too low for unequivocal analysis by on-site techniques, or by some of the off-site techniques currently being used. If this is the case, the designated laboratories will need to become well versed in tracing analytical methods and protocols for both scheduled and unscheduled chemicals. Some preparatory work in this direction is necessary.

5.8 Additionally, there may be a need, in incidents of investigations of alleged use, for there to be a capability to analyse biomedical samples. A small number of laboratories have undertaken research in identifying and analysing biomarkers resulting from poisoning by scheduled chemicals. There are good prospects that analysis of other biomarkers will soon be possible. These techniques need to be validated and shared, so that more laboratories are capable of carrying out such an analysis. There are many issues connected with this kind of analysis, including how to maintain expertise and standards. The Board suggested dealing with these issues as soon as possible.

Past recommendations by the Board on off-site analysis

5.9 In 2000, the Board had, at the request of the Director-General, reviewed the results of the Sixth Official OPCW Proficiency Test (see SAB-III/1, dated 27 April 2000).

It had then concluded that the current concept of OPCW proficiency testing may be counterproductive (see subparagraph 2.13 of SAB-III/1, dated 27 April 2000). At the administrative level, too much attention was being given to the mechanics of the scoring process, while too little attention was being devoted to an examination of the lessons to be learned from a test, and to the consequent refinement of sampling and analytical procedures. In the meanwhile, taking these comments into account, guidelines on the designation of laboratories for the analysis of authentic samples have been adopted by the Council (EC-XX/DEC.3, dated 28 June 2000). The Board would welcome a new, updated report on changes in the process of, and the reporting on, OPCW Proficiency Testing.

5.10 The Board had also been requested to address the issue of biomedical samples, but a temporary working group has yet to be established to study this issue (see subparagraph 2.10 of SAB-IV/1, dated 6 February 2001).

New developments

5.11 The Board then reviewed developments in chemical analysis relevant to off-site analysis by designated laboratories, taking into account the discussions at the IUPAC workshop in Bergen (Norway) 2002, and the penultimate draft (September 2002) of "Impact of scientific developments on the Chemical Weapons Convention – A report by the International Union of Pure and Applied Chemistry to the OPCW and its States Parties".

5.12 The IUPAC workshop spent considerable time reviewing new developments in analysis that could substantially affect the way the OPCW meets the analytical requirements of the Convention. The review, which was quite comprehensive, concluded that there were few developments that would drastically change the current potential in the near future. The above discussion of on-site and off-site analysis is based on this premise. One major problem was the cost of developing new equipment that would be specifically tailored to the OPCW's requirements. The one development necessary to meet OPCW needs seems to be the necessity to introduce immunoassays for toxins. The Board supported the need to have such techniques available to inspectors, as well as to designated laboratories.

5.13 Most other techniques referred to in the IUPAC workshop require specific development, or must await other developments for commercial purposes. The Board concluded that the only action necessary is for the OPCW (and the Board itself) to continue monitoring these advances, until such time that specific developments for the OPCW occur.

6. Destruction of chemical weapons and its verification

CW destruction technologies

6.1 The Board noted a recent publication that provided a comprehensive and authoritative overview on the chemistry underlying the current technologies for the destruction of chemical weapons (IUPAC Technical Report: Critical evaluation of proven chemical weapons destruction technologies, prepared for publication by Graham S. Pearson and

Richard S. Magee, Pure and Applied Chemistry, Volume 74, No. 4, pp.187-316, February 2002). The Board welcomed this publication.

6.2 The assessment and selection of destruction technology for chemical weapons, it was clearly recognised, is the responsibility of the individual State Party concerned. This will involve not only technological assessments, but also the consideration of other factors, including commercial factors.

Verification of CW destruction

6.3 In the past, the Board had already discussed measures to reduce the number of inspectors necessary for permanent on-site monitoring of CW destruction operations. It had concluded that the approach developed within the Secretariat was sound (see subparagraph 2.7 of SAB-IV/1, dated 6 February 2001). The Board's temporary working group on equipment will continue monitoring developments in relation to available instrumentation, but will not address any specific additional tasks in the near future.

6.4 The Board understands from the Secretariat that work is presently under way to further refine the verification approach for CW destruction facilities, and to develop proposals for methodological and instrumental solutions that would enable the inspection team sizes to be reduced, without compromising the verification objectives of the Convention.

6.5 The Board expressed its frustration that the Secretariat and the States Parties had not been able to make more progress in pursuing suggestions that steps be taken to reduce the number of inspectors at CW destruction facilities, by identifying the critical steps that require monitoring, and then in introducing statistically based methods for random, rather than continuous, inspections, and/or remote and CCTV monitoring.

6.6 In summary, the Board requested an early opportunity for its temporary working group on CW destruction technologies, to review the proposals that are presently being prepared.

