

International Union of Pure and Applied Chemistry A member of the International Council of Scientific Unions Division VI, Chemistry and the Environment Report to Bureau, April 2018 Submitted by Rai S Kookana, President

# I. Highlights and Executive Summary

Through world-recognized expertise and experience via its members and project teams, Division VI – Chemistry and the Environment (DCE) makes scientifically sound and timely contributions towards addressing the critical environmental issues at a global scale. We provide authoritative reviews and guidance on the fate, behavior and risks of chemical compounds in food and the environment by undertaking both fundamental and applied project activities to solve pressing environmental problems and enhance quality of life. Our salient features/achievements/activities are listed below.

## Expertise, Diversity and Inclusiveness

• We have brought together world-leading expertise in chemistry and other disciplines related to the environment from across the globe. Our team represents 20 nations and reflects gender balance (60% females), diversity and inclusiveness. We are undergoing a significant renewal in this biennium.

Project portfolio and leadership

- In collaboration with other Divisions (e.g. Div. III, V and VII) and Committees (e.g. COCI, CCE), we currently have a healthy list of active projects (section IV). We integrate, synthesize and deliver these via two subcommittees: (i) *The Advisory Committee on Crop Protection Chemistry* and (*ii*) *The Advisory Committee on Chemical and Biophysical Processes in the Environment* (section III).
- We have brought together industry, regulatory agencies, academia and researchers and provided global leadership on complex science issues (e.g. Nanomaterials/ Nanopesticides, e-waste, risk assessment projects – section III).
- We provided guidance on consideration of bioavailability of metals/metal compounds in risk assessment - <u>http://www.metal-bioavailability.org</u>.
- DCE is drawing strong interest and three approved projects had to be carried to 2018-19 for funding, as our allocated budget last biennium was fully spent.
- Steps are being taken for urgent completion of overdue projects.

Global outreach, technology transfer and collaborations

- We delivered a number of highly successful symposia,
  - three during the 46<sup>th</sup> World Chemistry Congress Sao Paulo, on (i) "*E-waste*" (*D* Purchase and H Garelick) (ii) "Nanomaterials" (S Obare), (iii) "Pesticides in Latin America" (J Unsworth)
  - one during ICOBTE 2017 (Switzerland) on "Trace elements analysis of environmental samples with X-rays" (R Terzano and B Miller), and another
  - during HPLC 2017 in JeJu Korea "Water and Environmental Analysis (IUPAC) " (DS Chung).
- Ecological Risk Assessment Workshops: following on from successful Workshops in Beijing, Bogota and New Delhi, San Jose in Costa Rica was host to the latest in the series. This Workshop was supported by IUPAC, ACS AGRO and CropLife International (Chemistry International <u>39</u>(4) 45-46 2017)

- To foster regional cooperation, a workshop was held in the Middle East on Sustainable Water Management of Transboundary Water (Shevah/ Garelick).
- To promote sustainable development and application of nanotechnology, a workshop on "Safety of Engineered Nanomaterials" was held during September 28-29, 2017 in Queretaro (Mexico), jointly funded by Division VII and VI.
- In collaboration with SETAC, we have organized a special IUPAC session in May 2018 Europe conference in Rome. Several projects are presenting works at this.
- Maintaining our long history in delivering Pesticide World Congresses every 4 years, we are helping organize the 14th IUPAC International Congress of Crop Protection Chemistry being held in Ghent, Belgium May 19<sup>th</sup> 24<sup>th</sup> 2019.

*The IUPAC 100 celebrations*: We are making significant contributions to IUPAC100 through committee co-chair, Laura McConnell.

# II. Plans and priorities for this biennium, and beyond:

## Overall strategy of the Division and alignment with IUPAC plan:

The Division's overall strategy to make evidence-based, scientifically sound (underpinned by both fundamental and applied sciences) and timely contributions towards addressing the critical environmental issues at a global scale is well anchored and therefore will remain the main thrust of our strategy. We will continue to provide authoritative reviews and guidance on the fate, behavior and risks of chemical compounds in food and the environment to solve pressing environmental problems. However, the scope of the chemistry and environmental issues being very broad, we will be selective and focused in our approach. The selection of projects will be guided by the unique leadership opportunity these may offer to IUPAC, i.e. asking the question why IUPAC and why now? Secondly, since the environment related projects are inherently multidisciplinary in nature, we would prefer to harness collective interdivisional capability and expertise of IUPAC which to some extent make IUPAC unique. We will continue to build on the strong track records of cooperation/ collaboration with large and successful organizations such as ACS and SETAC. We will ensure timely reporting and delivery on current projects. We plan to reach out and bring in new participants in divisional activities.

