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# Impact of scientific developments on the Chemical Weapons Convention (IUPAC Technical Report)*

Katie Smallwood[1], Ralf Trapp[2], Robert Mathews[3], Beat Schmidt[4], and Leiv K. Sydnes[5,‡]

*[1]Independent Consultant, Geneva, Switzerland; [2]International Disarmament Consultant, 74270 Chessenaz, France; [3]Defence Science and Technology Organisation, Australia; [4]Spiez Laboratory, 3700 Spiez, Switzerland; [5]Department of Chemistry, University of Bergen, 5007 Bergen, Norway*

*Abstract*: This document represents the final report of discussions and conclusions arising from the workshop on Developments in Science and Technology Relevant to the Chemical Weapons Convention, held in Spiez, Switzerland in February 2012.

*Keywords*: Chemical Weapons Convention; CWC; implementation; science and technology; Third Review Conference.

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*Sponsoring body: IUPAC Executive Committee: see more details on p. 876.
‡Corresponding author: E-mail: leiv.sydnes@kj.uib.no

## 1. INTRODUCTION

IUPAC organised an international workshop in Spiez, Switzerland on 21–23 February 2012 to review advances in science and technology with regard to their impact on the Chemical Weapons Convention (CWC). This was the third workshop of its kind: in 2002, IUPAC held the first workshop (Bergen, Norway) and in 2007, held a second workshop (Zagreb, Croatia). For each previous workshop, the program committee prepared a report with findings and recommendations to the States Parties of the CWC and the Organisation for the Prohibition of Chemical Weapons (OPCW) [1,2]. These reports were well received and recognised as providing an important independent contribution from the scientific community to the preparations for the First and Second Review Conferences. The reports informed the preparations by States Parties and the OPCW Technical Secretariat, and were also a major resource for the OPCW Scientific Advisory Board's (SAB) report to the First and Second CWC Review Conferences.

Discussions in 2011 between IUPAC and the OPCW led to an agreement to convene a third workshop, this time hosted by Spiez Laboratory in Spiez, Switzerland. IUPAC assembled both an international advisory committee and a program committee; the latter consulted with the OPCW Technical Secretariat but took primary responsibility for the organization of the workshop.

Review Conferences of the CWC are convened every five years in recognition of the evolutionary nature of the agreement. There exists an ability to adjust and modify the Convention in response to advances and changes, and the objective of the Review Conferences is to review the operation of the CWC, to assess the progress made with its implementation, and to provide strategic guidance for the coming years. The drafters of the CWC understood the need to periodically review the impact of advances in science and technology (S&T) on the CWC and specifically required Review Conferences to "take into account any relevant scientific and technological developments" [3]. Such advances may relate to the scope of the prohibitions set out in the CWC, affect the way it is being implemented, and create opportunities for advancing international cooperation among States Parties in areas such as protection against chemical weapons (CW) and the peaceful application of chemistry. Dialogue between the OPCW and the scientific community in evaluating scientific and technological progress also creates opportunities to advance awareness of the CWC and its requirements in the scientific, technological, and industrial communities.

Advances in chemistry, the life sciences, and other scientific disciplines and enabling technologies in recent years will undoubtedly create considerable benefits for humankind—advances which could lead to improved health, a better environment, and more sustainable development. At the same time, new scientific discoveries may lead to new risks, including the potential for new chemical compounds to be used as CW. In order to fully understand the impact of these new scientific and technological developments, IUPAC organised the Spiez workshop and prepared this report.

This report, which summarises the presentations, discussions, findings, and conclusions of the Spiez workshop, is being provided to support the report that the SAB will prepare for the Third Review

 

Conference and will be submitted to the States Parties and the OPCW to assist with their preparations for the Third Review Conference.

## 2. SUMMMARY OF FINDINGS AND RECOMMENDATIONS

The findings and recommendations of the workshop are organized into seven groups: (a) overall findings and recommendations; (b) scientific and technological advances that potentially affect the scope of the CWC; (c) new and ongoing developments that affect the practical implementation of the CWC; (d) advances relevant to the field of chemical verification; (e) advances relevant to the field of chemical protection; (f) evolution of the international S&T environment—issues relevant to international cooperation; and (g) approaches to expanding awareness of the CWC and understanding of its requirements, particularly in the academic community and in industry.

### 2.1 Overall findings and recommendations

2.1.1 The Spiez workshop provided an opportunity to reflect on recent developments in S&T, many of which are occurring in fields discussed at the previous workshops in Bergen (2002) and Zagreb (2007), and to explore the pace of advances over the past decade and their potential implications*. Overall, the Spiez workshop demonstrated that certain aspects of S&T relevant to the CWC are advancing at a rapid pace, in particular developments in the biological sciences. For example, research on neuropeptides and bioregulators is providing an increased understanding of how these molecules work, and advances in synthetic biology enable the possibility of large-scale production of toxins, bioregulators, and other biologically active molecules that could be used for hostile purposes. Other aspects of S&T relevant to the CWC are advancing less rapidly. For example, the use of microreactor technology, which was just over the horizon five years ago, is now being commercially applied on a limited basis for the production of specific classes of chemicals, including peptides. Thus, the pace and manner in which the advances in S&T have practical implications for the scope and implementation of the CWC vary considerably.

2.1.2 Advances in S&T relevant to the CWC are not yet at the point to cause major paradigm shifts. Key trends in chemical S&T and the infrastructure supporting scientific advances should continue to be monitored at regular intervals. Many are capable of significant discoveries, and developments will become more applicable, inexpensive, and broadly distributed. It will be important not only to monitor the key trends, but also to identify and monitor the significant drivers for these trends.

2.1.3 In addressing changes in S&T in the context of the CWC, the workshop discussions highlighted that the question of *utility* should not be ignored. Specifically, how certain new technologies could be applied to specific scenarios of CW development, production or use, or to protective purposes, including CW detection and decontamination, should be considered. The Spiez workshop identified, for example, that the potential to use S&T for purposes prohibited by the CWC will vary due to multiple factors including but not limited to: (1) the potential user(s) (e.g., individuals vs. non-state actors vs. governments); (2) user access to adequate levels of scientific, technical, and economic knowledge and resources; and (3) what the user is trying to accomplish.

*Some of the S&T developments discussed in Spiez 2012, Zagreb 2007, and Bergen 2002 include biological or biomediated processes for chemical synthesis; potential applications of nanotechnology to the CWC; microreactors and other novel chemical production methods (e.g., microwave, novel catalysis, photochemistry, etc.); development of new toxic chemicals; and advances in methods for CW detection (e.g., “lab on a chip”, DNA arrays, microbial sensors, etc.).

 

## 2.2 S&T advances and their impact on the scope of the CWC

2.2.1 The nature of the chemical risk spectrum is changing, with implications for both States Parties and non-state actors such as terrorists. It is recognized that traditional CW will continue to be a concern. The States Parties possessing CW are destroying their stockpiles, but this activity is not yet complete. In addition, non-States Parties may still have stockpiles of traditional CW agents. However, there are also potential opportunities for other types of toxic chemicals (i.e., nonscheduled chemicals, including toxic industrial chemicals) to be applied for prohibited purposes. This concern applies to both state and non-state actors, although in different ways and for different goals. New considerations also arise from developments such as the production of toxic chemicals, including toxins, through biological synthesis (an aspect of the convergence of chemistry and biology); encapsulation and delivery through nanotechnology; and flow microreactors, which enable types of chemical reactions under conditions that were not previously technically feasible. The increasing incorporation of green chemistry methods and technologies into industrial production may mitigate some risks, for example, by limiting the size of inventories of hazardous chemicals and reducing volumes of toxic chemicals produced either as byproducts or intermediates. On the other hand, the production of smaller quantities of chemicals may also mean that certain facilities may no longer be subject to inspection under the CWC's verification regime; and the new production processes could also potentially introduce new chemicals of concern. Developments in chemical research and in industry may also be altering the spectrum of risks of concern (see Section 2.3). These aspects of the changing environment have implications for the role of the CWC in disarmament and nonproliferation.

2.2.2 The field of chemistry is converging with many other scientific fields, including other physical sciences, mathematics, and biology, the latter of which is attracting significant attention. Chemistry is also taking advantage of enabling technologies offered by such fields as modeling and simulation, informatics, data storage and management, and distributed computing. Convergence of scientific disciplines in part fuels the rapid pace of discovery and is an inevitable outcome of scientific advancement. In preparing for changes brought about by S&T, the review and evaluation of S&T relevant to the CWC thus should not be limited to specific disciplines.

2.2.3 The workshop gave particular attention to the question of achieving greater technical understanding of the implications of the growing convergence between chemistry and biology for the CWC. New disciplines exist at this cutting edge of science, which may need to be considered in the context of the Convention. In addition, convergence of chemistry and biology has implications for areas that may overlap with the Biological and Toxin Weapons Convention (BWC).

2.2.4 Certain classes of chemicals affect biological organisms through action on the central nervous system (CNS) in a manner commonly referred to as incapacitating (e.g., fentanyl derivatives and other opioids). These chemicals are highly toxic (some with $LD_{50}$ values comparable to VX). Many biological factors, including age, gender, and preexisting health conditions, influence the individual effects of exposure to these chemicals at carefully managed therapeutic levels. The development of these chemicals and improved understanding of their mechanisms of action are being driven by medical research, such as the development of new anesthetics. Medical research is also driving significant interest in the continued development of effective methods for delivering chemicals into the CNS, particularly across the blood–brain barrier. Several medical applications for the delivery of therapeutics such as anticancer agents were discussed at the Spiez workshop. As these scientific developments related to CNS-modulating chemicals and the deliveries of such chemicals to targeted biological tissues intersect, they have implications for their potential use in law enforcement as so-called "incapacitating chemical agents" (ICAs). Unlike use of chemical agents in traditional CW contexts, which are used in excess amounts to saturate an area so as to ensure their intended effect, the employment of ICAs for law enforcement would require delivery techniques that "titrate" a target group (control the exposure) so that the desired incapacitating effect is achieved without an unacceptable level of lethality. This in itself would be a challenge but in addition, law enforcement uses would also have to ensure effect and selectivity across individual variations in characteristics such as age, health, or sensitivities to particular agents. The decision on the appropriateness of the development and use of ICAs for law enforcement purposes, including whether such use would be permitted under the provisions of the CWC, is an issue which requires political, legal, and other inputs. S&T on classes of chemicals which could possibly be employed as ICAs is continuing to advance*; however, the discussions at the Spiez workshop indicated that the currently available S&T does not have the capabilities required to enable the delivery of such "incapacitating chemical agents" for law enforcement purposes in a "safe" manner.

