IUPAC Analytical Chemistry Division (V)

Report to Council, 2003 – 2005

I. Executive Summary

- The Division has made significant moves to build partnerships with
  - organizations that have experience in developing countries (IAEA, UNIDO, IOCD, SEANAC),
  - other unions and expert bodies (IUPAP, BIPM, IUGS).

- The Division is coordinating a series of articles for *Chemistry International* on the topic of *"Emerging needs of developing countries".* This series should run for 8-10 issues and will carry contributions from several Divisions.

- The Division has started a significant number of inter-Divisional projects. These link us with Divisions I, III, IV, VI and VII, and with COCI.

- To ensure attention to critical areas it has identified a limited number of "priorities" for the biennium. It has focused its energy on these.

- To cultivate a spirit of "collective responsibility" it has formed seven Teams, each with responsibility for one priority area. All NR, AM and TM are assigned to one or two teams. The Team structure should facilitate continuity of effort into the next biennium.

- Communication within the Division and with other officers of the union is maintained through the electronic newsletter *"Teamwork".*

- The Division is working on the maintenance and updating of two key IUPAC publications, *The Compendium of Analytical Nomenclature* (Orange Book) and the *IUPAC Stability Constant Database* (SCDB).

- To facilitate the development of new projects the Division involved external experts in a mini-symposium on "*Metrological traceability*" held at the IAEA in conjunction with its even-year meeting.

II. Report on Division activities in relation to IUPAC goals

2.1. *IUPAC will provide leadership as a worldwide scientific organisation that objectively addresses global issues involving the chemical sciences.*

The Division has 'Core activities' as on-going responsibilities. But it also identified a set of priorities that are based on perceived emerging needs of the scientific community. These 'Emerging issues' are more time-dependent and are likely to change to some degree from one biennium to the next:

Core Activities*:*

Communication

Project initiation and management in the areas of:

- Quality Assurance
- Terminology – Orange Book: maintaining and updating
- Critical evaluation of data

Emerging issues in analytical chemistry:

- in bioanalytical chemistry
- in process chemistry and nano-chemistry
- in developing countries and scientific communities.

Teams of 4-6 members (TM + AM + NR) are formed for each priority area. Each Team has a collective responsibility and is encouraged to:

- Determine the scope of its responsibility and activities;
- Develop a strategy for effective communication between and by its members.
- Identify activities that advance the goals of IUPAC in its designated area.
- Achieve at least one significant output each year (*e.g*. letters to Editors; an IUPAC or ACD presentation at a Conference; an article for *CI*; a Project Proposal; etc.)
- Accept responsibility for leading Division activities in its designated area
- Facilitate a 'roll-over' of its activities at the end of the current biennium.

Communication.
The Division maintains communication with all its members, and officers of other Divisions and Operational committees, through its newsletter *Teamwork*.

The Division interacts with all Task Groups on a half-yearly basis (to be changed to eight-monthly) via a Project reporting system. The reports are read by all Division members and are reviewed at Division meetings. They provide an 'early warning system' for any projects that are struggling, alert the Division to the need for reviewers and allow re-assessment of Dissemination plans as the projects near completion. As from November 2004 these reports are appended to the respective Project pages on the IUPAC website, so that Project progress is in the public domain.

Global issues.
One global issue being addressed is the measurement of pH, through the project: *Comparable pH measurements by metrological traceability. Part I: Water quality monitoring and assessment; Part II: Clinical and biochemical matrices.* This project sees a continuation of work by the "pH task group" [Measurement of pH. Definition, Standards and Procedures. 2002] and it has the financial and professional backing of three Divisions and COCI.

Another global issue addressed is the concept of *'fair trade'*. Fair Trade can only arise between nations when all have adequate and *quality-assured laboratories* and their methodology meets the current requirements for *metrological traceability*. These issues are particularly relevant to the less developed nations. These concepts were the basis of:

(a) A successful joint project proposal with IOCD which includes two Division V members, titled: "*Standardisation of analytical approaches and analytical capacity building in Africa*". This project involves a melding of IUPAC technical expertise with IOCD appreciation of geopolitical issues in developing countries.

(b) Division V support for the WPQA in the preparation of an ICSU proposal on "*Measurement traceability – a fair basis for trade'*. This application for funds was not successful but the process of preparing the proposal generated very positive interactions with project partners UNIDO and IUPAP (including their participation in a WPQA/Division V workshop).

