



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 2016 – Submitted by Petr S. Fedotov, President

I. Highlights

Through its internationally recognized membership and project teams, Division VI – Chemistry and the Environment (DCE), provides unbiased and timely authoritative reviews on the behavior of chemical compounds in food and the environment. The DCE undertakes both fundamental and applied evaluations that contribute to solving environmental problems and enhancing the quality of food on a global scale.

- a. Division VI has made progress on a number of important projects over 2014-2015 and initiated six new projects in 2015:
 - i. 2014-023-2-600 (Letcher) – Climate Change: Observed Impacts on Planet Earth, 2nd Edition. This project seeks to provide an updated Edition of the original book with new chapters and updated information in other chapters. All chapters have been reviewed and submitted to the publisher.
 - ii. 2014-031-3-600 (Purchase) - The Environmental and health challenges of E-Waste and its management: an emerging 21st century global concern. This project aims to bring together global expertise to a) examine current research on the chemical nature of e-waste and its global distribution; b) evaluate its environmental and health impact of e-waste and related risk management tools and models; c) identify short-comings in present regulations and management strategies as well as future challenges; and d) develop a set of specific recommendations for management approaches that are science-based and globally informed.
<http://www.degruyter.com/view/j/ci.2015.37.issue-4/ci-2015-0415/ci-2015-0415.xml?format=INT>
 - iii. 2014-032-1-600 (Karpouzias) – Advances on the Assessment of Pesticides' Soil Microbial toxicity: New research and regulatory aspects in light of the recent methodological advances. Thus the project aims to review the current knowledge on soil microbial ecotoxicity of pesticides and propose a regulatory scheme on how pesticide soil microbial ecotoxicity should be assessed.
 - iv. 2014-026-3-600 (Obare) - Chemical speciation of anthropogenic nanoparticles. The objective of this project is to develop guidelines and provide a framework for understanding the chemical speciation of nanoparticles and the associated environmental health and safety issues.
 - v. 2014-038-2-600 (Unsworth) - Global Framework for Implementing Consistent Ecological Risk Assessment of Pesticides for Sustainable Agriculture: Workshop in Chile. This project is designed to organize an Ecological Risk Assessment Workshop in Chile as part of the 4th Latin American Pesticide Residue Workshop in Chile.
 - vi. 2015-048-1-600 (Unsworth and Lalah) - Ecological Risk Assessment Workshop for East Africa. The objective of this project is to conduct a focused workshop on Ecological Risk Assessment for scientists, students and government officials who will be attending the 3rd International Conference on

Innovation and Technology for Development in Nairobi, Kenya on February 23-25, 2016 (<http://conference.tukenya.ac.ke>).

- b. Division VI has established cooperation with the Division of Chemistry and the Environment (DCE) of the European Association of Chemical and Molecular Sciences (EuCheMS). Following an exchange by Petr Fedotov with EuCheMS a special session "Metals, Metalloids and Elemental Speciation" (conveners Petr Fedotov and Heinz Ruedel) has been organized at the 15th EuCheMS International Conference on Chemistry and the Environment (ICCE 2015, September 20-24, 2015, Leipzig, Germany).
http://www.icce2015.org/assets/program_monday_1.pdf
- c. Organized a satellite event on "The environmental and health challenges of E-Waste and its management: an emerging 21st century global concern" in the framework of ICCE 2015. A kick-off meeting related to project 2014-031-3-600 (Diane Purchase) has been also covered as part of the satellite event.
http://www.icce2015.org/se_2.html
- d. Division VI has partnered with CCE to organize the World Chemistry Leadership Meeting in Busan (August 2015) focusing on the UN Sustainable Development Goals. (<http://www.degruyter.com/view/j/ci.2015.37.issue-4/ci-2015-0420/ci-2015-0420.xml?format=INT>)
- e. Division VI has sponsored an Environmental Chemistry Poster Prize at the World Chemistry Congress in Busan. Approximately 100 presenters have competed for three prizes presented at the closing ceremony.
- f. Organized a symposium, "Novel Molecular and Supramolecular Theory and Synthesis Approaches for Sustainable Catalysis" at the World Chemistry Congress in Busan (August 2015). This symposium included speakers funded a special international call for proposals managed by IUPAC and funded by several national funding agencies to foster multi-national cooperation in sustainable chemistry.
- g. Successfully hosted the 13th IUPAC International Congress of Pesticide Chemistry in August 2014 at the American Chemical Society National Meeting and Exposition. www.iupac2014.org. At this Congress, presented the IUPAC International Award for Advances in Harmonized Approaches to Crop Protection Chemistry (<http://www.degruyter.com/view/j/ci.2015.37.issue-4/ci-2015-0408/ci-2015-0408.xml?format=INT>). Several publications are either completed or are in progress as a result of the Congress. The 14th Congress will be held in 2018 in Rio de Janeiro, Brazil.
- h. Published a special issue of Pure and Applied Chemistry resulting from a symposium at the World Chemistry Congress in Istanbul (<http://www.degruyter.com/view/j/pac.2014.86.issue-7/issue-files/pac.2014.86.issue-7.xml>).
- i. Sponsored the 4th Latin American Pesticide Residue Workshop in May 2015 in Santiago, Chile.
- j. Sponsoring the 3rd International Conference on Agrochemicals Protecting Crops, Health and Natural Environment, in January 2016, Delhi, India.
- k. Sponsoring the 9th World Mycotoxin Forum & XIVth International Symposium on Mycotoxins in June 2016, Winnipeg, Canada.
- l. As a means of consolidating activities and recruiting new members in Division VI, a new Subcommittee on Chemical and Biophysical Processes in the Environment was established in 2014, this subcommittee combined the earlier subcommittee on