2.2.5 The workshop did not identify any new developments in chemical S&T that are not covered by the Convention's comprehensive nature and its prohibitions in regard to all types of CW. The "general purpose criterion" (GPC) is expressed in the definitions of the CWC and states that toxic chemicals are CW unless intended for purposes not prohibited by the Convention and in types and quantities that are consistent with these purposes. This definition safeguards the Convention against being superseded by developments in S&T. Through the GPC, the CWC ensures that all toxic chemicals, past, present, and future and whatever their method of production, are captured by the provisions of the Convention. As noted above, advances continue in a number of fields, including some that the workshop was not able to address in depth, and surprises are always possible. The ongoing monitoring of trends in S&T to assess their relevance for and impact on the scope of the CWC will be important.

2.2.6 Combinatorial chemistry, high-throughput screening, and concerns about the commercial databases containing information on millions of biologically active experimental chemicals have been raised since the workshop held in Bergen in 2002. It would appear that no new toxic chemicals which have been developed by the pharmaceutical and agricultural companies have been used for CW purposes in recent years. With respect to the large number of new toxic chemicals being developed, the Zagreb report noted that "simply expanding the Schedules will not be a practical way of dealing with this risk" [2]. However, a number of participants at the Spiez meeting noted that it could be useful to review the Schedules in light of advances in chemistry and experiences in implementation of the Convention. Such a review could reflect the general scope of the CWC and could result in proposals for the addition of new chemicals to the Schedules or changes to the existing Schedules.

2.2.7 Some of the key scientific trends that will require regular monitoring because of their potential impact on the scope of the Convention include: (1) convergence of biology and chemistry because of the array of new products and production processes; (2) green chemistry because of the potential to produce an array of new chemicals through these production processes; and (3) production and use of nanomaterials.

### 2.3 Developments that affect the practical implementation of the CWC

2.3.1 One of the key trends highlighted in the workshop is the increasingly global nature of scientific research and collaboration, as well as the increasing globalization of the chemical industry. However, the global level of access to advances in S&T remains uneven. In particular, in many countries access to S&T is limited, which has implications for the national capacity of those countries to respond to a chemical event, including limited speed and scale of chemical

*See, for example, Technical Workshop on Incapacitating Chemical Agents; Spiez, Switzerland, 8–9 September 2011 [4].

detection, medical treatments (e.g., availability of antidotes), decontamination, and limited national capacity for availability and maintenance of equipment. The workshop noted that some countries are beginning to pool resources on a regional basis, which could have implications for implementation of CWC given its country-by-country approach.

2.3.2 There have been some significant shifts in the global chemical industry, going beyond the "BRIC-plus" countries*. New developments include rapid advances in, and diffusion of, technology encouraged by the pressures of market competition, regional migration of production locations, and the broadening of capabilities from large-scale production facilities ("world plants") to include custom manufacturing and specialization in a larger number of countries. Many companies are also increasingly disaggregating steps of their chemical production processes and subcontracting or outsourcing early production steps to other (sometimes overseas) facilities. These shifts have implications for the implementation of the CWC and direct consequences for the "other chemical production facility" (OCPF) regime. Some issues include the number and geographical distribution of OPCW inspections; the diversity of OCPFs to be inspected; methods for OCPF inspection; transparency in global trade and distribution of chemicals (i.e., including the ability to track and trace).

2.3.3 Developments in flow reactors, microreactors in particular, should be regularly reviewed for their potential impact on the Convention. Five years ago microreactors were still an experimental technology largely confined to research laboratories. However, with recent developments, microreactors have now entered the chemical production toolkit for certain kinds of operations. They alter the signature of chemical production infrastructure to some extent, although they are only one piece of a sequence of infrastructure, which includes tank farms and downstream processing with workup and isolation. Major advantages of microreactor technology include the safe production of hazardous, corrosive chemicals, as well as certain classes of biologically active chemicals, which could not be otherwise done under batch conditions. In a microreactor it is possible to perform highly energetic reactions, work with unstable intermediates, employ more reactive reagents, and use active catalysts more effectively that may enable novel production processes. The major potential risks to the CWC from microreactors and other novel production methods identified during the workshop include the potential for new types of synthetic/production pathways that may open the possibility of new routes to well-known Scheduled chemicals that would not start from the expected precursors (a point made in the report of the Bergen workshop). Such developments could have major implications for the precursors listed in the CWC Schedules and the inspection regimes. Microreactor technology also is an effective tool in process and product development that could shorten the time from the discovery of a new class of toxic chemicals to production of selected agents. There is also the possibility that other toxic chemicals (e.g., pharmaceuticals and peptides) could be produced in microreactors for prohibited purposes.

2.3.4 Some of the key trends related to infrastructure of S&T advances that will require ongoing monitoring because of their potential impact on implementation include: (1) advances in chemical manufacturing technology (e.g., flow microreactors), which may eventually require adaptation of national implementation and verification systems; (2) developments in miniaturization and portability of instrumentation, which is particularly important for first responders, but also has implications for the conduct of inspections; and (3) the changing international structure of S&T research and industry, which has growing potential for international collaboration and cooperation as well as the need to ensure compliance and good governance.

*The report on the 2007 Zagreb meeting referred to the BRIC countries (Brazil, Russia, India, and China). A number of additional countries have also been developing substantial chemical sectors since then.

## 2.4 S&T advances specifically relevant to verification

2.4.1 In regard to verification of the CWC, it will continue to be necessary to keep abreast of advances and new technologies and features of analytical technology. Specific considerations will include assessment of the versatility of the technology in different environments, with traditional and emerging chemicals and/or materials, and in chemicals embedded in complex matrices. In addition, the consequences of a false positive during verification could result in the need for a conservative approach to adoption of new analytical technology. As the OPCW expands the scope of its analytical capability to include methods of analysis of additional chemicals (e.g., toxins), the analytical technologies used to support verification will need to be carefully evaluated and validated for adherence to required specifications. The rapid developments in analytical capability in the areas of miniaturization, complex mixture analysis requiring reduced sample preparation, and increased sensitivity will present opportunities for improvement of the current verification systems, and continued, iterative development and evaluation of analytical technology will be necessary to address the evolving needs of the verification system. The existing technology development infrastructure within the OPCW and the technical working group structures are in the process of investigating possible new technologies for incorporation into the verification methodology, identifying gaps within the existing analytical capabilities, and building global networks of scientific expertise that can be drawn upon to assist in filling those gaps.

2.4.2 Chemical analysis for verification occurs in two settings within the CWC, on-site and off-site. On-site analysis occurs at inspection sites such as chemical industry production facilities; off-site analyses occur at OPCW-designated laboratories on samples collected at inspection sites. Instruments used for on-site analysis must, among other criteria, be transportable and rugged against physical stress (e.g., air transport, truck transport, on- and off-loading); must perform reliably after exposure to a wide array of environmental conditions (e.g., heat, cold, dust); must be operable within a short period of time after arrival on-site (short warm-up and calibration cycles); must have known, well-characterized responses; must complete analyses within a fixed time window; and must be capable of analyzing as broad as possible a range of different relevant chemicals. Inspectors require training to ensure the quality of the analyses and to allow for basic, in-field troubleshooting and resolution of technical problems. These requirements limit the ability to introduce cutting-edge technology into the on-site analytical suite, and favor the use of "multipurpose" methods and equipment that can be used for a broad range of chemicals. Since the 2007 workshop in Zagreb, the OPCW's internal analytical team has developed a new on-tube derivatization methodology that has reduced the sample preparation burden on the inspectors and reduced the time to analysis. This demonstrates the potential for iterative development of existing technology, and such efforts should continue. At the 2012 workshop, it was noted that theoretical and technological advances in miniaturization of gas chromatography-mass spectrometry (GC-MS; see Section 3.8) could provide opportunities for advances in on-site analytical instrumentation to improve portability and robustness. It is likely, however, to require significant development before this technology can be applied in the field for identification (rather than for screening or safety monitoring) purposes.

2.4.3 As off-site analyses are performed in controlled designated laboratory settings, opportunities exist for expanding analytical capabilities by incorporating cutting-edge technology. Indeed, as the OPCW moves towards trace analysis and the analysis of biomedical samples and considers implications for chemical–biological convergence for the development of new biologically active or derived chemicals and materials of concern, additional analytical capacity and capability will be needed. Presentations at the Spiez workshop highlighted two recently developed ionization methodologies for high-resolution MS that enable analysis with minimal sample preparation. These methods are appropriate for analysis of complex compounds at trace concentration levels in complex matrices, such as biological samples. These are two relevant developments within a field that is undergoing rapid development, and complex sample analysis should continue to be monitored and evaluated for their usefulness and applicability to the CWC regime.

2.4.4 One observation from the Spiez workshop, and one that was noted both in Bergen and in Zagreb, is that the pace of S&T development is accelerating in the area of chemical and biological convergence. It will be important for the OPCW to take advantage of these developments in order to enhance the OPCW's verification capabilities in the future. There is potential for off-site analytical facilities to act as test beds for emerging technologies and for evaluation of the potential of these new technologies to be translated and incorporated into the suite of off-site and on-site analytical instrumentation.

### 2.5 S&T advances specifically relevant to protection against CW

2.5.1 Chemical analysis related to protection against CW currently focuses more upon on-site *detection* rather than *identification**. Important ongoing trends in research and development (R&D) relevant to chemical detection include miniaturization (portable technologies), reduction of time of analysis (the ability to detect CW within a short time to provide rapid warning of the hazard and guide medical treatment and environmental decontamination), more accurate detection of multiple types of agents (traditional agents as well as toxic industrial chemicals, TICs), and improvement of the point-of-care methodologies. However, the translation of new technologies and methods for chemical detection into effective field devices for use by the military, first responders, OPCW inspectors, and other relevant authorities continues to be a challenge.

2.5.2 There have been no recent breakthroughs in portable instruments for the detection of CW. One challenge is that research for protection purposes (chemical defense) has tended to focus on traditional CW agents, which does not reflect potential risk from TICs, which are now a greater concern because of threats from non-state actors. Another potential challenge to rapid advances/breakthroughs are the differing drivers (sensitivity/specificity, portability, power supply, legal requirements, etc.) for R&D on instrumentation, depending on whether the equipment is to be used for on-site verification or incident response. Chemical identification to a high level of specificity, low false alarm rate, and identification of a large number of compounds often within complex matrices are a few important requirements for on-site verification analysis (for additional detail, see Section 2.4.2). Some of the characteristics important for incident response include rapid identification, class-level identification accompanied by targeted methods for triage, and equipment that must not require advanced technical knowledge by the operator. The drivers for incident response are accompanied by different technical challenges as compared to those for on-site verification. As such, commercial application of the next generation of portable detection instrumentation is likely to occur first (within 5–10 years) for incident-response applications.

