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The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

12 May 2015

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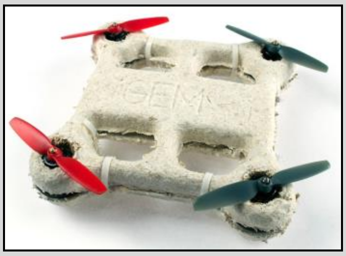


Image from [*wired magazine*]

Self-destructing biodrones are one of the many developments in the world of UAVs.

OPCW Inspectors during an Article VI Inspection.

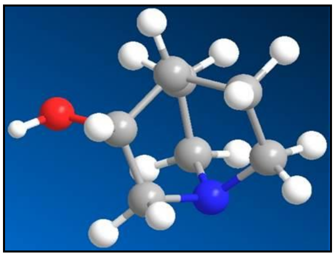
Inherent safety concepts applied to chemical production.

Welcome

Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

Today marks the 105th anniversary of the birth of Dorothy Crowfoot Hodgkin (1910 – 1994), who was awarded the 1964 Nobel Prize in Chemistry "for her determinations by X-ray techniques of the structures of important biochemical substances". We have previously highlighted the importance of X-Rays in understanding biomolecular structure; a relevant example to the CWC comes from work in the development of bioscavengers against nerve agents.

The S&T Puzzle



We congratulate our colleagues at the CTBTO, who were quickest to recognize 3-quinuclidinole (shown on the left), a schedule 2.B.09 chemical that is a key precursor to BZ (3-quinuclidinole benzilate, schedule 2.A.03). Thanks to all you who submitted answers!

This was by far the largest puzzle participation we have yet seen! Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1, and CTBTO 2.

Our next puzzle is a combination scavenger hunt and text analysis. We are looking for the five most frequently spoken words by our Director-General in public addresses from January to April 2015 (commonly used words such as "and", "the", etc. do not count). Without giving too much away, this covers 8 statements and 1717 words! Highest number of correct words identified in the top 5 wins the prize: a choice of requesting a featured topic, designing a puzzle, or receiving a beverage hand selected by the Science Policy Adviser. Send answers by email. There is also a bonus prize for the "best" visualisation of the Director-General's words. Good luck!

News and Updates

Recently published reports and newsletters:

Handbook of Toxicology of Chemical Warfare Agents (Second Edition); table of contents and abstracts can be viewed online.

Science Fun:

May is a month of many celebrations that inspire ideas for fun science which leads to hours of debate on what should fill the pages of science fun. The obvious choice for a May newsletter arrived (with great fanfare) on this months first Monday, greeting us with "May the 4th be with You!" in celebration of "Star Wars Day". Now, 38 years after the original movie was released, we take a look at the science of Star Wars and how far from reality it is today. While we encourage questioning of the science behind what we see on film (for example, laser physics and slow digestive processes), don't snicker: planets like Tatooine may actually exist (and not just one, but many), the force may already be with us and you might even be able to purchase some of it!

Was R2-D2 using technology based on graphene? Image: Screenshot from Star Wars/Lucasfilm/20th Century Fox (through *Science Alert*).

Following the original storyline, we begin with droids: here is one you can build at home (with simple instructions). With an appropriate neural network, you may be able to add Artificial Intelligence (AI) as an upgrade. Is there need for an emotion accessory too? Add some graphene, and the ability to generate 3D holograms could be the next addition (details here). Alternately, given all the wearable and implantable gadgets we cherish, should the droids receive the most enabling technologies?

Spiez Laboratory 2014 Annual Report.

A report on The Global Pandemic of Falsified Medicines: Laboratory and Field Innovations and Policy Perspectives.

Science and technology roadmap for graphene (details here).

The World Academy of Sciences (TWAS) Newsletter: The Power of Science Diplomacy.

United Nations Global Pulse 2014 Annual Report (highlighting Big Data innovation projects in sustainable development).

Reports on the use of Twitter by international organisations and world leaders.

April 22 issue of *inno4dev*, UNDP Innovation News.

April 2015 issue of International Council for Science (ICSU) Newsletter.

Science and education resources:

Celebrating Chemistry from the American Chemical Society (Earth Day Edition).

Infographic on CRISPR/CAS9 Targeted Genome Editing.

Open Labware: 3-D Printing Your Own Lab Equipment.

Disarmament education resources from the United Nations Office of Disarmament Affairs (UNODA).