Symposia and Workshops.
The Division attempts to capture external expertise to introduce and scope emerging issues or opportunities in analytical chemistry. This is assisted through mini-symposia held in conjunction with the Division even-year meeting and the GA.

From the mini-symposium on "*New Challenges for Analytical Chemists in Genomics, Proteomics, and Genetically Modified Organisms*" held during the Ottawa GA, two new projects were identified. One has been funded in this biennium ("*Standard definition of terms related to mass spectrometry*") while the other on "*Terminology related to analytical chemistry of metal forms in biological systems: metallomics*" has been thoroughly scoped and a Task Group identified.

At the even-year meeting in Vienna 2004 a mini-symposium on "*Metrological traceability*" was held jointly with IAEA staff and the WPQA. It attracted speakers from IUPAP, UNIDO, BIPM, IAEA and WPQA. The meeting identified several areas in which IUPAC expertise might be applied. We now try to identify possible 'concrete' outcomes from that meeting - IUPAC projects that could be crafted

around the ideas and concerns that were shared. IUPAC will benefit through any projects that link it with agencies that are working much closer to the geopolitical coal-face.

2.2. IUPAC will facilitate advancement of research in the chemical sciences through the tools that it provides for international standardisation and scientific discussion

Division V actively pursues these goals through its program of critical evaluations of data, the establishment of guidelines for Quality Assurance in chemical methods and associated sampling, and by the updating of analytical nomenclature and making it readily available via the web:

(a) ***The Orange Book***. This is now on-line at (http://www.iupac.org/publications/analytical_compendium/)

The route for updating terminology in the OB is via formal publication in *PAC.* Examples of issues being currently addressed through projects are: *Glossary of Terms related to Solubility; Revision of terminology in separation science; Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanlytical chemistry; Internationally agreed terminology for observations in scientific communications; Standard definitions of terms relating to mass spectrometry.*

The text will be progressively converted to ICTNS-accepted format; it will also be aligned with the Gold book version, so that there is only one version of terminology within the IUPAC database.

(b) ***The IUPAC Stability Constants Database*** (SCDB) is the most comprehensive compilation of stability constants available, covering the years 1877 to 2002. It is the primary source of data for the Critical evaluations of Stability Constants that are published on a regular basis by Division V. It is a major research tool for those involved in equilibrium modelling of environmental, biological and industrial systems.

Division V has in place a Project to continue the evaluation, collection and entry of data through to 2008. To minimise risk the data collection team has been expanded from one site to now involve experts in four countries.

The future of SCDB was the subject of a Division V presentation to the Bureau meeting in 2004. All aspects of the management of the database – program development, data conflation, advertising, marketing – have for the last 16 years been undertaken on behalf of IUPAC by the developers of the current database, Academic Software. This company has now signalled that it wishes to transfer the responsibility for management and maintenance of SCDB to IUPAC within about 3 years.

Division V has formed a consultative team (Folke Ingman, David Moore and Kip Powell) to work with Academic Software and the Executive to effect a successful transition to management by IUPAC or an alternative external systems manager. The Bureau meeting identified the future management of commercial databases as a generic issue that now needs to be addressed by IUPAC. It is possible that appropriate secretariat resources may need to be assigned in future.

(c) ***The Working Party on Quality Assurance*** continues to produce publications that are of value to chemists in analytical laboratories; e.g. *Revision of the IUPAC/ISO/AOAC protocol for proficiency testing; Harmonised guidelines for single-laboratory validation of methods of analysis; and Terminology for soil sampling*. The WPQA will make a major presentation at the GA on *"Metrological Traceability of Results in Chemical Measurement."*

(d) ***The Solubility and Solution Equilibrium Data sub-committee (SSED)*** has a very active program of projects that embrace the critical evaluation of solubility data related to (a) mobility of metals in the environment, (b) industrial processes, (c) human health. The outputs appear as papers in the Journal of Physical and Chemical Reference Data or as

book volumes and are thence transferred to the NIST-IUPAC Solubility Database: http://srdata.nist.gov/solubility/. A significant new project is a 25-Chapter book volume on "*Solubility for Industry*". Another project is concerned with *Chemical speciation of environmentally significant heavy metals with inorganic ligands.*

2.3. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement of the quality of life.

Chemistry-related industry is served by the active program of critical evaluations of solubility data and of solution equilibrium data, and by the continuance of data evaluation and compilation for the IUPAC Stability Constant Database. The current projects on pH (*Comparable pH measurements by metrological traceability.)* and metrological traceability *(Metrological Traceability of Results in Chemical Measurement*) are highly relevant to industry. The SSED were joint organisers of the 11th International Symposium on solubility phenomena (Aviero, 2004) at which there was significant emphasis on industrial issues and involvement of industrial chemists (*PAC*, 77(3), 2005).