II. Selected Accomplishments and Outcomes in 2014-2015 and early 2016 – According to IUPAC Strategic Plan

a. *IUPAC provides scientific expertise to address critical world needs.*

- i. The first workshop associated with the project titled “Guiding principles to facilitate a harmonized ecological risk assessment framework for nano-pesticides in the environment” (project 2012-020-3-600) was held in Europe at the University of York on 18-19 May 2013 coinciding with SETAC Europe meeting in Glasgow. The synthesis from the workshop discussions was captured in a “Perspective Article” published in April 2014 in Journal of Agriculture and Food Chemistry: [dx.doi.org/10.1021/jf500232f](https://doi.org/10.1021/jf500232f). The workshop was jointly sponsored and organized by IUPAC and APVMA (The Australian Pesticide and Veterinary Medicines Authority). APVMA is the regulatory agency in Australia dealing with nanomaterials for applications in agriculture and veterinary medicines. (<http://www.degruyter.com/view/j/ci.2014.36.issue-6/ci-2014-0617/ci-2014-0617.xml?format=INT>). The second meeting and symposium “Fate, Effects and Risks of Nanopesticides” was held at the 13th IUPAC International Congress of Pesticide Chemistry (August 2014, San Francisco, USA)
- ii. In the project “Environmental Chemistry, Green and Sustainable Chemistry” (2012-034-1-600 Garelick), a special issue of Pure and Applied Chemistry has been published as a result of three sponsored symposia held at the World Chemistry Congress in Istanbul Turkey. The aim of the special issue is to provide a critical review of both fundamental and applied aspects of specific contaminants behavior in the environment and to aid in future risk assessment that is based on appropriate consideration of their life cycle. (<http://www.degruyter.com/view/j/pac.2014.86.issue-7/issue-files/pac.2014.86.issue-7.xml>).
- iii. The 13th IUPAC International Congress of Pesticide Chemistry was held 10-14 August 2014, in San Francisco, USA. The Congress was organized by the AGRO Division of the American Chemical Society under the auspices of the IUPAC Division of Chemistry and the Environment (DCE). Two members of the DCE Committee served as co-organizers for the Congress, DCE President Laura McConnell and past-President Kenneth Racke. The Congress Scientific Committee was chaired by Cathleen Hapeman, AGRO Program Chair.

The theme of the Congress was “Crop, Environment, and Public Health Protection: Technologies for a Changing World”. The scientific program was organized into nine main scientific topics and 46 individual symposia. Topics ranged from discovery synthesis to environmental chemistry to residues in food to regulation. Each individual symposium included invited lectures, posters, and an interactive panel discussion or workshop discussion. More than 1000 lecture and poster presentations were included in the symposia. Each day of the Congress began with two plenary lectures that all participants attended, and the rest of the day involved nine concurrent sessions which participants could choose between. A synopsis of the meeting is available online (<http://www.iupac2014.org/wp-content/uploads/2009/06/IUPAC-ACSFall14.pdf>).

