The OPCW Science & Technology Monitor

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

14 April 2015 Volume 2, Number 5

Featured Content:

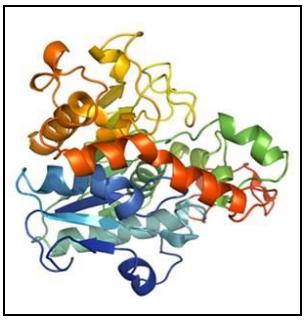


Image from Green Chem, 2015,17, 1756-1766.

Solvent free catalysis using enzymes immobilized in thin films.

Image from Soft Matter, 2015,11,1667-1676.

From insects to reptiles: technological advances discovered by studies across some of the "creepier" citizens of the animal kingdom.

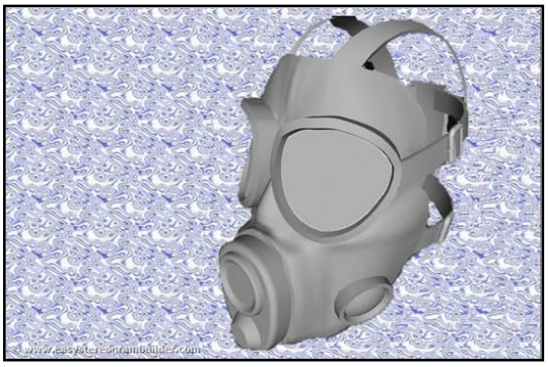
In this issue:

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.

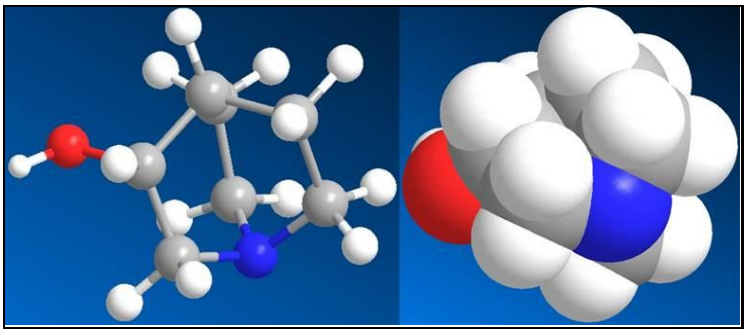
Today marks the 12th anniversary of the completion of the Human Genome Project. Tools and methods developed for studying genomics have applications for studying chemical warfare agents. Published studies include gene expression in survivors of sulphur mustard exposure and analysis of single-nucleotide polymorphisms of the genes involved in organophosphate detoxification.

The S&T Puzzle



Congratulations to Janaina Teixeira Pires do Couto from the Inspectorate, who was quickest to recognize the gas mask in our stereogram (look left for what you will see when viewing it correctly). Statistics now stand at: VER 4, OSP 2, OCS 1, INS 1, and CTBTO 1.

Moving on to this edition of the puzzle and considering all of our S&T communication channels, do you recognize the molecule below? Can you name it? Identify if it is on a Schedule (and if so, which one)? And tell us why it has relevance to the Chemical Weapons Convention? First person to correctly answer can choose a featured topic, design a puzzle, or receive a beverage hand selected by the Science Policy Adviser. Send answers by email. Good luck!



Science Fun:

With Koningsdag (Kings Day) fast approaching, we thought it only fitting to look at some of the science and technology that underpins life here in the Netherlands.

We are fortunate to live in a country with so much science to be observed, for example: innovative developments in water technologies, windmills (and continued development in wind and other renewables), greenhouses, laser armed trains, gouda cheese (a scientifically interesting food), solar powered bicycle paths (night photos here), wooden shoes and people whose average height has increased by 20 cm over the last 200 years (details here)!

Photo of Keukenhof.

Tulips: a dual-use biological material?

Perhaps more relevant to our Chemical Weapons Convention is the Tulip, a flower that was originally introduced to The Netherlands during the mid 16th Century. Tulips contain the chemicals Tulipalin A and B, which render these flowers toxic to dogs and cats and can induce dermatitis or eczema in humans. The bulbs also contain proteins capable

News and Updates

Recently published reports and newsletters:

Nature Index 2015 on Science in the Asia-Pacific Region.