2.5.3 S&T relevant to medical countermeasures has seen incremental progress, particularly in regards to antidotes and treatments. Many gaps still exist, and there have been few fundamental changes in how victims of CW are managed. These gaps are particularly concerning in light of research in other fields that advance our understanding of body chemistry, toxicity pathways, and other biochemical processes that contribute to acute and chronic adverse effects and/or recovery of individuals exposed to harmful chemicals. And there are increasing con-

*In this context, *detection* refers to the use of portable analytical instruments to demonstrate the presence or absence of hazardous levels of a toxic chemical or class of toxic chemicals. *Identification* refers to the use of tools and techniques that determine the molecular identity of the chemical.

 

cerns about the treatments for long-term effects of CW, including detrimental impacts on mental health, which may or may not be immediately evident.

2.5.4 The application of nanotechnology to improve materials and systems relevant for protection against CW and chemical decontamination is an area of gradual, but important development. Some areas of ongoing research that should continue to be monitored include the development of nanofibers for protective clothing, nanocatalysts for decontamination methods, and nano-based drug delivery mechanisms for medical countermeasures.

2.5.5 The ability and criteria needed to detect and analyze toxins, which cannot be performed using the methods developed for traditional CW agents, and the ability to rapidly analyze biomedical samples, are two of many challenges faced by the Convention. The convergence of chemistry and biology may lead to new materials and devices useful for addressing these and other challenges related to chemical detection and analysis, and medical countermeasures. For example, advancing research in microbiology is demonstrating methods for use of bacteria to screen for specific chemical or biological agents. Developing deployable chemical sensors based upon microbiology could be used in resource-limited areas; where accidents occur; where people are living (medical deployment into communities facing particular exposures); and in anticipated warfare situations with relatively little required technical knowledge. Discussions during the workshop highlighted that the combination of sensors with mobile applications and databases (e.g., accessible from a smart phone) may become a powerful method for rapid interpretation of results and access to information on targeted methods of treatment.

## 2.6 The evolution of the international S&T environment

2.6.1 In addition to the increasing globalization of both scientific research and industry discussed in Section 2.3, researchers in all parts of the world are taking advantage of improved information and communication technology (ICT) as well as lower prices and increased availability for many types of specialty chemicals and equipment to expand their research. This diffusion of these technologies remains uneven, and researchers in some countries still require assistance or face barriers in obtaining the knowledge and the technologies already available in other parts of the world, but the general trend is toward significant global access to S&T capabilities.

2.6.2 Expanding S&T capacity is yielding substantial opportunities for increasing cooperation and collaboration, along both traditional "North–South" lines as well as new "South–South" partnerships. So far the latter trend is less pronounced in chemistry than in life sciences because of the greater impetus for life sciences collaboration in public health and in developing a response capacity to outbreaks of disease, but it is nonetheless significant. All of these collaborations are greatly facilitated by the increasing ease of interdisciplinary teamwork in "virtual" laboratory settings.

2.6.3 The general trends of S&T expansion and collaboration can help promote a positive international environment, but certain conditions will need to be met to ensure that the developments support the goals of the CWC. A stable and equitable regulatory environment is very important for both the academic community and industry. More specifically, removing barriers to access must be accompanied by effective implementation of the CWC at the national level (including relevant legislation) and promotion of a robust culture of compliance with requirements regarding safety and security of chemical activities. The discussions at the Spiez workshop underscored important current deficiencies, for example, in terms of controls at the university level, which generally remains under the radar screen for the OPCW and CWC and also pose challenges to national implementation.

 

2.6.4 In addition to the existing activities of its international cooperation and assistance division, the OPCW can further contribute to the continued development of this environment by implementing its own cooperation programs as well as providing a platform for a broader stakeholder community to share views and experiences and promote practical steps to enhance chemical safety and security. Two recent developments in this regard are the task force appointed by the OPCW Director General to advise him on chemical safety and security and the new temporary working group on outreach and education for the SAB.

## 2.7 Extending support for the CWC via outreach and education

2.7.1 The existing CWC verification regime and national implementing legislation are reaching relevant communities such as those parts of the chemical industry that are subject to regulation because of the types and quantities of chemicals they produce, process, or consume. But as illustrated during the workshop's discussions of new developments in S&T, the changing nature of the R&D environment, and the increasing role of highly versatile small-scale facilities that produce quantities below the present OCPF threshold, the existing regime does not reach all relevant communities. The academic community, in particular, currently has little knowledge of the CWC and the responsibilities that it imposes.

2.7.2 In addition to any changes in more formal regulations, the future success of the CWC will thus depend on promoting awareness of the Convention and its requirements among a wider audience. This will support improved implementation at the national level and, by engaging the scientific community, will help ensure that its members do not inadvertently contribute to proliferation or other hostile purposes such as chemical terrorism.

2.7.3 To reach wider audiences, emphasizing relevant CWC provisions, domestic laws and regulations, and responsible conduct and a culture of safety and security will be especially important. In general, the subject should be introduced to chemists and those in related fields as part of a broader context of the social responsibility of science, as well as framing CW issues as part of a wider spectrum of risk. More specific education and training can follow as needed.

2.7.4 It is important to remember that there cannot be a "one size fits all" approach to the design of outreach and education programs. Programs must be framed in ways that will be most relevant and engaging for the particular audiences—students at various levels, academics, industry, policy makers, individuals in different countries and regions of the world, and so forth.

2.7.5 The CWC National Authorities need to engage other partners about CWC-related issues within their national government, academic, and industrial communities to encourage the discussion of chemical safety and security and education. For example, there would be a clear benefit to including ministries of education in the discussions on outreach.

2.7.6 IUPAC, which enjoys wide international recognition among the chemical sciences community, has already worked with the OPCW on education and could assist the organization in mapping out new program areas, seeking partnerships and identifying its role for the future. There is a clear need to avoid duplicating the valuable work being undertaken by other organizations in the area of chemical safety and security, and therefore careful consideration of the specific role of the OPCW is required. In turn, IUPAC can operate through its national adhering organizations and partners, including national chemical associations and national academies of science, to encourage discussion and debate about responsible conduct of chemistry and awareness of the CWC.

2.7.7 Given the emphasis during the workshop on the importance of the increasing convergence of chemistry and biology, and the considerable work already underway with regard to education about biological safety and security, there may be opportunities for the CWC and BWC communities to share information and, in spite of the differences between the conventions, perhaps consider some common messages in their programs.

## 3. THE WORKSHOP

The workshop consisted of eight topical plenary sessions and an informal technical discussion (see Appendix for the workshop agenda). For each plenary session, two or three speakers were invited to discuss aspects of a topic related to a given S&T advance. A chair coordinated the speakers' contributions, and a discussant provided feedback and reaction to the presentations. Open discussion was held following each set of presentations as time allowed. An informal technical discussion was also held during the workshop; it consisted of two short presentations by experts in practical application of chemical and biological analysis techniques and a moderated discussion. Breakout sessions and a concluding discussion period provided significant opportunities for participants to further consider the information presented in plenary and the potential implications of new developments, and to provide input to help inform the report (see Section 4 for a discussion of some of the themes that arose).

The plenary and technical discussion sessions focused on specific topics as follows:

1. Overview and Background
2. Convergence of Chemistry and Biology
3. New Synthesis and Toxicological Analysis Methods
4. Developing New Materials and Delivery Mechanisms
5. Technical Discussion: New Developments in Technology and Anticipated Technological Challenges
6. Advances in Industrial Production Methods
7. Chemical Safety and Security: Possession, Transfer, and Acquisition
8. Defense against CW Agents
9. Chemical Safety and Security: Engaging the Chemical Sciences Community

What follows are brief summaries of the presentations and discussion during each of the sessions, provided for the reader's reference. These summaries are based on notes and comments captured by rapporteurs during the workshop. It should be emphasized that the views presented in these summaries do not necessarily represent a consensus of the authoring committee members or of the workshop participants.

### 3.1 Overview and background

*Workshop Welcome, Minister Andreas Friedrich*

Minister Friedrich welcomed the participants on behalf of the Federal Department of Foreign Affairs and noted the strong support of the Government of Switzerland for the CWC. He stressed the importance of S&T for the future of the convention and the contributions that the workshop could make to assist in the preparations for the Third Review Conference.

*Perspectives on the Context of the CWC Review Conference, Ambassador Ahmet Üzümcü**

Ambassador Üzümcü, Director-General of OPCW, welcomed the participants and expressed his appreciation to IUPAC on its initiative in organizing the workshop. He noted that, although the work of destroying the world's existing stocks of CW will continue for some years to come, the OPCW needs a long term vision to take existing and emerging demands and trends into account. He noted universality, effective implementation, responses to the changing nature of the threat, and the impact of S&T as among the obvious challenges. He expected developments in S&T to be a major focus of attention at the Third Review Conference. He noted the importance of the workshop and similar endeavors to the future of the Convention:

*The full text of the Director-General's remarks may be found at http://www.opcw.org/index.php?eID=dam_frontend_push&docID=15319.

> The civil society, the scientists and the academics nourish and enrich debate. This intellectual endeavor is selfless. Because it is driven by knowledge and expertise, it provides energy and direction to policy. So, as we head towards the next Review Conference, I urge you to once again make your contribution in sensitizing, in informing and in advising policy makers on what you see as the challenges ahead. As the OPCW prepares to enter a new phase in its life, these inputs assume critical importance.

The Director-General described several aspects of the work of the OPCW to which S&T is particularly relevant, such as ensuring the continued effectiveness of the verification regime. He described the SAB, noting that the chair and several members were attending the workshop, and discussed its work. He also announced that the OPCW would be recruiting a science policy adviser to assist him in formulating policy for the Organization and creating more effective liaison with the scientific community. This is part of his general goal of strengthening cooperative relations with the global chemical industry as well as with scientific and academic institutions. He also stressed the importance of promoting ethical norms against the misuse of chemistry, and of raising awareness among scientists and engineers about the norms and regulatory requirements of the CWC. He indicated that he sees an important role for IUPAC in these endeavors and hopes that the Third Review Conference will provide additional impetus.