A total of 1216 scientists from 53 countries attended the Congress, with approximately one half originating from outside of North America. There was a strong emphasis on the participation of students and younger scientists as well as experts from scientifically emerging regions. More than 50 student travel grants were awarded and a “new investigator” award competition, open to those within 5 years of their Ph.D., generated a number of applicants from which three finalists were selected. A special graduate student luncheon was organized and included guest speakers who discussed international career opportunities.

Based on an IUPAC project grant, a world crop protection chemistry leadership workshop was organized during the first day of the Congress. This workshop focused on identifying opportunities for training the next generation of crop protection chemistry leaders for industry, government, and academia. A report outlining a set of consensus recommendations is being prepared by the DCE’s Advisory Committee on Crop Protection Chemistry. 2013-019-2 (Unsworth) - World Crop Protection Chemistry Institute: Developing Global Leaders for Research, Regulation and Stewardship in the 21st Century. (<http://www.degruyter.com/view/j/ci.2015.37.issue-2/ci-2015-0244/ci-2015-0244.xml?format=INT>)

- iv. Quantitative Review and Analysis of Pesticide Sorption and Its Effect on Degradation in Relation to Soil and Climate Project No. 2010-018-2-600 (Chen): This project while still underway has generated an ACS Symposium Series Book in 2014, “Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil” (<http://pubs.acs.org/isbn/9780841229785>).
- v. Book entitled “Climate Change. 2nd Edition. Observed Impacts on Planet Earth” has been published as an outcome of Project No. 2014-023-2-600 (Letcher) The book presents a multi-disciplinary overview of the Earth's changing climate, including models of climate change, geological history, and further engineering aspects. <http://store.elsevier.com/Climate-Change/isbn-9780444635242/>
- vi. Project No. 2014-031-3-600 (Purchase) “The environmental and health challenges of e-waste and its management: an emerging 21st century global concern” is underway. It aims to bring together global expertise to a) examine current research on the chemical nature of e-waste and its global distribution; b) evaluate its environmental and health impact of e-waste and related risk management tools and models; c) identify short-comings in present regulations and management strategies as well as future challenges; and d) develop a set of specific recommendations for management approaches that are science-based and globally informed.

Items *i,ii,v,vi* refer to *multidisciplinary projects addressing critical global issues*.

III. Other Substantive Information

- i. A divisional conference call was held on January 28, 2016 with 16 division members and 1 additional member participating.
- ii. The next annual meeting of the division will be held in London, UK on May 28-29, 2016.