Algae as a Potential Source of Food and Energy in Developing Countries.

Issue 27 of Dstl's *Insight*.

March 2015 Issue of PNNL's *Currents*.

Atoms for Peace and Development, Volume 56 Issue 1 from the IAEA.

Third issue of NASA's *Digital Technology Innovation Magazine*.

Issue 7 of *UNDP Skopje: Innovation Stories* (Innovation News Update).

2014 Intellectual property facts and figures from WIPO.

Documents from the commemorative event for the 40th Anniversary of entry into force of the Biological Weapons Convention.

Behind the Curve: New Technologies, New Control Challenges; report from the Small Arms Survey.

Defense Advanced Research Projects Agency (DARPA) report on *Breakthrough Technologies for National Security*.

2015 AAAS Science and Human Rights Report.

Science resources:

GLEAMviz a tool for modelling and visualizing epidemics.

Introduction to Ebola for journalists from the WFSJ.

Games that can be used to teach public health.

Infographic guides to scientific evidence and evaluating scientific work.

How good is your knowledge of scientific glassware? Answers can be found in this infographic visual guide.

Some news from world of science:

From the weeks of 15 – 21 and 22 – 28 March; 29 March – 4 April; and 5 - 11 April 2015 in chemistry.

New Technology for Chemical Production and Discovery

We pay considerable attention to devices and technologies for analyzing chemicals, but before we can identify and detect a chemical, it must somehow be prepared (whether by nature or in a lab).

of inhibiting DNA synthesis.

Of course biological materials and the chemicals they contain have multiple uses. These Tulip derived chemicals have anti-bacterial, cosmetic and biopolymer applications.

Finally, we can't ignore the fact that The Netherlands is a country of bicycles, a form of transportation that continues to evolve with technological innovation, lends itself to becoming a smart device and drives invention to keep riders safe. And we all know that if we can make our bicycles smarter and safer, we can also make them faster!

Crowdsourcing:

Do you have any photographs that convey the role Power Africa and energy innovation are playing in powering Africa?

Interested in designing a mobile app to educate children about good hygiene practices and sanitation?

Our crowd sourcing feature has primarily focused on alerting our readers to crowd source opportunities they can participate in. Have you ever wondered how good the crowd can be for providing information? Here are some reports on going to the "crowd" to detect clinical features of an eye condition from digital photography and to rank adverse drug reactions.

Not surprisingly, new concepts and technologies to make organic synthesis more efficient are changing the laboratory as chemists work toward the development of a "synthesis machine". Automated synthesis of peptides and nucleic acids has been accessible for many years, and we are now seeing machines that automate the assembly of a variety of small molecules (details here).

New chemistry to form carbon-carbon bonds employing boronate esters and functionalized olefin coupling under mild conditions are opening up new routes to synthesis. New approaches to using biological molecules in synthesis continue to emerge as well, such as enzymes that can be engineered to catalyse reactions not found in nature, the use of DNA to catalyse enantioselective reactions (details here) and solventless reactions using enzymes in thin films (details here).

To help contain the ever increasing cost of pharmaceutical development, enabling tools such as Computer-Aided Drug Design (CADD) to better identify drug leads (details here) and other computational methods for exploring "small molecule space" along with "Robot Scientists" that streamline drug discovery are being adopted (details here). These methods are themselves augmented by new ways to combine computational and functional studies with analytical tools in identifying and screening drug function (such as reduced risk of pain-killer dependency).

New methods for producing materials are likewise being invented, as demonstrated by a simple yet high volume method recently reported for graphene.

From Worms to Reptiles: Nature Inspired Science

We've spent considerable time thinking about the convergence of chemistry and biology, with much focus on the manipulation of microorganisms and plants. Yet, it is much more than just chemistry and biology that has converged and a significant amount of bio-inspired science and technology has developed from observations of multicellular organisms across the animal kingdom. Bio-inspired materials and venom component derived drugs are just two of the topical areas that can be explored in the scientific literature. We present here a sampling of convergent science inspired by observing some of natures less charismatic creatures.