7. Chemistry education, outreach and cooperation

7.1 The Board noted with satisfaction that the IUPAC, in its penultimate draft report for the CWC Review Conference, had stated that "greater efforts on education and outreach to the worldwide scientific and technical community are needed in order to increase awareness of the CWC and its benefits. An informed scientific community within each country can be helpful in providing advice to States Parties, and in disseminating unbiased information to the public. Education of, and outreach to, signatory States and non-signatory States could be helpful in increasing awareness of the importance of universal adherence to the Convention, thereby enhancing safety and security for all States".

7.2 The Board also recognised that the Secretariat had developed certain projects that supported these goals, in particular the Associate Programme and the Ethics Project.

7.3 The Board was convinced that efforts in the area of education and outreach are important to further the objectives of the Convention; these efforts include raising awareness, assuring that the principles of the Convention become firmly anchored in professional ethics and teaching, and promoting international cooperation in the field of chemistry. International cooperation and outreach were also important in respect to attracting additional countries to adhere to the Convention. The Board expressed a strong desire to further discuss and clarify its particular role in relation to education, outreach, and cooperation.

7.4 There are a number of opportunities in the area of outreach, education and international cooperation, and the Board will need to consider further which ones are the most useful ones to pursue.

7.5 To this end, the Board considered it useful for the OPCW to engage in a dialogue with other organisations, such as the IUPAC and its chemistry education division, professional and chemical industry associations, or national, as well as regional science academies.

7.6 The Board concluded that it will need to return to this issue at its next meeting, in order to further discuss practical and useful measures in relation to education, outreach, and international cooperation.

8. The technical capabilities of the Technical Secretariat

8.1 The Board noted the observations included in the IUPAC penultimate draft report to the Review Conference, and endorsed these statements. They are reproduced in the following three paragraphs.

8.2 “Given the rapid pace of developments in the screening of new unscheduled chemicals and in the development of new, more flexible production processes for chemicals, attention needs to be given to ensuring that the Technical Secretariat is kept up to date and has the necessary competence to take such developments into account in the implementation of the Convention.”

8.3 “For sampling and analysis only the highest standards are acceptable because of the importance of accurate results. Such standards, both in the OPCW Technical Secretariat and in the designated laboratories that support the OPCW analytical activities, cannot be achieved and sustained without all the staff involved being well trained and well practised. There is a need to review what training is provided, how it is provided and whether sufficient resources are available to sustain the process.”

8.4 “Consideration should be given to the organisation of periodic workshops to review relevant scientific and technological developments. Such workshops should be part of the ongoing training of staff members but could also benefit States Parties. Planning for such workshops is principally the responsibility of the Technical Secretariat and the OPCW Scientific Advisory Board, but IUPAC and other appropriate international scientific bodies might be consulted as appropriate.”

8.5 In addition, the Board strongly suggested that:

(a) previously agreed equipment specifications for approved equipment, that were adopted together with the list of approved equipment by the Conference, need to be updated by the Secretariat, as analytical techniques and instruments evolve, and supply situations change on the market; and

(b) there is a need to have a sufficiently flexible mechanism to approve new inspection equipment in order to increase verification efficiency, reduce costs, improve logistics, and/or improve the health and safety of inspection teams. That mechanism should give adequate authority to the Director-General to pursue the approval of new equipment, when needed. The States Parties should focus on the functionality of such proposals, as well as on such aspects as cost, improved verification effectiveness, improved protection of confidentiality and the like, rather than on the equipment itself.

8.6 From the perspective of a scientist, it needs to be said that inflexibility in adjusting the available approved equipment to progress in science and technology, as well as to supply situations, will inevitable lead to inefficiency and wastefulness in the conduct of inspections.

Annex 3

Status of the OPCW's Capabilities in Relation to Sampling and Analysis[3]

1. On-site analysis

1.1 Approved inspection equipment: The sampling and analysis (S&A) equipment from the list of approved equipment (C-I/DEC.71, dated 23 May 1997) has been packaged into special transport boxes, thus creating the OPCW mobile laboratory. The OPCW mobile laboratory is an independent field laboratory that is fully operational for GC/MS analysis, after a set-up time of three to four hours. It is operated by a minimum of two analytical chemists. The equipment includes items for sampling various types of solid, liquid and wipe samples, including environmental samples, sufficient to sample up to eight samples of each type. The on-site laboratory provides all the equipment necessary to prepare this number of samples for GC/MS analysis, in accordance with validated procedures, including derivatisation of non-volatile compounds. The equipment has been tested under laboratory and field conditions and – sometimes in close cooperation with a supplier – improvements have been achieved. Standards and chemicals brought on-site by the inspection team do not include any chemical listed in the Schedules of the Convention, to prevent any form of cross-contamination by the inspection team. The OPCW mobile laboratory, with equipment adapted to inspection requirements, is used for all types of inspections.