### Summary of the number and general types of projects

We currently have 21 active projects which cover a number of topics ranging nanomaterials, ewaste, pesticides and risk assessment, many of which require a multidisciplinary approach. These also are progressively building a body of work where IUPAC can make a substantial contribution as a result of synthesis from several projects.

Often environmental issues are inherently multidisciplinary in nature. We source the required expertise externally as well as internally within IUPAC. In fact, we have a strong track-record of multidisciplinary inter-divisional projects. A number of Div VI projects have been developed and are being undertaken in close cooperation with Division III, V, VII and interdivisional committees (e.g. COCI). Some of these are listed below.

I. 2017-035-2-600 (Kookana and Johnston) - Human Health Risk Consideration on Nano-enabled Pesticides for Industry and Regulators. This project has been jointly proposed with Div VII with equal financial support and the task group is being cochaired by Linda Johnston (Div VII) and Rai Kookana (Div VI). Our other interdivisional projects include: 2017-004-1-600 (Chung); 2016-045-2-700 (Kookana and Johnston); 2016-019-2-600 (Terzano); 2016-015-2-600 (Perminova); 2016-047-1-600 (Xing); 2016-035-1 (Purchase, Obare); 2016-045-2-700 (Johnston and Xing); 2017-040-1-700 (Gubala Div VII with Garelick Div VI and Apotheker CCE).

### III. An overall report of Division/Committee activities and achievements during 2016-2017

# Goal: Provide scientific expertise to address critical needs on Chemistry and the Environment:

To provide scientifically sound and timely contributions towards addressing the critical environmental issues at a global scale is our main goal. In collaboration with other Divisions (e.g. Div. III, V and VII) and Committees (e.g. COCI, CCE), we currently have 21 active projects (see full list and their status in section IV). Through these we are currently covering a range of chemistry and environment related topics (ranging from e-waste to nanomaterials, from metals to pesticides toxicants, from risk assessment to regulations) underpinned by fundamental understanding of biogeochemical processes governing the fate and behavior of chemicals in the environment as well as their exposure and risk assessment.

We integrate, synthesize and deliver these projects via two subcommittees, namely (i) *The Advisory Committee on Crop Protection Chemistry*, and (ii) *The Advisory Committee on Chemical and Biophysical Processes in the Environment*. Some of the activities of committees and projects under both of these subcommittees are listed as examples of achievements towards the above strategic goal of IUPAC.

### (i) The Advisory Committee on Crop Protection Chemistry

The Committee provides unbiased and authoritative views regarding environmental and human health aspects of crop protection chemistry. Through its timely projects, publications, and outreach activities the Committee seeks to advance research understanding and promote environmental stewardship.

The Advisory Committee on Crop Protection Chemistry has evolved from various IUPAC Commissions prior to the adoption of the project system: since 2002 the committee has been called the Advisory Committee on Crop Protection Chemistry. Minutes of meetings of the various bodies are available in pdf format from 1983 to the present.

The Committee is currently comprised of 28 members, from 14 different countries, representing both developed and scientifically emerging countries: Argentina, Australia, Brazil, Canada, China, Colombia, Costa Rica, Greece, Japan, The Netherlands, South Korea, United Kingdom, United States and Uruguay. Members are drawn from government, academia, industry and private consultancies, thus ensuring a wide spread of expertise and experience.

There is significant interest in the Committee and a category of "Affiliate Membership" has been set up. This consists of scientists that are interested in the work of the Committee and wish to be kept up to date on its current activities. There are currently 21 affiliate members from 16 countries: Australia, China, Germany, Greece, India, Israel, Kenya, Pakistan, Poland, Russia, South Africa, South Korea, Taiwan, Uganda, United Kingdom and the United States.