Starting with invertebrates, "worms in space" are informing astronauts how to mitigate bone and muscle loss in zero gravity. Moving to the world of molluscs, the stretchy material that makes up the teeth of a limpet was recently discovered to be one of the strongest materials in nature (details here). Cephalopods are masters at camouflage, their associated chemical and biological processes have inspired interesting reflective coatings. A recent scientific article accused cone snails of using "chemical weapons", perhaps not quite a concern for the CWC, but of interest to those who study insulin.

Upcoming S&T Related Events:

19 – 23 April 2015
ALLData2015 - The First International Conference on Big Data, Small Data, Linked Data and Open Data. Barcelona, Spain.

30 April – 1 May 2015
2015 AAAS Forum on Science and Technology Policy. Washington DC, USA.

6 – 7 May 2015
6th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague

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. The Hague, Netherlands.

15 – 19 June 2015
ACHEMA – World Forum for Chemical Engineering and the Process Industries. Frankfurt am Main, Germany.

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

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

Silk from insect cocoons has molecular properties that can be used to generate electricity or even dissipate energy (details here). Other insect inspired materials include antireflective coating discovered by studying moth eyes (more details here). Insect neural systems can be manipulated with technologies that produce "cyborg" drones (controllable by Smartphones, details here); actual non-hybrid drones inspired by butterflies and ants exist too. Spiders quite naturally have also inspired drone technologies.

Other examples of arachnid science focus on spider webs, a fascinating area of materials science that has inspired 3D printer design and breakthroughs in nanofiber and 3D cell printing (for tissue engineering) research. Sensors can also be designed to mimics a spider's sensory system to detect vibrations (such as those produced from the motion of an insect's wing; a video is available here). Looking to other arachnids, scorpion venom has shown potential for treating bacterial infections and in chemotherapy. Molecular components of arachnid venoms have been identified as drug development scaffolds and insect specific insecticides. Venom from ants, centipedes (details here), and other arthropods are studied for similar purposes.

Fish and reptiles have also contributed to scientific development in similar ways to many of the invertebrates already described. Consider oil repellent materials for diving goggles inspired by fish (and flowers too, details here) and potential therapeutics identified in the blood of alligators (details here). Perhaps the chameleon (details here) can give those cephalopods a bit of competition in camouflage too?

We'll end this survey of somewhat scary creatures and their scientific contributions with a plea to be kind to rats and a reminder that interesting discoveries inspired by nature often come from unexpected places (even slime molds, details here).

Codes of Conduct and Ethics in Chemistry

Codes of conduct and ethics in chemistry received renewed attention at OPCW when the Nineteenth Conference of States Parties to the Chemical Weapons Convention welcomed an initiative for a text of ethical guidelines for chemical professionals related to the Convention (see C-19/5, dated 5 December 2014, paragraph 23.3). In support of this initiative, 19 scientists participated in a workshop on 11 March to discuss the issue and think about how it might be taken forward. Participants included members of the American Chemical Society (ACS), Bangladesh Chemical Society (BCS), European Chemical Industry Council (Cefic), European Association for Chemical and Molecular Sciences (EuCheMS), Federation of Asian Chemical Societies (FACS), Gesellschaft Deutscher Chemiker – the German Chemical Society (GDCh), Indian Chemical Council (ICC), International Union of Pure and Applied Chemistry (IUPAC), Ministry of Industry and Information Technology of the People's Republic of China, The National Academies and the National Engineering & Scientific Commission – Pakistan (NESCOM). Those involved in the workshop are continuing their considerations and we are sure to hear more in the next few months.

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

6 - 13 August 2015
IUPAC 2015
48th General Assembly
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.

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

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

During the workshop a number of presentations were made on past, present, and on-going initiatives in developing ethical codes and this is where our focus for this feature comes in. As part of the discussion, a first pass text analytics study that encompassed sixty-three existing codes of conduct and ethics for chemistry (and/or broader scientific professionals that include chemists and chemical engineers). For those interested, the text of these codes is available upon request from us here at the *S&T Monitor*.

The study was meant to be insightful, not comprehensive. The codes in the data set represent international and regional organisations as well as organisations specific to the countries shown in Figure 1. The types and number of these organisations in the data set are reported in Figure 2. In some cases (several of the South American countries for example, the national chemical society was using a translated version of a code already included in the data set from another chemical society; in this instance we did not include the duplicate code).