*Workshop Objectives, Leiv K. Sydnes*

Professor Sydnes, a former president of IUPAC, began by noting the important role that developments in chemistry had played in human history, from the Bronze Age to modern pharmaceutical products and protection for crops. He noted that improved chemical safety has been achieved in recent years through several international initiatives, including Responsible Care, the Registration, Evaluation, Authorisation and Restriction of Chemical Substances (REACH regulation), and Strategic Approach to International Chemicals Management (SAICM). Although the resulting regulations now mainly affect the handling of chemicals used in the chemical industry, they will gradually also impact the use of chemicals in research laboratories. One consequence of the new regulatory environment created by these regulations and guidelines is that we will learn more about safety limits and toxicity of chemicals than we have done in the past. Such knowledge is in principle beneficial, but it may also be misused, and he provided several examples of such dual use to illustrate the relationship between chemical safety and security. He echoed the concerns expressed by Ambassador Üzümcü about the relative lack of knowledge among chemists and chemical engineers about the CWC and the limited attention currently given to ethical issues in chemistry education. Professor Sydnes also provided an overview of the activities of IUPAC and described the two workshop on trends in chemical S&T the union had organized for prior CWC review conferences. He then described the topics to be covered during the workshop, noting that a number of the topics offered the opportunity to build on the results of the previous workshops.

### 3.2 Convergence of chemistry and biology

*Advances in the Life Sciences, Andrew Pitt*

Science is now multidisciplinary and integrative, and the convergence of chemistry and biology (among many areas of science) is inevitable. This trend has had a significant impact on the manner in which biological research is undertaken. This is particularly true in the pharmaceutical sector where, in the postgenomic era, biological products are increasingly relevant in areas commonly dominated by relatively low-molecular-weight chemicals.

This process is driven by a growing understanding of the modulation of biology and of the more efficient targeting of specific genes. High-throughput next-generation sequencing, for instance, is being undertaken with broader scope, with smaller cell sampling, and by focusing on individual cell behavior. From 2007 to 2010, the number of complete genomes rose from 2519 to 6500 (the majority in 2010 being large eukaryotic organisms). There have also been fundamental changes in approaches to studying biology, from a focus on individual proteins to an increasing emphasis on complex systems and interacting molecular networks.

The rapid growth of new areas of interdisciplinary science, such as the "-omics", the study of biomarkers, and systems biology have appeared alongside waves of new *enabling technologies*. Nanotechnologies, bioinformatics, and systems biology have facilitated the transformation of information into knowledge about biological processes. These technologies have increasingly engaged mathematicians, modelers, and statisticians who are now involved in biology, along with biologists, chemists, and physicists.

#### *Synthetic Biology and Biomediated Synthesis of Organic Chemicals, Pawan Dhar*

In synthetic biology, which is the controlled construction of biological systems, systems are composed one part at a time. Recent developments in this area are promising, and products based on the use of synthetic biology have already found their way to market. For instance, companies are selling DNA printers to synthesize one's own DNA. Other products include antimalarial compounds (e.g., artemisinin), isoprenoid compounds, cosmetic surfactants, and bioacrylic paints.

Although predicting the direction of the science is difficult, the technologies currently indicate a trend towards faster, cheaper DNA synthesis, whole genome cloning, the automatic design of biological pathways, synthetic chromosomes, altered genetic codes, RNA structural engineering, customized genetic circuits, and applications based on synthesized cells and predictive genome engineering. Long DNA synthesis looks set to become a mature technology although the lack of absolute control (i.e., the ability to synthesize complete organisms) will continue. Progressing economies such as India will be big investors in this area.

One new area of research noted by Dr. Dhar, given the nickname "junkomics", has focused on the synthesis of molecules from segments of intergenic (non-coding) regions of DNA that show no evidence of transcription. Such research centers around the question of how such non-coding regions of DNA can be transcribed and translated into functional peptides and proteins. This research has revealed untapped potential in the unexpressed genome and evidence for potential therapeutic properties existing among the peptides and proteins produced. However, it is recognized that non-coding DNA might also be used to identify and produce toxic chemicals and biological molecules with harmful effects.

#### *High-Throughput Identification of New Antibiotics, Douglas Weibel*

The workshop heard of recent developments in the use of high-throughput methods for the identification of pathogenic agents. Current identification of pathogens is generally constrained to centralized laboratories using large equipment, large teams, and requiring large budgets. In addition, the challenges associated with sampling and sample transport continue to be a bottleneck and burden on rapid identification processes.

There is a clear requirement for remote (i.e., field-based) pathogen detection. Such detection techniques must be transportable, small, inexpensive, enable a fast turnaround, and function with no power source. They must also allow the sample to be collected and tested in the same place. Small, robust chemical devices now exist that can help to fulfill these criteria. For example, devices are being developed to screen metabolites and small molecules produced by bacteria (to enable bacterial identification based on a unique metabolic fingerprint). The analysis of data produced by such devices can in some cases be enabled by a mobile phone application. Bacteria that can degrade specific chemical agents have also now been produced.

The identification of specific bacteria has clear relevance for the BWC, but the additional ability of these techniques to detect and identify small molecules bears relevance to the CWC. Portable detection of select chemical agents is foreseeable as such types of technology further advance.

 

*Discussant, William Kane*

As Dr. Kane noted, with regard to the CWC, the boundaries between chemistry and biology were clearer in 1993 when the Convention was opened for signature. New developments in life sciences and other areas of technology show a clear and consistent trend towards the convergence of disciplines across biology, chemistry, engineering, and information technologies. Three themes characterize this convergence: the pace of change (things are speeding up), the spread of knowledge and documentation of it, and the teamwork involved.

The CWC recognizes the uses of toxic chemicals that provide benefits to mankind, and the existence of such chemicals means that they will always be available to misuse. However, this misuse of toxic chemicals is prohibited by the Convention regardless of origin or method of production. The definition laid out by the CWC is forward-looking, and biological processes are not excluded. However, a clear understanding of the term *production by synthesis* is still required for the implementation of the Convention.

When viewed in isolation, many of the advances in the biosciences may seem to be of little direct relevance to the CWC. However, when taken in combination with developments across the sciences, for instance, with the continued synthesis of new, highly toxic chemicals such as those used to fight cancer, some recent developments in synthetic biology do have some relevance to the CWC. As convergence continues to occur across the sciences, separate regulatory regimes continue to exist. Reconciling the changes in S&T with these disciplinary regimes is a likely ongoing challenge for the CWC and BWC States Parties.

## 3.3 New synthesis and toxicological analysis methods

*New Catalytic Methods/Biocatalysis, David StC Black*

Green chemistry is a relatively novel but increasingly important approach to doing chemistry which aims to enhance human welfare and quality of life, enhance environmental protection, and promote the sustainability of chemistry. It strives to reduce or eliminate the generation of hazardous substances and to reduce or eliminate the negative environmental impact of chemistry.

This process occurs throughout the scientific steps involved, not necessarily simply by eliminating the use of hazardous starting materials. Green chemistry involves the consideration of all materials used in experiments and their intrinsic risks with the goal of minimizing negative impact and maximizing process efficiency. The practice of green chemistry is based on the use of alternative (renewable, less toxic) feedstocks, the use of innocuous reagents, the employment of natural processes such as biocatalysis for efficiency and selectivity, the use of mild solvents and reaction conditions, and the minimization of energy consumption. Green chemistry has the potential to have significant positive economic impact due to savings in terms of regulation, control cleanup, and remediation. Developing and applying the principles of green chemistry may thus have positive implications for the CWC.

*High-Throughput Toxicological Screening, Andrew Pitt*

High-throughput toxicological screening has seen a number of developments and trends, particularly in the area of chemical genomics: understanding genetic regulation, phenotype characteristics, and biological pathways using small molecules as probes and modulators. Chemical genomics can either be target-based (often using protein binding assays or reporter gene assays) or cell-, organism-, or tissue-based (phenotype-based screening). Trends in this area include the use of techniques based on robotic systems and the use of large, validated single-compound libraries. This indicates that the science has moved away from the use of combinatorial libraries. In addition, there has been a marked decrease in the scale of traditional assays (from volumes of ~50 to ~4 µL) with faster throughput.

Methodological changes have had implications for the outputs of high-throughput screening. Readouts are providing information on a bigger scale, i.e., an understanding of the effects on the whole organism is being sought, not just on specific molecular targets. A crucial area of research is in predictive modeling methods to improve the extrapolation of data from in vitro to in vivo (systems pharmacology). In summary, screening of drugs for their effects in cellular systems is now faster and methods are being improved to present the overall physiological effects of drugs and chemicals.

*Discussant, Robin Black*

Dr. Black noted that clear benefits are drawn from the use of biocatalysis in chemical synthesis, and the chemical industry has clear drivers to do this. For chemicals that are listed in the Schedules of the CWC, all can be produced by relatively simple chemistry. Halogenation for the synthesis of nerve agents may be one area where additional vigilance should be applied in the context of the CWC, and particularly for the OPCW's verification activities. However, he noted that it is difficult to see many further applications of biocatalysis to the production of Scheduled CW. The use of such methods for the production of incapacitating agents is another question entirely, and here there are many possible applications.

In the area of chemical defense, soft decontamination measures have been an area of research which is of relevance to the CWC and to the activities of the OPCW. For instance, one line of research has studied the use of esterase compounds as catalytic scavengers as therapy against specific nerve agents.

Previous workshops have extensively addressed the issue of drug discovery. The potential of screening libraries and high-throughout methodologies has relevance to the identification of potential future CW agents, but currently there is no evidence that such techniques have been applied for this purpose. Advances in high-throughput drug screening assays have potential benefits in the development of therapeutics and detection devices, and it is important that the OPCW keeps abreast of developments in this field. These technologies thus have clear beneficial uses, and the latent potential for nefarious use has not so far occurred.

Participants of the workshop also noted that it was important to remember that traditional CW are not high-value pharmaceuticals. Much of the attractiveness of traditional CW is that they are based on simple S&T, which was at the forefront of science in the 1940s and 1950s.