IV. List of Publications

- a. Arancon, R. A. D., Tao Zhang, Y., & Luque, R. (2014). Nanotechnology management for a safer work environment. *Pure and Applied Chemistry*, 86(7), 1159-1168.
- b. Ambrus, A. International Harmonization of Food Safety Assessment of Pesticide Residues. *Journal of Agriculture and Food Chemistry*, Article ASAP. DOI: 10.1021/jf505854w
- c. Ambrus, A. Global harmonization of maximum residue limits (MRLs) for pesticides. *Journal of Agriculture and Food Chemistry*, Article ASAP. <http://dx.doi.org/10.1021/jf505347z>
- d. Berenbaum, M.R. Does the Honey Bee "Risk Cup" Runneth Over? Estimating Aggregate Exposures for Assessing Pesticide Risks to Honey Bees in Agroecosystems. *Journal of Agriculture and Food Chemistry*, Article ASAP. <http://pubs.acs.org/doi/pdfplus/10.1021/acs.jafc.5b01067>.
- e. Chalkiadaki, O., Dassenakis, M., Paraskevopoulou, V., & Lydakis-Simantiris, N. (2014). Experimental study of cadmium bioaccumulation in three mediterranean marine bivalve species: Correlation with selected biomarkers. *Pure and Applied Chemistry*, 86(7), 1189-1204.
- f. Chen, W., Sabljic, A., Cryer, S. A., Kookana, R. S. (Eds.) (2014). Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil. ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
- g. Chen, W., Laabs, V., Kookana, R. S., Koskinen, W. C. (2014). Coupled Sorption and Degradation Kinetics and Non-First Order Behavior. In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil*, pp 5-37, W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
- h. Farenhorst, A., McQueen, R., Kookana, R. S., Singh, B., Malley, D. (2014). Spatial Variability of Pesticide Sorption: Measurements and Integration to Pesticide Fate Models. In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil* (pp 255-274), W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
- i. Farrukh, A., Akram, A., Ghaffar, A., Tuncel, E., Oluz, Z., Duran, H., . . . Yameen, B. (2014). Surface-functionalized silica gel adsorbents for efficient remediation of cationic dyes. *Pure and Applied Chemistry*, 86(7), 177-1188.
- j. Fedotov, P. S. (2014). Estimating the bioavailability of trace metals/ metalloids and persistent organic substances in terrestrial environments: Challenges and need for multidisciplinary approaches. *Pure and Applied Chemistry*, 86(7), 1085-1095.
- k. Garelick, H., Miller, B., & Peijnenburg, W. (2014). 44th IUPAC congress: Environmental chemistry. *Pure and Applied Chemistry*, 86(7), 1083-1084.
- l. Kookana, R.S.; Boxall, A.B.A. ; Reeves, P.T., Ashauer, R. , Beulke, S., Chaudhry, Q. , Cornelis, G. , Fernandes, T.F., Gan, J. , Kah, M. , Lynch, I. , Ranville, J. , Sinclair, C. , Spurgeon, D. , Tiede, K., , Van den Brink, P.J. (2014). Nanopesticides: Guiding principles for regulatory evaluation of environmental risk. *Journal of Agricultural and Food Chemistry*, 62: 4227-4240. DOI: 10.1021/jf500232f
- m. Kookana, R. S., Ahmad, R., Farenhorst, A. (2014). Sorption of Pesticides and its Dependence on Soil Properties: Chemometrics Approach for Estimating Sorption. In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil*, pp 221-240, W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS

- Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
- n. Kustov, L. M., Al-Abed, S. R., Virkutyte, J., Kirichenko, O. A., Shuvalova, E. V., Kapustin, G. I., . . . Finashina, E. D. (2014). Novel Fe-Pd/SiO₂ catalytic materials for degradation of chlorinated organic compounds in water. *Pure and Applied Chemistry*, 86(7), 1141-1158.
 - o. Lawrence, G. D., Patel, K. S., & Nusbaum, A. (2014). Uranium toxicity and chelation therapy. *Pure and Applied Chemistry*, 86(7), 1105-1110.
 - p. Li, J., Zhang, Y., Herjavić, G., Wine, P. H., & Klasinc, L. (2014). Bibliometric analysis of research on secondary organic aerosols: Update. *Pure and Applied Chemistry*, 86(7), 1169-1175.
 - q. Liu, C., Guan, A., Yang, J., Chai, B., Li, M., Li, H., Yang, J., Xie, Y. Efficient Approach To Discover Novel Agrochemical Candidates: Intermediate Derivatization Method. *Journal of Agriculture and Food Chemistry*, Article ASAP. DOI: 10.1021/jf5054707.
 - r. Nick, S. T., Bolandi, A., Samuels, T. A., & Obare, S. O. (2014). Advances in understanding the transformation of engineered nanoparticles in the environment. *Pure and Applied Chemistry*, 86(7), 1129-1140.
 - s. Leonardo Pantoja Munoz, Diane Purchase, Huw Jones, Jorg Feldmann and Hemda Garelick (2014). Enhanced determination of As-phytochelatin complexes in *Chlorella vulgaris* using focused sonication for extraction of water-soluble species. *Anal. Methods*, 2014, 6 (3), 791 – 797.
 - t. Rüdell H*, Díaz Muñiz C, Garelick H, Kandile NG, Miller BW, Pantoja Munoz L, Peijnenburg WJGM, Purchase D, Shevah Y, van Sprang P, Vijver M, Vink JPO(2015). Consideration of the bioavailability of metal/metalloid species in freshwaters: experiences regarding the implementation of biotic ligand model-based approaches in risk assessment frameworks, Accepted for publication in *Environmental Science and Pollution Research*. Published online: 08 March 2015. DOI 10.1007/s11356-015-4257-5.
 - u. Sabljic, A., Nakagawa, Y. (2014). Biodegradation and Quantitative Structure-Activity Relationship (QSAR). In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil*, pp 57-84, W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
 - v. Sabljic, A., Nakagawa, Y. (2014). Sorption and Quantitative Structure-Activity Relationship (QSAR). In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil*, pp 85-118, W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.
 - w. Shevah, Y. (2014). Water scarcity, water reuse, and environmental safety. *Pure and Applied Chemistry*, 86(7), 1205-1214.
 - x. Stankovic, S., Tanaskovski, B., Zlatic, B., Arsenovic, M., & Pezo, L. (2014). Analysis of trace elements in surface sediments, mussels, seagrass and seawater along the southeastern adriatic coast -a chemometric approach. *Pure and Applied Chemistry*, 86(7), 1111-1127.
 - y. Sur, R. (2014). Terrestrial Field Degradation Based on Soil, Climatic, and Geographic Factors. In *Non-First Order Degradation and Time-Dependent Sorption of Organic Chemicals in Soil*, pp 39-56, W. Chen, A. Sabljic, S. A. Cryer, R. S. Kookana (Eds.). ACS Symposium Series 1174; American Chemical Society: Washington, DC, 2014. Oxford University Press. ISBN 978-0-8412-2978-5.