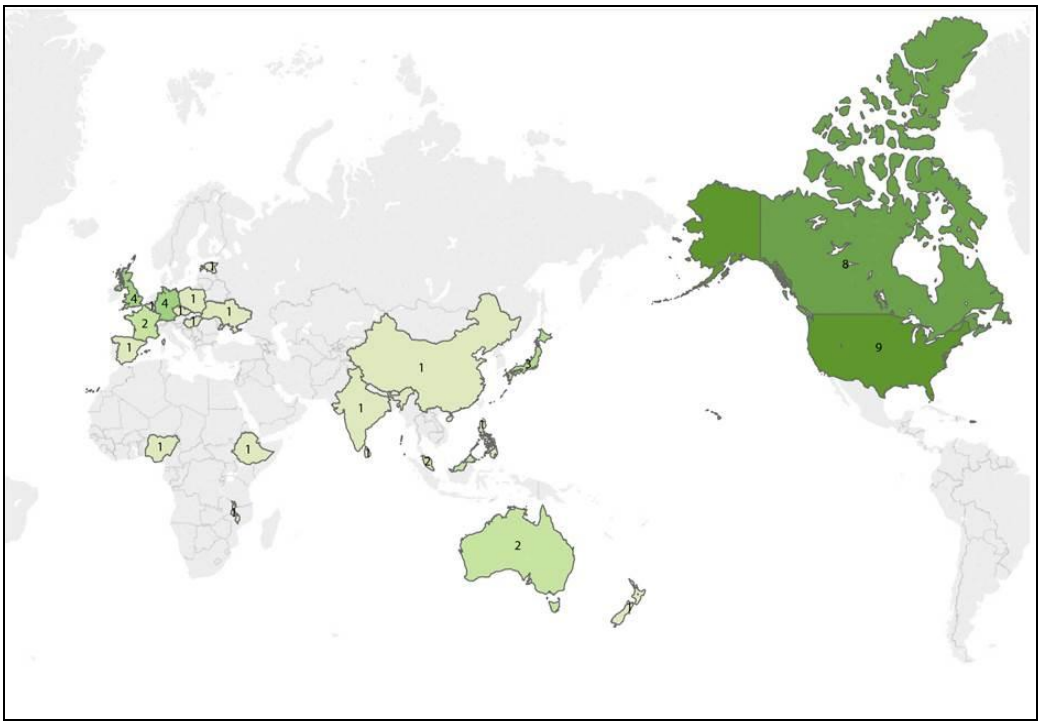


Figure 1: Map showing individual countries from where written codes of conduct or ethics in chemistry and chemical engineering were available (and how many codes came from each country). In addition there were eight codes from organisations that represented regional and international scientific organisations and some national societies used identical codes (which were not duplicated in the data set).

The analysis sought to discover patterns in the existing codes to provide an in-depth insight. The analysis was performed using Provalis QDA Miner software (available in OSP and the OPCW the Library). In this feature we report an introductory summary of the cluster analysis that was performed. Cluster analysis is a data reduction method by which a large number of items are grouped into a number of clusters of similar items. When applied to textual data, cluster analysis can be used to identify themes or broad classes of concepts that are common between documents placed into their respective clusters (groups). For purposes of this summary, one can think of all the codes found in the same

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cluster to have text that is similar to one another and divergent from the text of the documents in the other clusters. Additionally the closer the distance between the codes within a cluster, the more similar the documents actually are. Figure 3 illustrates the first pass cluster analysis, indicating the documents considered to be (by their authors) codes of conduct or codes of ethics).