The Committee tries to meet formally in association with an IUPAC-sponsored Congress or regional workshop. The last full meeting of the Committee was held on August 9th, 2014 in San Francisco, USA, immediately prior to the 13th IUPAC Pesticide Congress.

Main outcomes from IUPAC projects managed via this committee are review papers, technical reports or books on certain topics. Recent examples are a book on the *biophysico-chemical processes and toxicity of engineered nanoparticles*, a review paper on the *consideration of bioavailability for the risk assessment of metal species in waters*, or a *guidance paper on substance-related environmental monitoring strategies regarding soils and waters*. Some project activities demonstrating the outputs and outcomes associated with the core objective above are listed below.

HIGHLIGHTS FROM CURRENT PROJECTS OF BOTH COMMITTEES

Project Name (No.)	Leader	Status
Inventory of developments in the field of RNAi-based pesticides and potential needs for international harmonization of regulatory safety requirements 2013-029-2-600	Kleter	Presentation on human and animal safety considerations of RNAi technology, both for GM- plant-incorporated dsRNA and dsRNA used as pesticide active ingredient, during the iPlanta conference on RNAi plant applications in Poznan, Poland, on February 15th, 2018, which also highlighted the IUPAC project, among others (http://iplanta2018.home.amu.edu.pl/) Collection of articles and data on RNAi by team members ongoing Continuation of preparation of a review manuscript highlighting regulatory and safety considerations, based on textual inputs already received from various team members, to be collated and finalized this spring (2018)
Advances on the Assessment of Pesticides' Soil Microbial toxicity: New research and regulatory aspects in light of the recent methodological advances 2014-032-1-600	Karpouzas	The conclusions drawn from this project and a proposal for the regulatory framework regarding the assessment of the soil microbial ecotoxicity of pesticides will be summarized in a paper which will be published in a relevant journal as open access to increase visibility.
Guidance for Industry and Regulators on Assessment of the Environmental Fate and Risks of Nano-enabled Pesticides 2016-016-2-600	Kookana	Based on the Nantes workshop and subsequent work by the project team, an article entitled "Ecological risk assessment of nano enabled pesticides: A perspective on problem formulation" has been developed that has now been accepted by the Journal of Agricultural and Food Chemistry (DOI: 10.1021/acs.jafc.7b02373) in the special issue Nanotechnology applications and implications of agrochemicals toward sustainable agriculture and food systems' under the "Perspectives" category. In this paper, a group drawn from regulatory agencies, academia, research and the agrochemicals

Development of three technical symposia on environmental chemistry at the 46 <sup>th</sup> IUPAC World Chemistry Congress: 2016-035-1-600	Obare/	industry offered a perspective on relevant considerations pertaining to the problem formulation phase of the ecological risk assessment of nano-enabled pesticides. Delivered three highly successful symposia, three during the 46 <sup>th</sup> World Chemistry Congress Sao Paulo, on (i) " <i>E-waste</i> " ( <i>D Purchase and H</i> <i>Garelick</i> ) ( <i>ii</i> ) "Nanomaterials" ( <i>S Obare</i> ), ( <i>iii</i> ) "Pesticides in Latin America" – (J Unsworth). All three symposia were well-attended and well-
	Purchase	received, raising awareness of the three important topics associated with the work and expertise of Division VI membership. They also provided the opportunity to address specific regional problems and expand current, mainly EU and US based networks.
Water and Environmental Analysis - a Symposium part of HPLC 2017: 2017-004-1-600	Chung	The IUPAC symposium was highly successful, it comprised 1 keynote lecture, 10 invited talks, and up to 10 contributed talks in a half-day session and a poster session. The session was well attended.
Consideration of bioavailability of metals/metal compounds in the aquatic environment. 2011-060-1-600	Rüdel	The project has provided information on metal and metalloid bioavailability and the application of Biotic Ligand Model and bioavailability-based software tools for freshwater risk assessment. A first outcome of the project is a review on the current state of the application of bioavailability- based approaches in risk assessment approaches. The findings from this project is being disseminated via a websites http://www.metal-bioavailability.org/ on the bioavailability of metals. Similar websites for other projects (e.g. on e-waste is currently under development. Finding from this project will also be presented in the special IUPAC symposium during the SETAC 2018 conference in Rome.
Trace Elements Analysis of Environmental Samples with X-Rays: From Synchrotron to Lab and from Lab to Synchrotron 2016-019-2-600	Terzano	A one-day special Symposium entitled "TRACE ELEMENTS ANALYSIS OF ENVIRONMENTAL SAMPLES WITH X-RAYS" was organized during the ICOBTE 2017 Conference, which took place in Zurich (Switzerland) from 16 to 20 July 2017. A total of 30 abstract were received from 16 countries out of which 10 contributions (from 8 countries) were selected for oral presentation (6 regular + 4 short). 18 contributions were presented as posters. Two