Some news from world of science:

From the weeks of 12 – 18 and 19 – 26 April, 27 April – 3 May and 3 – 10 May in chemistry.

Images to celebrate 25 years of the Hubbel telescope.

Drones

The development of unmanned autonomous vehicles (UAVs), whether terrestrial, aerial, or aquatic (and combinations thereof) has experienced significant growth in recent years for personal, economic and utilitarian purposes. We are continually seeing proposals of new applications and demonstrations of capabilities. Examples include drone-based deliveries (where delivery locations might update in real-time using the addressees Smartphone as a locator), aerial drones for security, delivery of blood to critically injured patients, delivering life preservers to struggling swimmers, tracking stray dogs and even sheep herding.

The majority of drone based measurements that we have seen involve photography and video; applications include mapping, high resolution 3D imaging and search operations where aerial surveillance may have limitations.

What about all those fantastic vehicles? How fast do the land speeders really go? This question is being addressed in a most scientific manner. Can you determine if the calculations are accurate? For most of us, the prospect of owning a space craft is only realistic if we build it from Lego®. Although with a sufficient budget, a Tie Fighter engine can be had! Achieving light speed capability however, may remain difficult.

We often hear about science fiction predicting the future, is it true, or is it a case of science fiction inspiring people to build what they see? No matter the answer, we can be sure that in another 38 years, science can only become more fun!

The ambulance drone that could save your life. Photo from *Daily Mail Online*.

As sensors become smaller, integration of devices (Smartphones for example) is a foregone conclusion (and there are many potentially portable and miniaturised devices available). This concept has appeared in patent literature for many years (with some patents focusing on CBRN specific applications). Agriculture is another sector where we are seeing UAV platforms integrated with sensors and other technologies; examples include evaluating leaf water use efficiency and applying pesticides. Other examples involve pollution and environmental monitoring, and environmental sample collection.

With the proliferation of UAVs into more and more everyday uses, a need for "air traffic control", miniaturized radar and advanced autopilot systems is critical for collision free sky (and there are certainly other unforeseen situations that may arise). UAVs can challenge regulations, prompting policy-makers to review existing laws and propose UAV specific measures. Self-driving cars have prompted conceptually similar discussions. There are also security concerns that have lead to net carrying interceptor drones to counter potential threats from small UAVs. Privacy concerns have likewise emerged, with calls for no fly zones over private property.

We end this feature by noting that UAVs have not been spared from the list of technologies converging with biology, as demonstrated by a "biological UAV" that is intended to self-destruct and dissolve upon impact. It was designed to avoid leaving behind litter in pristine eco-systems. Interested in creating your own "biodrone"? The inventors have made the procedure available.

Chemical Weapons Inspectors and Industry Verification

When we reflect on the work of the OPCW and its accomplishments in demilitarisation and non-proliferation, we rarely hear directly from OPCW inspectors. Yet without them, these accomplishments would not have been possible. Likewise, OPCWs demilitarisation activities (representing more than 13,000 inspector days in 2014) overshadow another important aspect of the Chemical Weapons Convention verification regime: the inspection of industrial chemical facilities (Article VI Verification). In 2014, OPCW inspectors conducted 241 Article VI missions adding up to nearly 3,000 inspector days; this amounts to about 8 OPCW inspectors on mission somewhere in the world where declared (and inspectable) Article VI facilities exist (see Figure 2) on any given day of the year!

For this feature, we sat down with a few Inspection Team Leaders (ITLs), Chemical Production Technologists (CPTs) and an Analytical Chemist from the OPCW Inspectorate to learn about them and their work in Article VI verification activities. For those with further interest in the facts and figures presented, we refer you to OPCW Annual Reports.

Crowdsourcing:

The IUPAC Committee on Chemistry Education seeks a new logo. If you are a chemistry student with a flair for design, they need your help!

How do we establish a sustainable human presence on Mars? NASA is looking for proposals (while this may not get you on a flight, creative ideas might win you a cash award).

Interested in a Smartphone App that can help save lives of children born prematurely? Your photographs of newborn babies feet, eyes and ears could turn it into a reality.

Crowdsourcing to verify social media information for emergency response? Here's what is being done in Nepal following the recent earthquake.

Upcoming S&T Related Events:

OPCW Calendar of Events June to December 2015.

26 – 30 May 2015

International Conference on Robotics and Automation. Seattle, Washington, USA.
The Amazon Robot Contest will take place at this event.