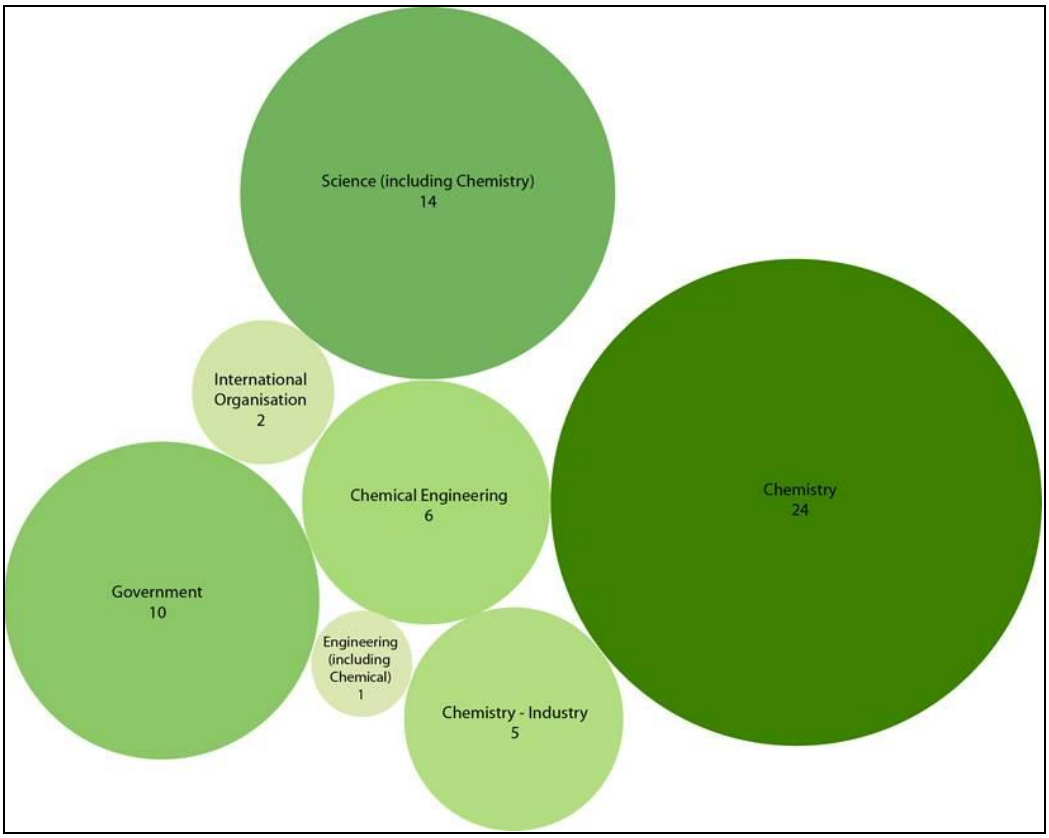

Figure 2: Illustration of number and types of organisations represented by the codes used in the analysis.

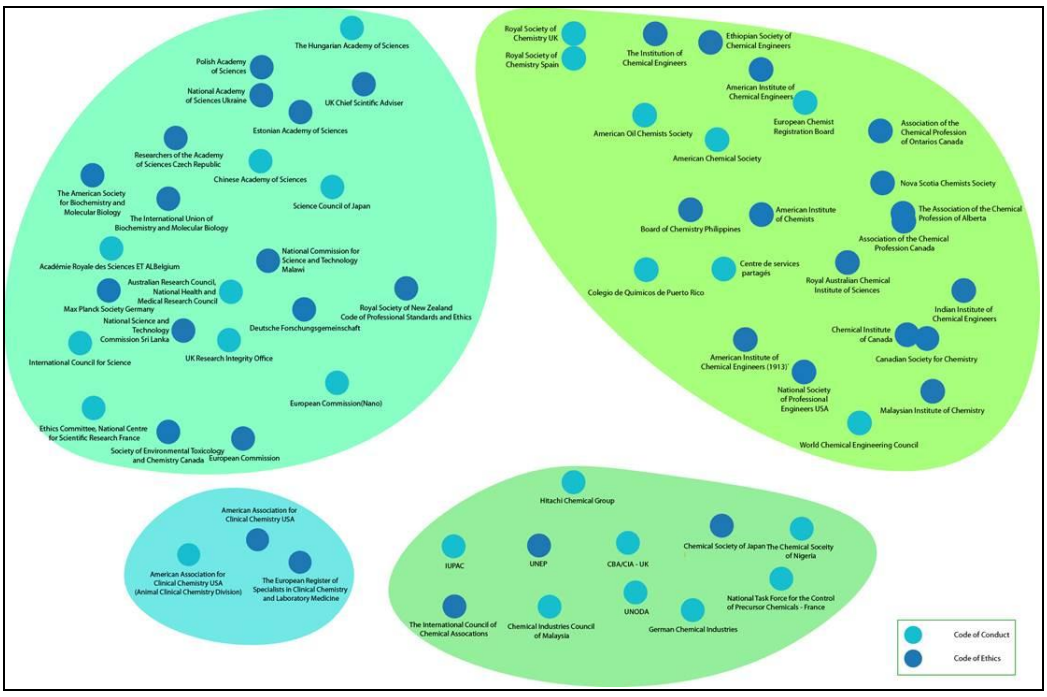

Figure 3: The codes separated into four clusters (groups of documents with similar text content). The cluster here is visualised with each code indicating if it is a code of conduct or a code of ethics (as defined by its authors and purpose).