- z. Tepavitcharova, S., Rabadjieva, D., Todorov, T., Kovacheva, A., Dassenakis, M., & Paraskevopoulou, V. (2014). Chemical speciation in fresh, saline and hyper-saline waters. *Pure and Applied Chemistry*, 86(7), 1097-1101.
- aa. Unsworth, J.B., Corsi, C., Van Emon, J.M., Farenhorst, A., Hamilton, D.J., Howard, C.J., Hunter, R., Jenkins, J., Kleter, G.A., Kookana, R.S. Developing Global Leaders for Research, Regulation, and Stewardship of Crop Protection Chemistry in the 21st Century. *Journal of Agriculture and Food Chemistry*, Article ASAP, <http://pubs.acs.org/doi/pdfplus/10.1021/jf5060744>.
- bb. Wang Xiaonan, He Xiongkui, Andreas. Herbst, et al. Development and performance test of spray drift test system for sprayer with bar[J]. *Transactions of the Chinese Society of Agricultural Engineering*, 2014, 30(18): 55-62.
- cc. Zhang Wenjun, He Xiongkui, Song Jianli, et al. Effect of adjuvant S240 on atomization of water dispersible granule and emulsion solution[J]. *Transactions of the Chinese Society of Agricultural Engineering*, 2014, 30(11): 61-67.
- dd. Ziska, L.H., McConnell, L.L. Climate Change, Carbon Dioxide, and Pest Biology: Monitor, Mitigate, Manage. *Journal of Agriculture and Food Chemistry*, Article ASAP, DOI: 10.1021/jf506101h
- ee. Farenhorst A, McQueen DAR, Kookana RS, SINGH B, Malley D. (2015). Spatial variability of pesticide sorption: measurements and integration to pesticide fate models. Non-first order degradation and time-dependent sorption of organic chemicals in soil. Washington DC: American Chemical Society Publications: 255-274.
- ff. Kookana RS, Ahmad R, Farenhorst A. (2015). Sorption of pesticides and its dependence on soil properties: chemometrics approach for estimating sorption. Non-first order degradation and time-dependent sorption of organic chemicals in soil Washington DC: American Chemical Society Publications: 221-240.
- gg. Unsworth JB; Corsi C; Van Emon JM; Farenhorst A; Hamilton DJ; Howard CJ; Hunter R; Jenkins JJ; Kleter, GA; Kookana RS; Lalah JO; Leggett M; Miglioranza KSB; Miyagawa H; Peranginangin N; Baruch R; Saha B and Shakil NA. (2015). Developing global leaders for research, regulations, and stewardship of crop protection chemistry in the 21st Century. *Journal of Agricultural and Food Chemistry*, DOI: 10.1021/jf5060744.
- hh. Rüdél H, Díaz Muñiz C, Garelick H, Kandile NG, Miller BW, Pantoja Munoz L, Peijnenburg WJ, Purchase D, Shevah Y, van Sprang P, Vijver M, Vink JP (2015). Consideration of the bioavailability of metal/metalloid species in freshwaters: experiences regarding the implementation of biotic ligand model-based approaches in risk assessment frameworks. *Environ. Sci. Pollut. Res. Int.* 22, 7405-7421.