		keynote lectures were given by invited speakers, whose participation costs were covered by Bruker Gmbh. The symposium was attended by about 100 participants. Three poster prizes (220\$ + award plaque) sponsored by IUPAC Division VI were awarded to: Barbara Lopata (Poland), Kathryn Spiers (Germany) and Antonio Caporale (Italy).
Workshop on Middle East Regional Cooperation and Sustainable Water Management of Transboundary Water. 2017-018-3-600	Shevah/ Garelick	To foster regional cooperation, a workshop was held in the Middle East <i>on Sustainable Water</i> <i>Management of Transboundary Water</i> was held on 15 <sup>th</sup> December 2017. The workshop was held as part of the bi-annual Malta Conference Foundation (MCF) – MALTA VIII, titled "Frontiers of Chemistry: Research and Education in the Middle East - a Bridge to Peace". The MCF is an independent nonprofit organization, promoting science cooperation as a bridge to peace in the Middle East.

#### Goal: Capability development and technology transfer:

- Ecological Risk Assessment (ERA) Workshops: Following on from successful Workshops in Beijing, Bogota, New Delhi, San Jose in Costa Rica was host to the latest in the series. This Workshop was supported by IUPAC, ACS AGRO and CropLife International. This Workshop was held as part of LAPRW2017. (Chemistry International <u>39</u>(4) 45-46 2017).
- Divisional members gave presentations at the Latin American Pesticide Residue Workshop (LAPRW2017) held in San Jose, Costa Rica in May 2017 and also took part in the symposium "Fate of Pesticides in Latin American Environments" as part of the 49th IUPAC General Assembly held in Sao Paulo, Brazil.
- 14<sup>th</sup> IUPAC International Congress of Pesticide Chemistry: plans are being formalised for the 14<sup>th</sup> Congress, originally planned for Rio de Janeiro, Brazil, which will now take place in Ghent, Belgium, May 19<sup>th</sup> - 24<sup>th</sup> 2019.
  - The next award for "Advances in Harmonized Approaches to Crop Protection Chemistry" will be given in 2019 at the IUPAC Pesticide Congress in Ghent. The presentation was originally scheduled for 2018 in Rio de Janeiro. A new call for nominations will be made.
- The proposed 4<sup>th</sup> International Conference on Agrochemicals Protecting Crops, Health and Natural Environment – "Discovery and Development of Synthetic and Natural Products for Pest Management" has been provisionally scheduled for January 2020 in New Delhi, India.
- Technical symposia on topical issues:

We organized and delivered five highly successful symposia, including three during the 46<sup>th</sup> World Chemistry Congress Sao Paulo, namely on

- (i) E-waste an emerging global environmental challenge (D Purchase and H Garelick)
- o (ii) Global Environmental Challenges of Nanomaterials (Chair S Obare),
- o (iii) Fate of Pesticides in Latin American Environments (Chair J Unsworth) and
- (iv) "Trace elements analysis of environmental samples with X-Rays" (*R Terzano*) during ICOBTE 2017 from 16 to 20 July 2017 in Zurich (Switzerland).