There are several observations from Figure 3 to point out. First, the

smallest cluster (bottom left in Figure 3) containing only three codes represents clinical chemistry organisations – all of whose codes contain similar text and whose organisations have a clinical focus that is not represented by organisations found in other clusters. Next, the actual written codes do not distinguish themselves within the clusters by whether they represent codes of conduct or codes of ethics. Figure 4 delves into other unique factors represented by the codes and organisations to further compare the content.

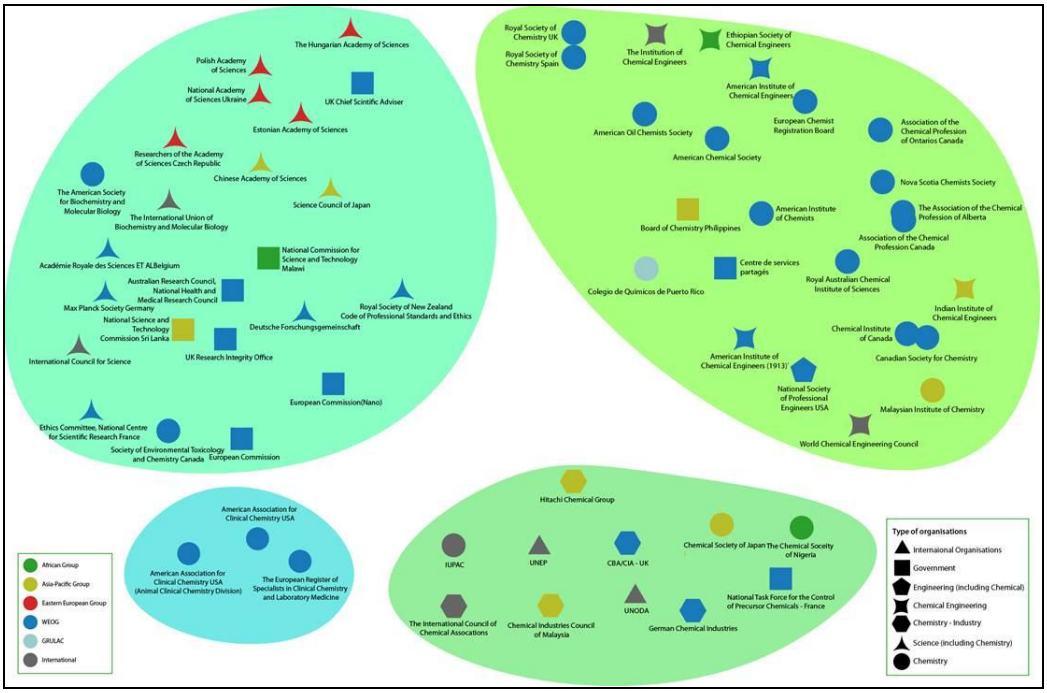

Figure 4: Visualisation of the codes within each cluster indicating the regional affiliation and type of organisation represented by the code.

In Figure 4, the clusters also do not segregate themselves by region. The majority of codes come from countries in the Western Regional Group and these codes are found in every cluster. Despite smaller representation over the sixty-three codes, Asian and African Regional organisations also appear in all clusters not representing clinical organisations (there are no clinical organisations from these regions in the data set). The only region which falls into a single cluster is Eastern Europe (top left in Figure 4). However, on closer inspection it can be seen that all the organisations from this regions are Academies of Science and all the Academies of Science from across the data set fall into this same cluster.

Other organisational groupings observed within the clusters are the chemical engineering organisations all in the top right cluster; and international and industrial organisations in the bottom right cluster (showing that international organisation and industrial codes distinguish themselves from the other types of organisations represented in the data set). The major attribute which appears to define to which cluster a document belongs, is the type of organisation that the code is written for, not the geographical region, nor the type of document (e.g. a code of ethics vs. a code of conduct).