2.4. IUPAC will foster communication among individual chemists and scientific organisations, with special emphasis on the needs of chemists in developing nations.

Analytical Chemistry in Developing countries
The Division seeks to expand activities in this area. "Emerging needs in developing countries" is one of its priority areas and is the responsibility of one Team. The Division is fortunate in having several members with established professional links with the African continent (Jan-Åke Jönsson, Walter Lund and Roger Smith). Nelson Torto (Botswana) has joined the ACD as a Provisional Member representing the IUPAC Associate Organisation, SEANAC. The Division is significantly involved in the project with IOCD: "*Standardisation of analytical approaches and analytical capacity building in Africa*".

To increase awareness of the needs of developing countries the Division has arranged a series of 8-10 articles for *Chemistry International.* These articles on *Emerging issues in developing countries* commenced in the March 2005 issue. Division V is well-supported by other Divisions in this venture.

Building bridges with other organisations.
The SSED works actively with NIST in the preparation of critical evaluations for publication in the NIST-IUPAC Solubility Data Series. The joint Division V - WPQA meeting in Vienna showed that many new dynamics can be brought to our activities by discussion and collaboration with other organizations, in this case IUPAP, IAEA, UNIDO.

Through the WPQA the Division is represented on the Coordinating Committee on Chemistry and Materials, ISO-Committee on Reference Materials, the International Committee on Weights and Measures, the Consultative Committee for Amount of Substance (BIPM), EURACHEM and CITAC.

Better Communication.
Dissemination of project outcomes is a crucial issue for improving the impact of our work in the chemistry community. This is overseen by the "Communications" team. The ACD website has been made more intuitive. Working with Dr. Meyers we are attempting to make it better attuned to the needs of those who are not familiar with the IUPAC system and processes. Improved lines of communication between TG chairs and the Division have been facilitated by the establishment of a 6-monthly Project reporting system in which the TGC responds to questions re progress, milestones, difficulties, and opportunities for further work, etc. These progress reports are now filed on the web on the respective project pages.

The Division has been pro-active in recommendations for improved IUPAC representation at conferences. It considers that there is scope for enhanced involvement of IUPAC representatives at IUPAC-sponsored conferences. This could be aided if conference organisers were required to discuss the nomination of an IUPAC representative with the relevant Division ahead of submitting the AIS. It is all too easy for Conference programs to be 'finalised' ahead of representative appointment, or without reference to IUPAC requirements.

2.5. IUPAC will utilise its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Division was represented in the Task Group for the project: *Chemistry's contributions to humanity.* It actively participates in the General Assembly Young Observers scheme. The question of career development for young chemists from developing countries was raised in one of the *CI* articles.

2.6. IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.

Division V has in place a strategy, which is communicated to the Nominations' Committee, to ensure the widest possible geographic representation. The Division actively sought participation of Nelson Torto as a Provisional Member representing the ANO, SEANAC. Within its own structures, the Division works to ensure **active** involvement of all AM, TM and NR.

III. Challenges and Solutions

The principal challenges to the ACD are typical of many IUPAC Divisions:

- The breadth of its portfolio.
- The generation of members' collective responsibility for
    - the goals of the Division
    - the needs of countries not represented
    - the long-range goals of IUPAC
- Maintaining momentum through the biennium and with the change of biennia.

Strategy adopted by the ACD to address these challenges:

- Identification of a manageable number of priorities for the biennium.
- Formation of Teams, each with collective responsibility for one priority area.
- Effort focused on the needs of developing countries and on links with other agencies.
- Use of mini-symposia to bring in external expertise.
- Maintaining active communication between members, e.g. through the newsletter, *Teamwork*.