### 3.4 Developing new materials and delivery mechanisms

*Development and Applications of New Nanomaterials, Ijeoma Uchegbu*

The development of new polymers, lipids, and other carrier materials for drugs or genes is an area of active research. These carriers may be used as components of nanomedicines, in which the properties of the carrier influence the biodistribution of the therapeutic agent that is bound or complexed with it. Both the chemical properties of the carrier (e.g., the relative hydrophilicity and hydrophobicity or the conjugation of "functionalizing" molecules to target particular cellular receptors) as well as physical properties (such as size and shape) influence the uptake and residence time of a drug in the body. These types of nanomedicines have a wide range of applications, including improved delivery across biological barriers such as the blood–brain barrier, prolonged residence time in the blood (reduced clearance in the liver), and improved targeting to particular cell types. Several examples of nanomedicine systems can be identified, including the delivery of drugs to the brain and the delivery of chemotherapeutic agents to tumors. A significant motivation in the development of nanocarrier delivery systems is a desire to improve medical treatments, and continued development and movement of such products into the clinic is anticipated. However, the knowledge that enables the improved delivery of therapeutic drugs and genes may also have potential misapplication to the delivery of agents such as CW. As a result, continued awareness of developments in the field as it advances will be useful.

*Report on Incapacitating Chemical Agents Workshop, Stefan Mogl*

A summary was given of a technical workshop on incapacitating chemical agents (ICAs) held at the Spiez Laboratory in Switzerland on 8–9 September 2011 [4]. VERIFIN and Spiez Laboratory organized a joint workshop with a technical focus on ICAs with the objective of bringing together policy and technical experts to clarify the technical questions that affect policy discussion on these agents. The principal findings of the workshop covered the nature of ICAs, their possible effects, how they may be produced and the impact of new technologies for their production, how they may be used, their detection, and how to prevent abuse.

*Discussant, Neil Davison*

Issues relating to ICAs may be divided into four areas: effects, definitions, utility, and broader risks. In terms of effects, Dr. Davison noted that there is no such thing as a "safe" incapacitating chemical. The use of anesthetic agents for these purposes involved carrying out anesthesia on numbers of people where dose adjustments are not possible, continuous medical care is not possible, and exposure is nonconsensual. No agreed definition for ICAs currently exists, and there is no clear scientific line between a chemical warfare agent and an incapacitating agent. A range of potential risks is associated should ICAs be used for law enforcement or other purposes, and any use will require training, aftercare, antidote treatment, and complex logistics. There are also broader risks associated with ICA proliferation, including the likelihood that such chemicals will undermine the norms of the CWC. Advances in S&T are not likely to resolve these potential technical and ethical issues, and discussions on ICAs and their relationship to the CWC will involve political, legal, and other inputs.

*Discussant, Jürgen Altmann*

Scientists are beginning to understand some general principles and strategies for the encapsulation of drugs, genes, and other materials and are gaining an increased understanding of how specific biological targets can be accessed using encapsulation as a delivery strategy. Within the set of active research on new delivery mechanisms, Dr. Altmann noted that the use of nanotechnology to develop systems that can be delivered through inhalation or aerosol exposure would be the most relevant to concerns regarding misuse. Some topics he highlighted for additional thought and discussion include:

(a) Expanded genomic knowledge—how might this new knowledge affect possibilities for genetic targeting?
(b) Synthetic biology and the do-it-yourself synthetic biology communities—how does the risk change if people can, for example, create their own viruses?
(c) Verification issues—how do small-scale activities in nonmilitary environments interact with current nonproliferation regimes? Will the current regimes remain relevant as the technological advances described here continue to develop?

Maintaining the current verification regimes may become increasingly challenging as technology becomes more useable at an individual level, and the community might need to adjust or modify some elements of the current arms-control regimes. It will be critical to have valid, trusted technology assessment to inform any changes. It would be beneficial to identify ways to enable in-depth assessments of the potential for new and emerging technologies to be used for malign purposes.

## 3.5 Technical discussion

### *New Developments in Technology and Anticipated Technological Challenges, Oliver Terzic and Mattias Wittwer*

There are numerous analytical challenges for inspection and verification under the CWC regimes today, and additional challenges may emerge in the future as new manufacturing methods are developed. Some new manufacturing methods may even use biological systems to manufacture chemicals, which is a factor not considered under the current analytical methods used for inspection and verification. Drs. Oliver Terzic and Mattias Wittwer presented to the workshop on these challenges and some emerging technology that may help address those challenges. The session began with an overview presentation by Dr. Terzic, who outlined the basic constraints imposed under the inspection protocols. In chronological order, analytical equipment must be moveable and durable enough for transport, by air and by truck. Facilities are often located in remote areas, and the level of vibration from transport across unpaved roads, for example, must be taken into account in instrument design. The equipment must also be tolerant of a wide range of environmental conditions (dust, humidity, cold, etc.). Once in place, the equipment must be online and calibrated as quickly as possible as inspectors have a limited window of time for sample collection and on-site analysis. The instruments must also be appropriate for users with limited technical training. Finally, as inspectors may face a variety of manufacturing methods, samples may be prepared from a variety of matrices (solid, liquid, tar, etc.). In the future, as OPCW considers the use of biomonitoring, new analytical challenges are expected.

Dr. Wittwer presented on some of the developments in the use of mass spectrometry to analyze complex samples contained within complex matrices. In particular, he highlighted work using matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) that uses a so-called "soft" ionization method that enables the direct analysis of large biological molecules. It is hoped that, through the development of new libraries of biomarkers and data analysis techniques, a "universal tool" for identification of biological samples in complex matrices can be developed. Today, even some whole, intact biological molecules can be analyzed. If thoroughly developed, this type of direct analysis could significantly reduce the need for sample cleanup and preparation, but it is in a very early stage of development. Such instrumentation represents a significant advance in capability, but also introduces new challenges. In particular, identification of complex spectra emerging from such complex samples requires the development of new data analysis methodologies and libraries. Though currently still being examined at the basic research level, this technique could be a powerful tool for analysis under the OPCW, especially for biological-based samples.

### 3.6 Advances in industrial production methods

*Changes in the Chemical Industry, Detlef Männig*

Changes in the global production of chemicals continue to occur, and many of these developments are striking in the Asian region. From 2001 to 2010, the number of OCPFs declared in Asia more than tripled, with current chemical production in Asia equaling the sum of European and American figures. China showed the most significant growth in Asia, representing approximately half of the market. In 2010, China was the biggest producer of chemicals in the world, with an industry worth over €570 billion. China and the Asia-Pacific region represent approximately 75 % of the global investment in chemical production.

Changes in technology and economy have also resulted in changes to chemical production. Some trends include the use of larger plant sites that may include "industrial parks". These can take the form of small, unconnected chemical production facilities co-located in a geographic area or plant site that allows for companies that are integrated with each other (e.g., one supplies materials for another or uses the waste products of a plant to manufacture materials). These changes may have direct implications for the definition of a "plant site" and verification activities under the CWC. However, it should also be noted that in addition to these larger facilities, there has also been a trend towards specialized, automated, and smaller chemical production sites. Overall, the types and scope of chemical manufacturing facilities are changing rapidly around the world.

The increased number and variety of regulation to which the chemical industry is subject, as well as the new strategic opportunities presented by sustainability, have driven a shift in chemical industry business models from products to solutions. New strategic alliances with other industries, such as the automobile industry, have been formed. Changes in speed have also occurred across the industry, impacting such areas as modeling, time to market, life-cycle analysis (i.e., during early product development one looks forward to issues post-marketing), rapid screening, and supply chains. Outsourcing to service companies continues to increase and continues to be an issue for OPCW inspections. It is currently unclear what the implications of these changes might be for the OPCW and the CWC, but awareness of the changes should be maintained.

 

Globally speaking, CAS Registry numbers (which indicate new chemical products or derivatives) show a sharp increase in the numbers of new substances since late 1990. Currently, ca. 12 000 new substances are registered daily.

The recent Ekeus report, published by the OPCW Technical Secretariat, made a number of recommendations, some of which are directed towards the relationship between the OPCW and the chemical industry [5].

*Microreactors, Petteri Elsner*

Continuous-flow reactors such as microreactors have now entered into chemical production. Although the mainstream production of pharmaceutical chemicals still takes place in batch processes, a number of specialized companies are increasingly applying continuous processes to the bulk production of fine chemicals, including pharmaceuticals.

The use of continuous-flow reactors for the production of such chemicals in industry demonstrates a technological change that has taken place in the last five years. The scale-up of chemical production requires robustness that until recently, flow reactors could not provide. A toolbox approach that employs batch and continuous processes in a manner that enhances flexibility, speed, and modularity is becoming an attractive option for companies specializing in large-scale production of pharmaceuticals and fine chemicals.

Microreactors play a central role in the continuous synthesis of chemicals. They enable continuous processes based on plug flow reactors with minimal volume of reagents, rapid dynamic responses and robustness, good temperature control, and efficient mixing. Various specifications exist for industrial microreactors, some are used for development chemistry (low flow rates to test channel geometries) whilst others are used for production (these are a key part of the scale-up process and are multipurpose and modular). Microreactors are now designed with scale in mind, with microreactors used for sample (gram scale) to large-scale (>50 tonne campaigns). Parallelization ("scale-out") is now avoided. Technological hurdles remain, however, and a greater degree of flexibility is required. The current state of the art makes three types of reaction suitable to microreactor production:

- Type A: very fast (<1 s), controlled by mixing process, yield increase is achieved through more efficient heat exchange;
- Type B: 10 s to 30 min, predominately kinetically controlled;
- Type C: >30 min, might be converted into type A or B reactions through process intensification; requires ability to process high temperatures and pressures.

Any reaction that forms a precipitate, either as a product or as an intermediate during a reaction, poses challenges for microreactors that are as yet insurmountable. In addition, care must be taken when adding additional synthetic stages to the series of reactors. Any addition can have effects that influence the rest of the reaction system, and intensive modeling and evaluation are required prior to a successful production system. Further developments resulting in greater flexibility and robustness of these systems may result in broader application of these systems to manufacturing processes.

*Flexible Manufacturing/Synthesis Systems: Modular Systems, Mark Ladlow*

Continuous-flow devices for use in drug discovery phases of chemical production are now on the market (about 10 types of device exist). Flow rates usually are approximately 50 mL/min on each channel. These devices employ multiple pumping channels, offer flexible configurations, and are software-controlled to enable multiple experiments.

Such devices could be used to create combinatorial libraries, but this is not generally recommended. So far, microreactors are only used on a widespread basis for reactions that are difficult under batch conditions, or that are hazardous (e.g., nitrations). The synthesis of pharmaceutical drugs has been successfully demonstrated. For instance, Prozac has been synthesized with continuous chemistry, and the methods were found to be efficient and scalable. Achievable conversion was not 100 %, so purification through conventional methods was required. Opioid agonists have also been synthesized using these methods in an automated system, including in-line purification of intermediates, and the process yielded a greater amount of product than conventional synthesis methods.