7 – 12 June 2015

2015 AAAS-TWAS Course on Science Diplomacy.
Trieste, Italy.

8 – 12 June 2015

Twenty-Second Session of the OPCW Scientific Advisory Board.
OPCW Headquarters, The Hague, Netherlands.

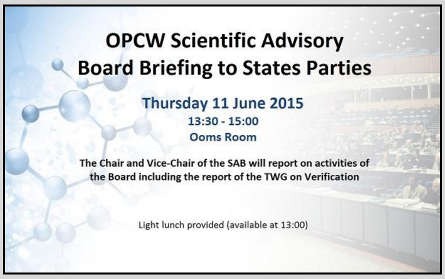


Figure 1: OPCW Inspectors at a chemical production facility (Article VI inspection).

The current staff of the OPCW Inspectorate Division numbers 163. This includes inspectors, Inspectorate management and support staff; they collectively make up 55 unique nationalities (which means up to 86 different "official" languages might be heard as you walk down the hallway). Inspectors join OPCW from a wide range of professional backgrounds. Some are former military or come to OPCW from governmental and/or international agencies; while others draw their experience from the chemical industry, manufacturing plants and/or science and engineering laboratories.

Many have backgrounds in chemistry (especially analytical chemistry), chemical engineering (including the division director) and other science/engineering disciplines. Several inspectors also hold an MBA.

Article VI inspections are intended to build confidence amongst the States Parties to the CWC through verifying the absence of undeclared Schedule 1 Chemicals (chemicals with limited or no use for peaceful purposes) and activities banned by the Chemical Weapons Convention. The broad expertise within the inspectorate is necessary to be able to inspect facilities that span a wide spectrum of declared purposes (this is illustrated by the product group codes in Appendix 4 of the *Declarations Handbook*). Knowledge about scheduled and non-scheduled chemicals, chemical synthesis and, methods and equipment for producing chemicals are needed. As is a sufficient level of familiarity with the laboratory equipment, production equipment, safety (containment) infrastructure and other features of the inspection site in order to recognise consistency with declared purpose. Some missions (a total of nine in 2014) include Sampling and Analysis (S&A), where training in analytical chemistry is required. The work of an inspection team may provide an unusual degree of access to a plant site, requiring that operating procedures concerning confidentiality are strictly followed (as described in the Confidentially Annex of the CWC).

22 – 26 June 2015
CTBT Science and Technology Conference (SnT2015)
Vienna, Austria.

8 July 2015
"Science for Diplomats". The science of medical countermeasures.
13:30 – 15:00 Ooms Room
OPCW Headquarters, The Hague, Netherlands.

14 – 26 July 2015
19th Annual Green Chemistry and Engineering Conference.
Bethesda, ML, USA.

19 – 22 July 2015
12th World Congress on Industrial Biotechnology.
Montreal, Canada.

6 – 13 August 2015
IUPAC 2015
48th IUPAC General Assembly and 45th World Chemistry Congress.
Busan, Republic of Korea

10 - 14 August 2015
Biological Weapons Convention Meeting of Experts.
Geneva, Switzerland.

27 September – 1 October 2015
ECCE10 (10th European Congress of Chemical Engineering); ECAB3 (3rd European Congress of Applied Biotechnology); and EPIC5 (5th European Process Intensification Conference)
Nice, France.

5 - 8 October 2015
SOLVE.
Cambridge, MA, USA.

15 October 2015
Smart Manufacturing Summit.
Livermore, California, USA.

31 October - 2 November 2015
The Port Hackathon.
CERN

16 – 19 November 2015
Malta Conference.
Rabat, Morocco.