IV. CURRENT PROJECTS

*Interdivisional projects

1999-044-2-500 - Terminology for the description of peak asymmetry in chromatography
1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands
2000-003-1-500 - Ionic strength corrections for stability constants
2000-004-2-500 - IUPAC stability constants database - completion of data collection up to 2000+
2001-041-2-500 - Recommendation on the use of countercurrent chromatography in analytical chemistry
2001-063-1-500 - Revision of terminology of separation science
2001-072-1-500 - Low activation materials for fusion technology: State and prospects
2002-002-2-500 - Recent advances in electroanalytical techniques: characterization, classification and terminology
2002-003-2-500 - Performance evaluation criteria for preparation and measurement of macro and microfabricated ion-selective electrodes
2002-009-2-500 - Optical spectrochemical analysis using waveguides and optical fibers; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
2002-058-1-500 - Definitions and fields of application of the terms robust and rugged and the characteristics or qualities of robustness and ruggedness in analytical chemistry

2003-015-2-500 - Terminology, quantities and units concerning production and applications of radionuclides in radiopharmaceutical and radioanalytical chemistry
2003-037-1-500 - Optical biosensors and bioprobes; Series on Nomenclature, Symbols, and Units in Spectrochemical Analysis
2003-056-2-500 - Standard definitions of terms relating to mass spectrometry*
2004-005-2-500 - Comparable pH measurements by metrological traceability*
2004-016-2-500 - Guidelines for potentiometric measurements in suspensions
2004-017-1-500 - Standardization of analytical approaches and analytical capacity-building in Africa*
2004-041-1-500 - Uncertainty estimation and figures of merit for multivariate calibration

INTERDIVISIONAL WORKING PARTY ON HARMONIZATION OF QUALITY ASSURANCE

2001-010-3-500 - Metrological traceability of measurement results in chemistry
2003-004-1-500 - Interdisciplinary harmonised approach to metrological traceability of chemical measurement results

SUBCOMMITTEE ON SOLUBILITY AND EQUILIBRIUM DATA

2001-052-1-500 **-** Solubility of volatile and gaseous fluorides in all solvents
2002-025-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Inorganic actinide compounds
2002-031-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Alkaline earth metal carbonates
2002-032-1-500 - Solubility data of compounds relevant to mobility of metals in the environment. Metal carbonates
2002-033-1-500 - Solubility data related to oceanic salt systems. Part I - Binary systems containing sodium, potassium, and ammonium sulfate
2002-034-1-500 - Solubility data related to oceanic salt systems. Part II - magnesium chloride-water and calcium chloride-water and their mixtures
2002-035-1-500 - Solubility data of compounds relevant to human health. Solubility of substances related to urolithiasis
2002-036-1-500 - Solubility data of compounds relevant to human health. Solubility of hydroxybenzoic acids and hydroxybenzoates
2002-037-1-500 - Solubility data of compounds relevant to human health. Solubility of haloganated aromatic hydrocarbons
2002-038-1-500 - Solubility data of compounds relevant to human health. Antibiotics: peptide antibiotics and macrocyclic lactone antibiotics
2002-042-1-500 - Solubility data related to industrial processes. Lead sulfate
2002-043-1-500 - Solubility data related to industrial processes. Carbon dioxide and the lower alkanes at pressures above 2 bar: methane to butane
2002-044-1-500 - Solubility data related to industrial processes. Carbon dioxide in aqueous non-electrolyte solutions
2002-045-1-500 - Solubility data related to industrial processes. Solids and liquids in supercritical carbon dioxide
2002-050-1-500 - Solubility data related to industrial processes. Acetonitrile: ternary and other multicomponent systems
2003-018-1-500 - Mutual solubility of hydrocarbons and water (update of SDS Vol 37 & 38)
2005-006-1-500: Mutual solubility of alcohols and water (update of SDS Vol 15)

OTHER INTERDIVISIONAL PROJECT

2003-011-3-600 - A critical compendium of pesticide physical chemistry data
2003-060-2-400 - Terminology on separation of macromolecules
2004-021-1-300 - Reference methods, standards and applications of photoluminescence
2004-023-1-700 - Internationally agreed terminology for observations in scientific communication

PROJECTS NEAR COMPLETION / IN PRESS

510/31/95 - Nomenclature for X-ray emission spectroscopy
550/64/97 - Non-selective sensors arrays ("Electronic Nose", "Electronic Tongue") chemical analysis: classification and characterization
2001-055-1-500 **-** Critical evaluation of stability constants of metal complexes of complexones for biomedical and environmental applications
2001-038-2-500 - Recommendations for NMR measurements of high pK values and equilibrium constants in strongly basic solutions
2001-009-1-500 - Revision in the international harmonised protocol for the proficiency testing of (chemical) analytical laboratories

PUBLISHED REPORTS (2004-2005)