Laboratory-scale flow synthesizers provide excellent control of reactions, allow novel reaction conditions that are not possible in batch chemistry, and are scalable. There are current limitations (e.g., suspensions are difficult to handle), and these are being addressed through devices such as tube-in-tube reactors. However, these integrated systems are still at the R&D stage. The skills and training of the scientists working with flow reactor systems remain at least as important as for more conventional batch production chemistries.

### 3.7 Chemical safety and security: Possession, transfer, and acquisition

*Libraries/Stockpiles of Chemicals and Toxic Materials, Hikmat Hilal*

An-Najah University is one example of how chemical safety and security can be managed in an academic setting. The university uses a multifaceted strategy and maintains a documented chain of custody for chemicals from purchasing to disposal. When designing the storage facilities, care was taken to consider the full range of events and activities that could result in a release of hazardous materials. As a result, the facility uses engineering and procedural measures to minimize the probability of release or loss and to reduce the impact if such an event occurs. University chemical stocks are maintained in a central store, and purchase orders are documented in an online database. Smaller amounts of chemicals sufficient for weekly research and teaching needs are held in departmental stores, with withdrawals also documented. Only limited amounts of chemicals are stored on laboratory benches or shelves, and a teacher oversees student laboratory activities. Any excess chemicals are returned to the central store at the end of the week. The chemical storage facilities incorporate various chemical safety features, including separated storage for chemicals such as acids and bases, fire sensors and sprinklers, and systems to help prevent chemical spills during events such as earthquakes. Finally, the university provides training and outreach on safe chemical practices, including making available student pamphlets written in Arabic. Although these types of systems and policies require funds to implement, they help to provide a framework for safe chemical management. Though no one system can be employed across all schools, Dr. Hilal indicated that An-Najah University is ready to help others as requested in addressing the safe handling and storage of chemicals.

*Delivery and Storage Mechanisms for Research Materials and Chemicals, Wayne Temple*

The United Nations Globally Harmonized System (GHS) of classification and labeling of chemicals is a global approach to defining and classifying hazardous chemicals (through physico-chemical hazards and their effects on human health and the environment). New Zealand is one country that has adopted the GHS into its own legislations, through the Hazardous Substances and New Organisms (HSNO) Act (1996). All universities in New Zealand must adhere to this act through an HSNO Code of Practice. This code of practice included standards for laboratories, requirements for hazardous substances, and laboratory security. The code puts in place a management structure of authorized users and laboratory managers that are accountable for all purchasing, transport, and storage of chemicals in their universities. Chemical suppliers require proof of HSNO compliance, provided through certification. New Zealand universities often use tracking software to account for chemicals from receipt to disposal.

*Issues with Chemical Acquisition and Transfer, Muhammad Iqbal Choudhary*

Some developing countries have significant gaps in regulating the acquisition and transfer of chemicals, with the weakest link being the distribution to end-use customers. Local agents, middle men, suppliers, and contract manufacturers are all common sources for procurement of chemicals. This is due, in part, to the business structures that can exist within developing countries where there are often only a few large chemical suppliers, but many middle men and local agents. Often the result is that any chemical traveling from the manufacturer to the distributors and then to the end-user first passes through long chains of individuals and small-scale operators before arriving at its final destination. This presents significant challenges for monitoring, tracking, and controlling chemicals nationally because the intermediaries may not have detailed or appropriate storage protocols, facility security, or record-keeping in place.

One area where this system can be seen is in academic procurement of chemicals. For example, universities in India must procure chemicals through open bidding systems to be in accord with institutional auditing requirements. As it is an open process, disreputable distributors cannot be excluded from the bidding process. In addition, this procurement process can be quite lengthy, and as a result, no system for just-in-time purchasing exists. To maintain adequate quantities of chemicals on-site for education and research purposes, chemicals are often bought in bulk and then stored for long periods of time. However, little regulation may be exerted on universities with regard to compliance, and institutions may have a strong culture of academic freedom. As a result, few internal controls are in place to monitor chemical purchasing, and the situation can signal an overall lack of accountability and transparency. Thus, scientists tend to procure chemicals themselves through alternate means, and bartering systems exist between students for sharing and distributing chemicals. Often no system for tracking these purchases or maintaining inventories of purchases is in place to monitor these activities.

*Discussant, Patrick Lim*

Dr. Lim noted that speakers highlighted a number of points regarding inventory control, regulation, and legislation as aids to nonproliferation efforts. With regards to inventory, there are three key areas to consider: libraries of materials, accountability, and record keeping. Care must be taken to ensure that all of these items are linked and maintained. This training should begin in the university, where education in laboratory practice could integrate chemical safety and security. This integration could eventually aid the States Parties by encouraging best practices and facilitating a culture of safety and responsibility within academic settings. In response to a question regarding mass balance in inventories, it was noted that both inputs and outputs from the system should be recorded, and inclusion of chemical wastes is one way to retain an understanding of the mass balance of materials within an organization.

Many industrial settings must adhere to regulatory requirements that support safety and security practices. Academic settings have specific features that also must be considered with regards to safety. Unlike industrial settings, the volume of material on site, especially of chemicals of concern, is usually rather small. However, in some cases, procurement procedures necessitate the stockpiling of chemicals in order to meet research and educational needs. If it takes 3–6 months for a chemical to arrive after being ordered, advance planning is required. It should also be noted that in a university setting, there is an abundance of chemical expertise available. This can be an advantage for understanding the risks posed by certain compounds.

The increase in online ordering of chemicals was also noted. For example, 42 % of Aldrich research sales are reported to be online, and chemicals can also be purchased through online auctions in some cases. This may become a greater issue of potential concern in the future.

### 3.8 Defense against CW agents

*Detection Techniques for CW Agents and Related Compounds, Robert Simonson*

Detection techniques have applications in verification and compliance (requires adherence to the OPCW proficiency standards), weapon demilitarization (to ensure destruction of the materials), and personnel protection (such as detect-to-warn systems). Given these applications, portability, clear requirements and standards, and a clear understanding of the strengths and limitations of different analytical method are required.

Technical requirements should be considered in the context of the application. Common concerns include whether sample cleanup is needed, the time available for the analysis, and the limit of detection for the instrument. One often-cited area where improvement is desired is in miniaturization to support portable, reliable analytical methodology at the site where a sample is collected. The talk focused on the work being done to miniaturize gas chromatography coupled with mass spectrometry (GC-MS)*, a common analytical technique.

GC is a technique where the chemical constituents of a sample are injected in gas form into a column where the components are then separated based on their differential affinity between the chemically treated column and the gas. This allows separation of the components, which then enables the analysis of the individual compounds by MS or an alternative identification method. Methods for enabling optimal separation of complex mixtures with similar composition to chemical agents have been achieved, though one particular advance—improved injection technique on a small scale—has been only recently identified and resolved. The understanding of how to do fast GC injections is being applied to develop micro-GC systems today, which also often take advantage of multiple columns in series, each with a different chemical affinity, to improve analytical capability.

MS presents additional challenges because of the fact that the analysis must be done in a vacuum chamber, which requires large pumps. Work is being done to make high-pressure, portable MS a reality, but these are in the research phase. Note that the potential improvements in GC described above would simplify the analysis with MS, but would require an increase in the rate at which the analyses could be done, which adds an engineering challenge to the problem.

Finally, it is important to note that there are many different forms of chemical detection, including swipe tests, the use of reactive materials exposed to the environment, and others.

### *Analysis of Complex Compounds, Volodymyr Zaitsev*

Development in high-resolution MS in recent decades has generally occurred in two areas: improved mass resolution and dynamic range for detectors (e.g., Fourier transform ion cyclotron resonance and Orbitrap) and introduction of ionization techniques that allow for analysis of large molecules in complex matrices, some even at atmospheric pressure [electrospray (ESI), matrix-assisted laser desorption (MALDI), and surface-assisted laser desorption-ionization (SALDI)]. ESI, MALDI, and SALDI are all considered “soft” ionization techniques, meaning that large molecules, such as polymers and biomolecules, are not broken into small segments by the method, but ionized in such a way that allows for analysis of large segments, whole molecules, and aggregations of molecules. These techniques allow the user to take advantage of the large dynamic range of the newer mass detectors. MALDI is quite common these days, but suffers from a few disadvantages, the greatest of which is the effects from the matrix upon which the samples are placed, which contains organic acids that are ionized along with the sample. These effects make it difficult to analyze compounds under 1000 Da in size and can interfere with the analysis of complex mixtures, such as those containing whole cells or organisms.

SALDI takes a different approach by using an inorganic matrix, such as porous silicon or carbon-based materials (graphene), within which to mount the sample. This new method complements the existing ionization methods and allows for analysis of small molecules within biological samples, which expands the range of targets appropriate for MS analysis considerably. Focusing particularly on the application of porous silicon, a technique known as DIOS (desorption-ionization on silicon), to SALDI, it is possible to demonstrate the technique’s applicability to the analysis of forensic compounds, screening for enzyme inhibition, and identification of metabolic products and proteomics. Chemical modification of the silicon surface, such as with fluorinated compounds, can provide additional benefits, such as reducing the susceptibility of the surface to dirt. Other modifications, such as doping the surface with metals or with nanoparticles, can allow for benefits such as increased sensitivity, but it is important to recognize that any modification can change the physical and chemical properties of the sample matrix, and the effects must be characterized completely. It is clear that SALDI-MS,

*The gas chromatography serves to separate the constituents or compounds from each other so they can then be individually analyzed and identified with the mass spectrometer. GC-MS is a useful technique for identification of CW because it allows for the analysis of complex mixtures and samples of the type found in manufacturing facilities.

using commercial or modified surfaces, provides new opportunities for analysis, but the technique is not widely adopted yet. This active area of research will continue to add functionality for mass spectrometric analysis and may enable significantly reduced separation and sample cleanup prior to analysis in the future.

*On-site Response: Medical Countermeasures and Decontamination, Peter Blain*

Discussions of on-site countermeasures for incidents involving CW are driven to some extent by the different civil vs. military requirements for response. With respect to the treatment of individual chemical agents, and in terms of human decontamination, further attention is required.