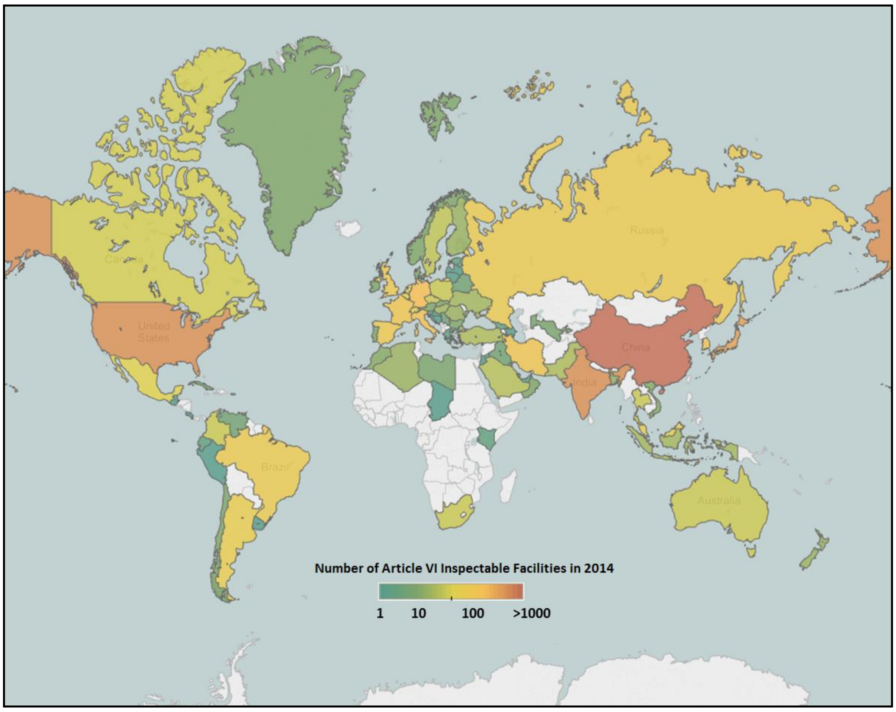


Figure 2: Declared and inspectable facilities under Article VI in 2014.

Team size and mission duration for Article VI inspections vary with the types of facilities inspected and whether or not S&A is to be performed. Schedule 1 and 2 facilities typically require three to five inspectors, while facilities producing unscheduled Discrete Organic Chemicals (DOCs) typically have inspections teams of two to four; in cases where a plant site has multiple inspectable facilities, larger teams might be dispatched. On S&A missions, teams of five are normally required (an ITL with two CPTs and two ACs).

Missions involving S&A are the most demanding. In preparation of the mission, ACs must ensure their instruments are calibrated and in some cases they may need to synthesise relevant chemical standards and controls (to ensure the highest levels of accuracy, this may include known and anticipated components/impurities of the samples to be tested – another example of where knowledge of chemistry becomes important). A mobile laboratory that includes a GC/MS (gas chromatograph/mass spectrometer), generators, portable fume hoods, sample preparation equipment and a variety of laboratory supplies (20 pieces taking up more than 5 m^3 and weighing more than a ton, see Figure 3), is shipped and assembled at the inspection site. Number and locations of sampling points at a chemical facility are negotiated with the inspected States Party prior to the analysis; they can include key points in a chemical production process along with random sampling points such as a waste water stream. As an S&A mission is typically three days in duration, the inspectors have limited time to assemble the lab, collect samples (see Figure 4) and run their analysis, making the logistical aspects of these missions critical for success.

18 – 21 November 2015
16th Asian Chemical Congress.
Dhaka, Bangladesh.

22 – 27 November 2015
2nd African Conference on Research in Chemical Education (ACRICE)
University of Venda,
Thohoyandou, South Africa.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii, USA.

Contact Us:

Questions, ideas, comments, suggestions, want to make a contribution, or be added to the mailing list? Please contact us through the OPCW Office of Strategy and Policy (OSP).

For more frequent updates, Visit us on the web or follow us on Twitter at @OPCW_ST.

Figure 3: Sample collection at an industrial chemical facility.

As S&A missions are labour intensive, chemists from OPCW have developed improved methods for sample collection (from liquids and air), derivitization and sample desorption from solid supports to streamline the analysis. The work-horse on-site analytical tool is the GC/MS; in Article VI inspections, the primary analysis is the comparison of measured mass spectra and GC Retention Indexes to reference data contained in the OPCW Central Analytical Data Base (OCAD; see chapter 7 of Chemical Weapons Convention Chemical Analysis).

The OCAD only contains reference data for scheduled chemicals. For routine analysis, chemicals in collected samples are only identified if there is a match to data contained within OCAD. This allows verification of the presence or absence of scheduled chemicals while maintaining confidentiality on sensitive information related to industrial (i.e. commercial) facilities. Further information on the OCAD can be found in the October 2014 *S&T Monitor* feature on the "40th Meeting of the OPCW Validation Group". A report from the 41st Meeting of the Validation Group is also available.

Figure 4: The OPCW Mobile Laboratory.