- (v) Water and Environmental Analysis symposium during HPLC 2017 in Korea (*Chung*).
- To foster regional cooperation, a workshop was held in the Middle East on Sustainable Water Management of Transboundary Water (Shevah/ Garelick).
- To promote sustainable development and application of nanotechnology, a workshop on "Safety of Engineered Nanomaterials" was held during September 28-29, 2017 in Queretaro (Mexico), jointly funded by Division VII and VI.
- In collaboration with SETAC we have organized a special IUPAC session in May 2018 Europe conference in Rome entitled, "Improvements in Environmental Exposure Assessment: Development and Application of Tools across Industry Sectors, Regulatory Agencies, and International Boundaries". Several divisional projects are presenting works at this. A total of 12 oral presentations and 34 poster presentations will be included in the session.

### IV. Tabular material.

## Selected publications (2016-2017)

- 1. Walker, G, Kookana, RS, Smith NE, et al. (2017). Ecological risk assessment of nano-enabled pesticides: A perspective on Problem Formulation. J. Agric. Food Chem. 65, DOI: 10.1021/acs.jafc.7b02373.
- 2. Unsworth JB and Carazo E. (2017). Ecological Risk Assessment. Chemistry International <u>39</u>(4) 45-46.
- 3. Saha BB. (2017). IUPAC 2017- World Chemistry Congress and IUPAC general Assembly. Chemistry International <u>39 (4)</u> 46-49.
- Perminova IV. (2017). Database on molecular compositions of natural organic matter and humic substances as measured by high resolution mass spectrometry. *Chemistry International*. 39 (2) 21–21. <u>DOI</u> <u>10.1515/ci-2017-0213</u>.
- 5. Kookana RS (2017). Environmental Fate and Risks of Nano-enabled Pesticides. Chemistry International. Chemistry International <u>39 (1)</u> 24-25.
- McConnell LL, Racke KD, Hapeman KJ, Seiber, JN. (2017). 13th IUPAC International Congress of Pesticide Chemistry: Crop, Environment, and Public Health Protection, Technologies for a Changing World. J. Agric. Food Chem., 64 (1), 4-5.
- Berenbaum MR. (2017). Does the Honey Bee "Risk Cup" Runneth Over? Estimating Aggregate Exposures for Assessing Pesticide Risks to Honey Bees in Agroecosystems. J. Agric. Food Chem., 64 (1), 13-20.
- Ambrus, A. (2017). International Harmonization of Food Safety Assessment of Pesticide Residues. J. Agric. Food Chem., 64 (1), 21-29.
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- 11. Anderson JA, Harrigan GG, Rice P and Kleter G. (2016) Challenges and opportunities in supporting sustainable agriculture and food security. Overview of the 13th IUPAC International Congress of Pesticide Chemistry Symposia on Agricultural Biotechnology (Editorial). J. Agric. Food Chem., 64(2), 381–382.

- Xing B, Vecitis CD and Senesi N. (2016). (Eds) Engineered Nanoparticles and The Environment: Biophysicochemical Processes and Toxicity. Volume VI in Wiley-IUPAC series. ISBN 978-1-119-27582-4.
- 13. Gras N. and Unsworth JB. (2016) Latin American Pesticide Residue Workshop -Food and the Environment, Chemistry International 38(2) 28.
- 14. Unsworth JB and Gras N. (2016) Ecological Risk Assessment Latin America, Chemistry International 38(2) 29.
- 15. Unsworth JB. and Lalah JO. (2016) Ecological Risk Assessment Workshop -Kenya, Chemistry International 38(5) 32.
- Unsworth, JB, Shakil NA and Kumar J. (2016) New Chemistries for Phytomedicines and Crop Protection Chemicals, Chemistry International 38(6) 34-36.
- 17. Pantoja Munoz L, ,Purchase D, Jones H, Raab A, Urgast D, Feldmann J and Garelick H. (2016) The mechanisms of detoxification of As(III), dimethylarsinic acid (DMA) and As(V) in the microalga Chlorella vulgaris. Aquatic Toxicology, 175 . pp. 56-72. ISSN 0166445
- Chan WC, Wildeboer D, Garelick H, Purchase D. (2016) Mycoremediation of Heavy Metal/Metalloid-Contaminated Soil: Current Understanding and Future Prospects. In Fungal Applications in Sustainable Environmental Biotechnology, pp.249-272. DOI: 10.1007/978-3-319-42852-9\_10.
- Joao Gatica, Vijay Tripathi, Stefan Green, Celia M. Manaia, Thomas Berendonk, Damiano Cacace, Christophe Merlin, Norbert Kreuzinger, Thomas Schwartz, Despo Fatta-Kassinos, Luigi Rizzo, Carsten U. Schwermer, Hemda Garelick, Edouard Jurkevitch, and Eddie Cytryn (2016). High throughput analysis of integron gene cassettes in wastewater environments. Environmental Science and Technology. 50 (21):11825–11836.DOI: 10.1021/acs.est.6b03188.
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- Ermolin MS and Fedotov PS, (2016). Separation and characterization of environmental nano- and submicron particles. Rev. Anal. Chem. 2016. doi: 10.1515/revac-2016-0006
- 22. Ermolin MS, Fedotov PS, Ivaneev AI, Karandashev VK, Tatsy YG. (2016). Assessment of elemental composition and properties of copper smelter affected dust and its nano- and micron size fractions. Environ. Sci. Pollut. Res. 2016. doi: 10.1007/s11356-016-7637-6
- Kördel W. (2016). Substance-related Environmental Monitoring Strategies Regarding Soil, Groundwater and Surface Water. Chemistry International 38(3-4), 31-33.