Cyanide, for example, is both difficult to diagnose and difficult to treat, and yet some of the most efficient improvised devices have used cyanide. It is generally accepted that the best treatment is oxygen, and if unconscious, dicobalt edetate, sodium nitrite and thiosulfate, or hydroxocobalamin. Novel antidotes such as cobinamide do exist, which has been shown to be effective orally and through intramuscular injection. Victims of sulfur mustard poisonings undergo symptomatic treatment, but no long-term treatment currently exists, even though over 50 000 victims still suffer from long-term health effects (most commonly these present as respiratory diseases and/or bone marrow cancer). The current treatment of nerve agent poisoning also remains unsatisfactory. For instance, due to the extremely rapid binding of soman to acetyl cholinesterase, no oximes are currently able to act as an antidote. Countermeasures for other nerve agents include bioscavengers and broader spectrum oximes. New research has also shown that intra-osseous lines are extremely effective routes for administering nerve agent antidotes. The rapid removal of clothes has recently been shown to be an effective step in decontamination. However, effective strategies for human decontamination need more attention in all three of its key objectives: to prevent further absorption, to prevent rescuer contamination, and to contain the hazard and prevent environmental spread.

*Discussant, Ralf Trapp*

As Dr. Trapp discussed, the issues of countermeasures and detection of CW are context-dependent. They depend on what chemical agents are available, what requirements exist for agents, and the nature of the threat. Different threat contexts will also have specific requirements and objectives for field equipment (i.e., warning, field analysis, verification, etc.). Although new developments have not yet been revolutionary in the field of detection, they have superseded some of the current OPCW technologies. For instance, high-resolution MS may have significant impact in investigations of alleged use of CW. However, when developing new instrumentation and procedures, or adapting those for inspection and validation purposes, it is important to recognize that the specifications will differ between instruments used on-site at a facility vs. off-site at an approved laboratory. In terms of how the development of effective medical countermeasures for CW have evolved, it is clear that short-term effects are not the only concern. Long-term effects, including those that will impact on mental health, are now also a relevant concern.

### 3.9 Chemical safety and security: Engaging the chemical sciences community

*Treaties Need Tending—The Importance of Outreach and Education, Robert Mathews*

The CWC was negotiated both as a revolutionary and an evolutionary treaty. It is revolutionary because, among other things, it is comprehensive and nondiscriminatory, it has routine inspections that intrude into civil industry, and it contains an anytime/anywhere inspections provision (the challenge inspection). It is evolutionary because it was designed to change and adapt with time, and indeed there exists within it a formal amendment procedure for technical alterations to the treaty—the treaty text is not set in stone.

If treaties are to be tended (i.e., looked after), an important theme when tending to the CWC is awareness-raising, education, and outreach. Following the joint IUPAC-OPCW Oxford meeting on this subject in 2005 [6], education was firmly placed in the wider context of multiple uses of chemicals.

Additional work was carried out on Codes of Conduct from 2005 to 2011, and this work sought to highlight the international obligations under the CWC, CWC-related laws and regulations, dual-use concerns, and inadvertent assistance to prohibited activities.

A new SAB Temporary Working Group on Outreach and Education will convene in April 2012 to discuss future work in this area. It will build on past work to develop tools and strategies for outreach and will learn from other regimes such as the BWC. Efforts on raising awareness for the BWC have highlighted that progress relies on long-term engagement and that effective metrics and indicators are essential in monitoring success.

Industry and academia have essential roles to play in this area, especially in the identification of *champions* to carry out much of the awareness raising. Champions may not be scientists; they could be located in politics. However, there is clearly value in high-profile scientists supporting such outreach activities.

## 4. FINAL THOUGHTS

The workshop included discussion sessions where participants were able to consider developments in S&T and their potential implications in greater detail. Key points arising from these small-group sessions were presented and discussed in plenary. Several themes emerged from these discussions and are briefly summarized below; these themes helped inform the report.

### 4.1 Continued progress in multiple areas of S&T

Science and technology continue to progress steadily in multiple areas covered at the workshop. For example, the synthesis and production of chemicals may be improved through the use of flow microreactors, which provide safety advantages for certain types of exothermic reactions or for reactions that involve toxic chemicals and byproducts. However, significant development work is required to optimize chemical processes in microreactor systems, and the flow chambers can become clogged by solids. Although the use of microreactors has become more widespread since the last CWC Review Conference, a trend that is likely to continue, dramatic advances have not been observed. It remains unclear whether use of microreactors will have significant implications for the production of CW.

Chemicals may also be produced through biomediated processes, an area that highlights increasing convergence between chemistry and other scientific disciplines, including biology. Developments in synthetic biology are also relevant to this trend. Toxins and bioregulatory molecules exemplify chemicals that are prohibited by both the BWC and CWC. As a result, both of the communities associated with both Conventions will need to continue considering how best to monitor relevant developments and address potential implications.

Delivery technology is another field in which steady progress continues to occur, driven largely by the development of improved medicines or chemotherapeutic agents. These delivery advances include encapsulation in nano- or micro-scale carriers, improved targeting and uptake in biological tissues, and improved ability to deliver large-molecular-weight molecules across biological barriers. Participants noted that new methods for the delivery of therapeutics could potentially be employed for more effective weaponization and delivery of toxic chemicals, although it was also emphasized during the workshop discussions that there is no evidence for this having taken place so far.

Developments continue in a variety of analytical tools, and opportunities exist to increase the technical convenience and applicability as part of the development of next-generation analysis and detection systems. In particular, systems that are simple and robust to use and that combine multiple types of analysis would be extremely useful. Although such devices are not currently available and the detection of toxins remains less reliable, participants suggested that it is only a matter of time before the technology meets necessary portability, robustness, and selectivity requirements. Miniaturization is also a key focus for future developments in field detection.

In the area of countermeasures, several continuing gaps were noted in capacity to respond to incidents involving CW. Further research on absorbents for decontamination purposes will likely be needed, and strategies such as regional support systems to help provide capacity for the effective medical treatment of CW victims may be useful.

The ethical, legal, and operational concerns surrounding riot control agents and incapacitating chemical agents will also continue to be a topic considered by the OPCW. Technological developments such as advances in effective delivery to targeted biological systems may be relevant. It remains a matter of consideration whether policy solutions such as new chemical schedules or the creation of international norms surrounding the use of these types of chemicals will be needed in the context of the CWC.

### 4.2 Pace and nature of advances

During the discussions, workshop participants noted that the pace of advances in S&T has quickened. Particularly in the medical and biosciences, a number of innovations, such as inexpensive and rapid DNA sequencing and synthesis, are driving advances forward rapidly. Chemistry is also increasingly taking place on ever smaller and more precise scales.

It was clear from the workshop discussions that developments in S&T are exciting and continue to be evolutionary, but the workshop did not identify disruptive and game-changing developments for the CWC. In the 10 years since the first IUPAC workshop, held in 2002, significant progress has continued to occur, but technologies have not yet had a dramatic impact on how CW could be produced or used. The nonlinear trajectory of new innovations makes them hard to predict, however, and changes and developments in S&T should continue to be monitored. It was noted that any application of new technologies to the production of traditional CW would depend on consideration of many factors, the outcome of which would depend on the country concerned. Many of the technologies discussed at the workshop may not yet be available to all developing countries or to all would-be proliferators. The availability of crude chemical mixtures, containing chemicals that are highly toxic, remains a concern.

Participants also noted that advances in S&T have numerous positive uses and are more likely to be beneficial than to be misused. The CWC seeks to strike an appropriate balance between preventing the use of toxic chemicals as weapons while not impeding the development and application of S&T for beneficial purpose; achieving this balance will continue to be important in the future. As the pace of technological advances continues, the OPCW's role in providing developing countries with opportunities to receive equipment and training will continue to be important.

### 4.3 Changing context of the CWC

The changing context of the CWC cannot be ignored. States Parties have traditionally been concerned with large-scale CW use and state-sponsored CW programs. The Chemical Schedules and inspection regimes also focus on certain types and quantities of chemicals, while the changing nature of chemical production may make other types of chemicals or facilities also relevant. As the CWC continues to evolve, it may be necessary to think about the relevance and effectiveness of the Chemical Schedules in the context of new developments in synthesis, production, and delivery as well as the changing nature of the global chemical industry.

Scenarios of smaller-scale CW production or of CW use by non-state actors may also differ from those of large state-sponsored programs. These differences extend beyond the agents and associated delivery systems that might be of greatest concern to differences in the requirements for effective detection and monitoring.

A central concept noted during the workshop is knowledge, and access to it. For example, scientific literature can now be accessed to a much greater extent on open-source search engines and information technology is an important enabler. As advances continue to be made, a trend toward the democratization of S&T is likely, and may have implications for the ongoing monitoring of relevant scientific progress and potential implications. There is also a fundamental issue of surprises in scientific developments that must be kept in mind. As a result, it will continue to be important to consider how surprises can be dealt with at the technological and institutional level.

### 4.4 Strategies for monitoring and planning

Workshop participants noted the need for a systemic approach to tracking and evaluating advances in S&T. Monitoring developments at key nodes of the innovation process might include the use of strategies such as open-source tracking and regular review of both published and "grey" literature, horizon scanning, and increased transparency by States Parties. As a result of global changes in the chemical industry, including the increasing use of contract manufacturing and networks of secondary chemical distribution, chemical supply chain concerns could potentially be mitigated (though not solved) by the development of global chemical tracking systems. Governance and stakeholder approaches may also include the promotion of responsible conduct as well as other methods such as national implementing legislation and regulation.

Scenario planning may be helpful to examine the concrete implications and/or applications of specific S&T developments in different contexts. Participants also highlighted the need to look at the system as a whole, and the utility of ongoing monitoring and assessment of relevant progress in S&T as part of this whole picture.

### 4.5 Education, outreach, and partnerships

Finally, the workshop discussions emphasized the roles that may be played by many communities in promoting chemical safety and security. Education, outreach, and awareness-raising will be vital, and issues related to CW may be effectively embedded within a broader context of risk and messages about the responsible acquisition, use, and disposal of chemicals. As has been raised in previous such workshops, any future work in the field of chemical safety and security should take place in conjunction with other initiatives such as Responsible Care, Green Customs, the WHO's International Program on Chemical Safety, etc. The value of regional approaches was noted in this context. National authorities, policy communities, civil society organizations, and scientific groups such as IUPAC and national chemical societies will also have complementary roles to play.