In addition to the technical skills and knowledge just described, "soft skills" that aid in negotiations and promote team work are equally important. One might say that the ITL is a "technical diplomat", requiring a thorough understanding of the Chemical Weapons Convention (what is and what is not allowed during an inspection), the necessary technical knowledge to perform the inspection and the ability to maintain a cooperative interaction with the teams escorts (National Authorities and staff of the inspected facility).

Several of the team leaders have been known to prepare presentations to explain the purpose of the inspection and bring awareness of the CWC and its goals. In effect, some of our greatest assets for the OPCWs Education and Outreach work are the inspectors themselves; OPCW staff who regularly interact with people involved at an operational level in chemistry, chemical production and chemistry commerce.

Inherent Safety

Through the Chemical Weapons Convention (CWC), the OPCW works toward a world free of chemical weapons, a world that becomes more secure in the process. Chemical security is another means to strengthen this drive toward a chemical weapon free world and receives much attention within security focused communities. Just as the OPCW inspects industrial facilities for security reasons, industrial facilities are inspected with high frequency for safety reasons. Chemical safety seeks to ensure the safety of people, the environment and property from harmful chemicals. We often describe the focus of chemical safety as preventing accidents rather than addressing the potential of intentional misuse; yet, chemical safety compliments (and benefits) chemical security.

Chemical and chemical engineering societies (such as the ACS and AIChE) place great importance on chemical and process safety. Both are important to keep people safe who work in chemistry laboratories or chemical production plants (occupational safety). There are many aspects to ensuring the safety of people handling chemicals, personal protective equipment (PPE) is critical (with more hazardous chemicals requiring more effective protection).

Of course, many hazards surround us in our day to day life. The gasoline (something all of us with motor vehicles are exposed to) is a chemical hazard and the speed at which you ride your bike can be a hazard if you don't pay attention to those around you. For an engineer on a chemical facility, potential hazards include toxic chemicals and industrial equipment. This is where the concept of inherent safety comes into the picture. The goal of inherent safety is to reduce hazards, and by doing it also promotes good practices for chemical safety and security.

We are all aware of a number of tragic events involving accidents in chemistry laboratories and high profile industrial incidents such as Bhopal and the Flixborough. While we can learn from past accidents, we must also strive to prevent future incidents. Toward this end, in 1977 Trevor Kletz defined the concept of *Inherent Safety* as a response to 1974 Flixborough Disaster where on a Saturday afternoon, 1st of June 1974, a loud explosion occurred at the Nypro site at Flixborough, United Kingdom. The incident was triggered by a cyclohexane leak that found a source of ignition. After investigating the incident, it was found one of the reactors (number 5) had a crack and in order to continue production, a temporary bypass assembly was placed between reactors 4 and reactor 6. Unfortunately, the bypass failed releasing a cloud of cyclohexane vapour. Twenty eight workers were killed that day, had it been a weekday, the number of casualties would likely have been higher.

Key principles of inherent safety are substitution, minimization, moderation and simplicity.

Substitution is the replacement of hazardous chemical with a less hazardous material in a process. The use of water based paint instead of solvent based paint for example; the substitution reduces a fire hazard and the water based paint is less toxic and more environmental friendly.

Minimization is the reduction in quantity of hazardous materials. For example, in processes where hazardous materials must be used, reducing pipe diameters can help minimize the amount of material that spills from an unexpected leak.

Moderation is reducing safety risk for processes utilizing hazardous materials. This could be the running a reaction at less severe process conditions or the dilution of a hazardous material to a concentration range that provides an acceptable safety and environmental risk. Interested readers may wish to read a report on the application of the dilution principle using hydrazine as an example.

Simplicity is a reduction in the complexity of plant design. Using less complex equipment for certain critical processes, for example, in order to minimize the number of possible failure modes. The use of gravity flow systems in place of electric or mechanical pumps (where process tolerance permits) would be an example of simplicity.

Inherent safety is an important concept in plant design and there are a number of publications illustrating specific case studies of the application of its principles, including for batch and semi-batch processes in pharmaceuticals.

Adopting the concepts of inherent safety is only one aspect of building an effective safety culture. Keeping informed on new developments and maintaining proper safety training are equally important. Many resources are available to help promote chemical safety (and bring with it benefits to chemical security).

High quality inspections can eliminate potential safety risks in production plants. Photograph Copyright by BASF (used here under a creative commons license).