To explore the relationship between significant keywords within the

documents and the types of organisations (the most prominent distinction between the clusters), a cross-tabulation analysis was performed. Figure 5 summarises the observations of word frequency for keywords of interest across the codes.

Figure 5 illustrates the most common words found across the documents and it is noteworthy to point out that terms such as Chemical Weapons Convention, Biological Weapons Convention, Weapons of Mass Destruction, Dual-use, Multiple-use, and Security are observed in a very small number of codes. The heat-map indicates the most frequent topics in the codes of this data set focus on safety, health, and welfare. It also indicates that not all types of organisations are concerned equally about these issues.

The workshop participants are following up on their meeting to identify key elements of CWC relevant ethical guidelines, principles and best practices for drafting ethical guidelines and how they might establish synergy with other similar initiatives (both past and present). The text analysis study presented here, while by no means comprehensive, may usefully inform their work. A more detailed publication (with more codes included) is currently being considered as a follow up.

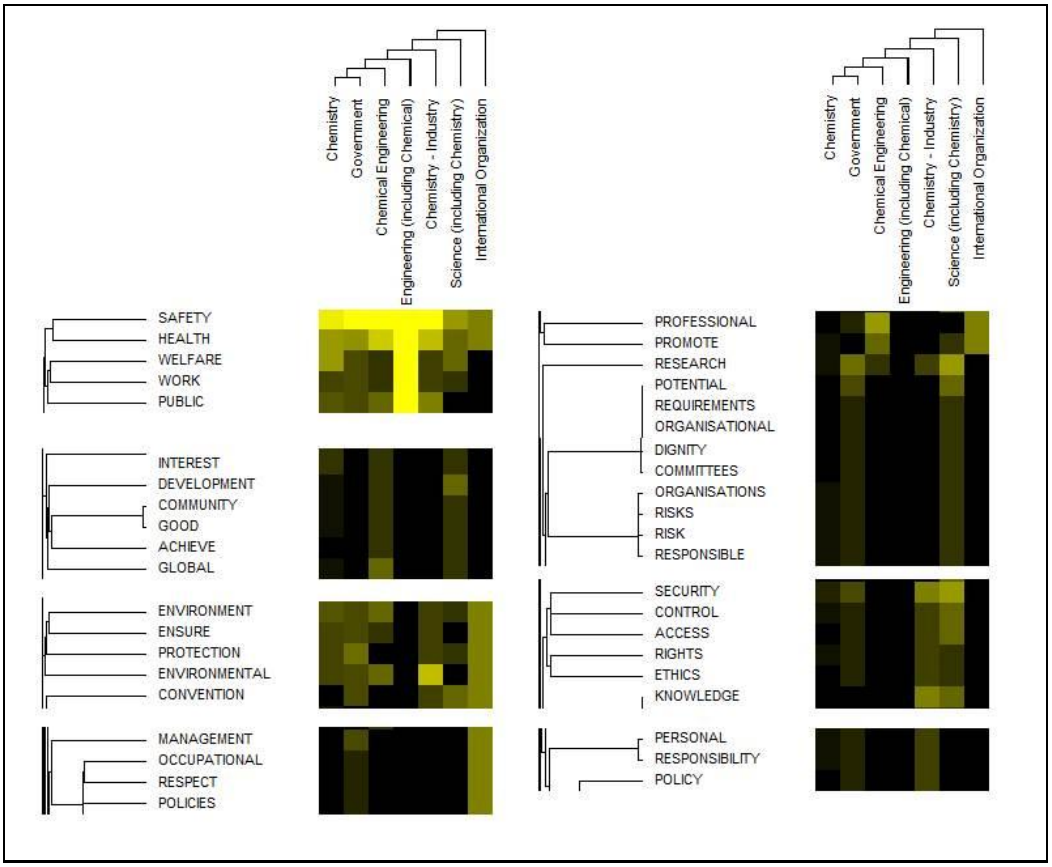

Figure 5: Heat map of word associations and frequencies across data set organised by the type of organisation represented by the code. Brighter colour indicates higher frequency of a specific word or word association across the documents.