## 5. ABBREVIATIONS

| | |
|---|---|
| BRIC | Brazil, Russia, India, China |
| BWC | Biological and Toxin Weapons Convention |
| CAS | Chemical Abstract Services |
| CW | chemical weapons |
| CWC | Chemical Weapons Convention |
| DIOS | desorption-ionization on silicon |
| DNA | deoxyribonucleic acid |
| ESI | electrospray ionization |
| GC | gas chromatography |
| GC-MS | gas chromatography-mass spectrometry |
| GHS | Globally Harmonized System |
| GPC | general purpose criterion |
| HSNO | hazardous substances and new organisms |
| ICA | incapacitating chemical agent |
| ICT | information and communication technology |

 

| | |
|---|---|
| IUPAC | International Union of Pure and Applied Chemistry |
| MALDI | matrix-assisted laser desorption ionization |
| MALDI-TOF | matrix-assisted laser desorption ionization-time of flight |
| MS | mass spectrometry |
| OCPF | other chemical production facility |
| OPCW | Organisation for the Prohibition of Chemical Weapons |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemical Substances |
| RNA | ribonucleic acid |
| SAB | Scientific Advisory Board |
| SAICM | Strategic Approach to International Chemicals Management |
| SALDI | surface-assisted laser desorption ionization |
| S&T | science and technology |
| TIC | toxic industrial chemical |
| VX | notation for a nerve gas |
| WHO | World Health Organization |

## 6. MEMBERSHIP OF SPONSORING BODIES

***Workshop Organizing Committee*****:** IUPAC Workshop, Spiez, Switzerland, 21–23 February 2012: K. J. Hughes; K. Sawyer; K. W. Bowman; J. L. Husbands; L. Brüggeman; J. Lodding.

***International Advisory Board*****:** IUPAC Workshop, Spiez, Switzerland, 21–23 February 2012: D. StC Black (Australia); H. Chaimovich (Brazil); P. Coleman (South Africa); R. M. Hartshorn (New Zealand); A. Hay (UK); N. Jackson (USA); I. Makalinao (Philippines); A. J. McQuillan (New Zealand); G. Ogunmola (Nigeria); N. Senesi (Italy); D. Škare (Croatia); R. van Sloten (Netherlands); D. M. Templeton (Canada).

Membership of the IUPAC Executive Committee for the period 2012–2013 is as follows:

***President*****:** K. Tatsumi (Japan); ***Vice President*****:** M. Cesa (USA); ***Secretary General*****:** R. Deplanque (Germany); ***Treasurer*****:** J. Corish (Ireland); ***Past President*****:** N. Moreau (France); ***Elected Members*****:** S. Penczek (Poland); N. Tarasova (Russia); Q.-F. Zhou (China).

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## 9. APPENDIX: WORKSHOP PROGRAM

A list of workshop participants is available online at http://dx.doi.org/10.1351/PAC-REP-12-11-18.

**Monday, 20 February 2012**

18:00–21:00 **Welcome Reception**, Hotel Royal St. Georges, Interlaken

Early Registration
Welcoming Remarks

**Tuesday, 21 February 2012**

7:30 Buses depart from hotel for Spiez Laboratory

8:00–8:30 Late Registration, Spiez Laboratory

8:30–9:15 **Plenary Session 1: Overview and Background**

**Chair: Nicole J. Moreau**, former President, International Union of Pure and Applied Chemistry

**Speakers:**
Workshop Welcome, **Minister Andreas Friedrich**, Federal Department of Foreign Affairs, Switzerland

Perspectives on the Context of the CWC Review Conference, **Ambassador Ahmet Üzümcü**, Director-General, Organisation for the Prohibition of Chemical Weapons

Workshop Objectives, **Leiv K. Sydnes**, University of Bergen, Norway

9:15–10:45 **Plenary Session 2: Convergence of Chemistry and Biology**

**Chair: Gabriel Babatunde Ogunmola**, former President, Nigerian Academy of Sciences, Nigeria

**Speakers:**
Advances in Life Sciences, **Andrew Pitt**, Aston University, UK

Synthetic Biology and Biomediated Synthesis of Organic Chemicals, **Pawan Dhar**, Symbiosis International University, India

High-Throughput Identification of New Antibiotics, **Douglas Weibel**, University of Wisconsin-Madison, USA

**Discussant: William Kane**, USA

10:45–11:05 Coffee & Tea

11:05–12:30 **Plenary Session 3: New Synthesis and Toxicological Analysis Methods**

**Chair: Danko Škare**, Ru er Boškovi Institute, Croatia

**Speakers:**
New Catalytic Methods/Biocatalysis, **David StC Black**, University of New South Wales, Australia

High-Throughput Toxicity Testing, **Andrew Pitt**, Aston University, UK

**Discussant: Robin Black**, Defence Science and Technology Laboratory, UK

12:30–13:30 Lunch

13:30–14:40 **Plenary Session 4: Developing New Materials and Delivery Mechanisms**

**Chair: Alejandra Graciela Suárez**, Universidad Nacional de Rosario, Argentina

**Speakers:**
Development and Applications of New Nanomaterials, **Ijeoma Uchegbu**, University College London, UK

Report on Incapacitating Chemical Agents Workshop, Sept. 2011, **Stefan Mogl**, Spiez Laboratory, Switzerland

**Discussants: Neil Davison**, International Committee of the Red Cross, Geneva
**Jürgen Altmann**, University of Dortmund, Germany

14:40–15:30 **Informal Discussion** w/Coffee & Tea: **New Developments in Technology and Anticipated Technological Challenges**

**Guests: Oliver Terzic**, Organisation for the Prohibition of Chemical Weapons; **Matthias Wittwer**, Spiez Laboratory, Switzerland

15:30–17:00 **Break-out Discussion Session 1**

**Four parallel sessions:**

A) Chair: **Irma Makalinao**, University of the Philippines Manila, Philippines
Rapporteur: **Katie Smallwood**, UK
Room: TH-2

B) Chair: **Beat Schmidt**, Spiez Laboratory, Switzerland
Rapporteur: **Kathryn Hughes**, US National Academy of Sciences, USA
Room: TH-15 (basement)

C) Chair: **James McQuillan**, University of Otago, New Zealand
Rapporteur: **Catriona McLeish**, University of Sussex, UK
Room: TH-70

D) Chair: **Malcolm Dando**, University of Bradford, UK
Rapporteur: **Catherine Jefferson**, The Royal Society, UK
Room: TH-16 (basement)

17:15 Buses depart from Spiez Laboratory for Hotel Royal St. Georges

Dinner on your own

**Wednesday, 22 February 2012**

7:30 Buses depart from hotel for Spiez Laboratory

8:30–9:15 **Oral Report from Break-out Sessions and Discussion of Day 1**

**Chair: Nariyoshi Shinomiya**, National Defense Medical College, Japan

Presentations from Rapporteurs of Day 1 Breakout Sessions

Discussion

9:15–10:45 **Plenary Session 5: Advances in Industrial Production Methods**

**Chair: Amy Smithson**, James Martin Center for Nonproliferation Studies, USA

 

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| | **Speakers:**<br>Changes in the Chemical Industry, **Detlef Männig**, European Chemical Industry Council (Cefic) |
| | Microreactors, **Petteri Elsner**, Lonza, Switzerland |
| | Flexible manufacturing/synthesis systems; modular systems, **Mark Ladlow**, Uniqsis Ltd, UK |
| 10:45–11:05 | Coffee & Tea |
| 11:05–12:30 | **Plenary Session 6: Chemical Safety and Security: Possession, Transfer, and Acquisition** |
| | **Chair: Nancy Jackson,** Sandia National Laboratory, USA |
| | **Speakers:**<br>Libraries/Stockpiles of Chemicals and Toxic Materials, **Hikmat Hilal**, An-Najah University, Jordan |
| | Delivery and Storage Mechanisms for Research Materials and Chemicals, **Wayne Temple**, New Zealand National Poisons Center, New Zealand |
| | Issues with Chemical Acquisition and Transfer, **Muhammad Iqbal Choudhary**, University of Karachi, Pakistan |
| | **Discussant: Patrick Lim**, University of San Carlos, Philippines |
| 12:30–13:30 | Lunch |
| 13:30–15:00 | **Breakout Session 2** |
| | **Four parallel sessions: A, B, C, D** |
| | *Coffee and Tea will be available 14:30-15:00 to take into Breakout or Plenary Sessions* |
| 15:00–16:30 | **Session 7: Defense against CW Agents** |
| | **Chair: Mahdi Balali-Mood**, University of Medical Sciences, Mashhad, Islamic Republic of Iran |
| | **Speakers:**<br>Detection Techniques for CW Agents and Related Compounds, **Robert J. Simonson**, Sandia National Laboratories, USA |
| | Analysis of Complex Compounds, **Volodymyr Zaitsev**, University of Kiev, Ukraine |
| | On-site Response: Medical Countermeasures and Decontamination, **Peter Blain**, Newcastle University, UK |
| | **Discussant: Ralf Trapp**, CBW Consultant, Germany |
| 16:30–18:00 | **Breakout Session 3** |
| | **Four parallel sessions: A, B, C, D** |
| 18:15 | Buses depart from Spiez Laboratory for Hotel Royal St-Georges |
| 19:00 | Conference Dinner, Hotel Royal St-Georges |

 

**Thursday, 23 February 2012**

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| 7:30 | Buses depart from hotel for Spiez Laboratory |
| 8:30–9:15 | **Oral Report from Break-out Sessions and Discussion of Day 2** |
| | **Chair: Serhiy Komisarenko**, National Academy of Sciences Ukraine, Ukraine |
| | Presentations from Rapporteurs of Day 2 Breakout Sessions |
| | Brief remarks, **Philip Coleman**, Chair, OPCW Scientific Advisory Board, South Africa |
| | Discussion |
| 9:15–10:30 | **Session 8: Chemical Safety and Security: Engaging the Chemical Sciences Community** |
| | **Chair: Alastair Hay**, University of Leeds, UK |
| | Treaties Need Tending—The Importance of Outreach and Education, **Robert Mathews**, Defence Science and Technology Organisation, Australia |
| | Facilitated Discussion on Engagement |
| 10:30–10:45 | Coffee & Tea |
| 10:45–12:00 | **Workshop Conclusions** |
| | **Chair: Leiv K. Sydnes**, University of Bergen, Norway |
| | Facilitated Discussion of Workshop |
| | Findings and Conclusions |
| 12:00–13:00 | Tour of Spiez Laboratory and Workshop Photograph (Pre-registration required) |
| 12:15 | First buses depart from Spiez Laboratory for those who are not attending the tour or lunch |
| 13:00 | Workshop Adjourns (lunch buffet available with pre-registration) |
| 14:15 | Second buses depart from Spiez Laboratory for Hotel Royal St-Georges |