523/2/89 - Determination of trace elements bound to soil and sediment fractions. *Pure Appl. Chem.* 76(2), 415-442, 2004
550/47/89 - Electrochemical detection in flowing media: Classification and recommendation. *Pure Appl. Chem.* 76(6), 1119-1138, 2004
510/35/97 - Guidelines for calibration in analytical chemistry. Part 2: multicomponent calibration. *Pure Appl. Chem.* 76(6), 1215-1225, 2004
550/62/97 - Electroanalysis with piezo-electric devices. *Pure Appl. Chem.* 76(6), 1139-1160, 2004
1999-050-1-500 - Chemical speciation of environmentally significant heavy metals and inorganic ligands. Part I Mercury. *Pure Appl. Chem.*, 77(4), 739-800, 2005. Chemical speciation of Hg(II) with environmental inorganic ligands. *Australian J.Chem.*,**57**, 1-8 (2004)
2000-033-1-500 - Assessment of uncertainty associated with soil sampling in agricultural, semi-natural, urban and contaminated environments (SOILSAMP). *Pure Appl. Chem.* 77(5), 827-841, 2005
2001-021-1-500 **-** Analytical electromigration techniques. *Pure Appl. Chem.* 76(2), 443-451, 2004.
2001-025-1-500 - Critical evaluation of the state of the art of the analysis of light elements in thin films. *Pure Appl. Chem.* 76(6), 1161-1213, 2004
2001-075-1-500 - Compilation of k0 and related data for NAA in the form of electronic database. *Pure Appl. Chem.* 76(10), 1921-1925, 2004
2001-085-1-500 - IA and IIA azoles, cyanates, cyanides and thiocyanates. *J. Phys. Chem. Ref. Data* 2004, **33**, No. 1, 1-176.

IUPAC REPRESENTATION AT CONFERENCES

Inaugural Conference for the Southern and Eastern Africa Network of Analytical Chemists (SEANAC), 7-10 July 2003, Gaborone, Botswana.

Colloquium Spectroscopicum Internationale 33rd Colloquium Spectroscopicum Internationale, 2003,7-12 September 2003, Granada, Spain.

Solubility Phenomena 11th International Symposium on Solubility Phenomena, Including Related Equilibrium Processes (11th ISSP), 25-29 July 2004, Aveiro, Portugal.

Trace Elements in Food, 2nd International Symposium on Trace Elements in Food (TEF 2),7-8 October 2004, Brussels, Belgium.

Analytical Forum 2004, July 2004, Warsaw, Poland.

8th International Conference on Nuclear Analytical Methods in the Life Sciences - NAMLS8. Rio de Janeiro, Brazil; April 2005

Analytical Chemistry and Chemical Analysis, (AC&CA-05). Kiev, Ukraine; September 2005.

International Union of Pure and Applied Chemistry

A member of the International Council of Scientific Unions

Division of Chemistry and the Environment (DCE - VI)

Report of Activities

January 2004 – June 2005

Kenneth D. Racke

1. HIGHLIGHTS

1.1 Terms of Reference

Through its internationally recognized membership and project teams, the Division of Chemistry and the Environment (DCE) will provide unbiased and timely authoritative reviews on the behavior of chemical compounds in food and the environment. The DCE will undertake both fundamental and applied evaluations that contribute to solving environmental problems and enhancing the quality of food on a global scale (revised May-2004).

1.2 Organization

The Division Committee is currently comprised of 10 TM's, 7 AM's, and 6 NR's. The 7th AM was a new position added during 2004 to accommodate a closer working relationship with IOCD. A new Division President assumed responsibilities during 2004. Several of the newly elected members for the 2004-2005 biennium are from outside the IUPAC family and have brought fresh perspectives. The work of the Division Committee is assisted by the efforts of several sub-committees, which help identify new priority project areas, stimulate proposals and recruit potential project leaders, and facilitate external communication encompassing the broad areas of environmental and food chemistry:

- Food Chemistry (Chair: Dr. Patrick Dysseler)
- Biophysico-Chemical Processes in Environmental Systems (Chair: Prof. Nicola Senesi)
- Chemistry of Environmental Compartments (Chair: Dr. Yehuda Senesi)
- Crop Protection Chemistry (Dr. Ken Racke)

Unfortunately Dr. Dysseler has been hospitalised with a serious illness for a significant portion of this reporting period.

1.3 Projects

Projects sponsored by the DCE generally fall into three broad categories. First, state-of-the-art **authoritative reviews** of a particular area of environmental chemistry are developed and published in book form. To this end, the Division has a long-standing working partnership with Wiley Press. Second, **technical evaluations** focus on critical assessment and development of specific recommendations for an area of environmental chemistry so as to assist and influence research and