1.2 Approved S&A procedures: The Secretariat and the OPCW Laboratory have built up a complex network of procedures for sampling and analysis, and for related activities. Methods for sampling and sample preparation are based on recommended validated procedures published by VERIFIN. The experience gathered during inspections, training, exercises, and proficiency tests led to the improvement of existing methods, and to the development of new ones. Approved Standard Operating Procedures and Work Instructions, which are part of the OPCW Quality System, describe the process of on-site sampling and analysis. The process of preparation, validation, and packing of GC/MS instruments before dispatch from the Secretariat is accredited by the Dutch Accreditation Council, in accordance with the requirements of ISO/IEC 17025.

1.3 QA/QC measures: On-site procedures include a series of steps to assure and control analytical results. These measures are: prevention of contamination of sampling equipment through one-time use of originally packed and sealed items; control of procedures and equipment by taking background, equipment, and method blank samples; and performance test and calibration of GC/MS instruments with an approved OPCW test mixture, which contains 16 unscheduled chemicals, and is used to control GC and MS performance and to calibrate retention indices. Stringent acceptance criteria must be fulfilled by a GC/MS instrument, if it is to be validated for on-site analysis.

1.4 Mass spectral library: During the post processing, AMDIS data analysis software compares GC/MS spectral data to the on-site target library, which is created on-site when the instrument is being set up. The on-site target library contains mass spectral data from the OCAD. In its present version, the e-OCAD (version 2), from which the

---

3 Information provided by the OPCW laboratory.

on-site target library is created, contains about 833 mass spectra and 333 retention indices of 576 compounds. Version 3 of e-OCAD (to be released in September) will contain about 1491 mass spectra and 810 retention indices of 1158 compounds. All analytical data contained in the OCAD is provided by Member States, validated by the Validation Group, and is approved by the Council. The OPCW Laboratory is accredited in accordance with requirements of ISO/IEC 17025 for the organisation of the OCAD, and the extraction to on-site databases.

1.5 Protection of (commercially) confidential information: Extensive technical measures have been implemented to allow the inspected State Party to protect commercially confidential information during on-site analysis. These measures include the restriction(s) resulting from the list of approved equipment, but in particular, the development of the blinding feature of the GC/MS operating software and the security level filters of AMDIS, the GC/MS raw data post processing software. Both features can be applied separately or in combination, allowing the inspected State Party a gradual restriction of information displayed by the instrument, while maintaining a high confidence level of reported identifications.

1.6 Performance of inspectors: The capability to set-up the OPCW mobile laboratory on-site to be fully operational within four hours has been demonstrated repeatedly during inspections, training, and exercises. OPCW inspectors have carried out sampling on inspections and during exercises under various conditions. Inspectors are trained in sampling procedures, including live agent sampling using various types of personal protective equipment. OPCW analytical chemist inspectors perform sample preparation and GC/MS analysis on a regular basis during inspections, training, exercises, and in the OPCW Laboratory. The capability to provide reliable analytical results has been demonstrated repeatedly. Various samples, including proficiency test samples, have been analysed, using on-site equipment and procedures.

2. Off-site analysis

2.1 OPCW Proficiency Tests: The OPCW Laboratory is accredited in accordance with the requirements of ILAC G13 for the conduct of proficiency tests. Laboratories seeking or maintaining designation need to demonstrate their capability to perform off-site sample analysis by participating in at least one test per year. Various types of samples containing low levels of CWC related compounds (scheduled and unscheduled) in difficult matrices have been analysed successfully in eleven proficiency tests, both by the OPCW Laboratory using Secretariat on-site procedures, and the test participants using their methods, which are similar to the Secretariat procedures, and which are based on the methods published by VERIFIN. The OPCW Laboratory, together with the test participants, has developed a stringent set of criteria for reporting and evaluation of analysis results based on the requirements adopted during the first Conference. These procedures include criteria to avoid the reporting of irrelevant results, in order to protect confidential (commercial) information.

2.2 Designated laboratories: The Director-General designates laboratories which successfully perform in OPCW proficiency tests, and which fulfil additional requirements as defined by the Member States. As of now, the list of designated laboratories includes 13 laboratories in three geographical regions. If samples are

sent for off-site analysis, the Director-General will select at least two different laboratories to perform the analysis. Guidelines for designated laboratories on the handling of off-site samples and related activities have been developed by the Secretariat.

2.3 Handling of off-site samples: A set of quality documents describing the process of sending samples for off-site analysis has been developed, based on the status of the informal consultations on this issue between Member States. Secretariat procedures include packing of samples at the inspection site in accordance with international transport requirements, handling of samples at the OPCW Laboratory, and a stringent chain of custody requirements. Split fractions (4-5) of an authentic sample will be sent from the inspection site to the OPCW Laboratory, where they are re-packaged (without opening of original sample containers), together with control samples and matrix blanks, before being sent to designated laboratories. Designated laboratories receive none-indicated vials containing the actual sample, a control, and a blank. Procedures for preparing and analysing the control samples and matrix blanks at the OPCW Laboratory have been developed and tested. The Secretariat plans to extend the accreditation of the OPCW Laboratory to cover the process of control sample preparation and analysis.

- - - o - - -