Project Number	Task Chair	Title	Status
2010-060-1-600	Unsworth	A Support Team for Enhancing, Maintaining and Ensuring the Future of the Pesticides Properties Database (PPDB)	In abeyance
2011-019-1-600	Xing	Engineered Nanoparticles and the Environment: Physicochemical Processes and Biotoxicity	On-going
2011-023-2-600	Harris	Critical review of approaches to dietary risk assessment for pesticides	On-going
2012-018-5-600	Parker	Development of IUPAC Good Modeling Practice (GMP) Guidelines for Pesticide Aquatic Ecological Exposure Assessment and Risk Management	On-going
2012-019-1-600	Unsworth	The Importance of Chemistry in Maintaining a Secure Food Supply	On-going
2012-020-3-600	Kookana	Guiding principles to facilitate a harmonized ecological risk assessment framework for nano-pesticides in the environment	Essentially complete
2013-024-2-600	Molyneux	Recommended Methods for the Structural Identification of Biologically Active Compounds in Food and Flavor Chemistry	On-going
2013-029-2-600	Kleter	Inventory of developments in the field of RNAi-based pesticides and potential needs for international harmonization of regulatory safety requirements	On-going
2014-026-3-600	Obare	Environmental Chemistry - Development of Three Technical Symposia at the 46th IUPAC Congress, São Paulo 2017	On-going
2014-031-3-600	Purchase	Environmental Chemistry - Development of Three Technical Symposia at the 46th IUPAC Congress, São Paulo 2017	On-going
2014-032-1-600	Karpouzas	Advances on the Assessment of Pesticides' Soil Microbial toxicity: New research and regulatory aspects in light of the recent methodological advances	On-going
2015-010-3-600	Keen	Standardization of electrical energy per order (EEO) reporting for UV/H2O2 reactors	On-going
2016-016-2-600	Kookana	Guidance for Industry and Regulators on Assessment of the Environmental Fate and Risks of Nano-enabled Pesticides	On-going
2016-019-2-600	Terzano	Trace elements analysis of environmental samples with X-rays: from synchrotron to lab and from lab to synchrotron	On-going
2016-025-1-600	Carazo	Ecological Risk Assessment Workshop for Central America	On-going
2016-035-1-600	Purchase	Fate of Pesticides in Latin American Environments (one of 3 symposia at IUPAC 2017)	On-going
2016-047-1-600	Xing	Multi-scale Biogeochemical Processes in Soil Ecosystems: Critical Reactions and Resilience to Climate Changes	On-going
2017-004-1-600	Chung	Water and Environmental Analysis - a Symposium part of HPLC 2017	On-going
2017-013-1-600	Racke	Crop protection chemistry in Latin America: Harmonized approaches for environmental assessment and regulation	On-going
2017-035-2-600	Kookana	Human Health Risk Consideration of Nano-enabled Pesticides for Industry and Regulators	On-going
2015-056-3-600	Kalderis	Glossary of terms used in biochar research	On-going