

**Teamwork**  
- Issue No. 10 - July 2005 -

< [Issue No.9](#)

> [Issue No.11](#)

**This issue of 'Teamwork' includes:**

- o [General Assembly in Beijing: Workshop on "Future Opportunities and Challenges for the Analytical Chemistry Division"](#)
- o [New projects of the Analytical Chemistry Division](#)
  - . Comparable pH Measurements by Metrological Traceability, an interdivisional project, led by F. Camoes
  - . Guidelines for Potentiometric Measurements in Suspensions, led by S.F. Oman
  - . Uncertainty Estimation and Figures of Merit for Multivariate Calibration, led by A.C. Olivieri
- o [IUPAC Vice President on the ACD move to the project system](#)

**General Assembly in Beijing: Workshop on "Future Opportunities and Challenges for the Analytical Chemistry Division"**

During the GA in 2003 in Ottawa our Division initiated a series of workshops aimed at alerting the Division to issues that should be addressed and to stimulate the project development process. In Ottawa we held a meeting on *New Challenges for Analytical Chemists in Genomics, Proteomics, and Genetically Modified Organisms* and a year later, in Vienna, we held a meeting on *Emerging Issues in Metrological Traceability*.

The Beijing workshop will be held on a much broader canvas and with an "in house" format. Several members of the Division (or associated with the Division) are going to make forward-looking presentations on their specific field or area of responsibility within the Division. The objectives will be to:

- (i) identify important trends and new developments in the respective fields of analytical chemistry,
- (ii) identify any Division priorities for the future,
- (iii) stimulate forward and lateral thinking,
- (iv) clarify the philosophy of the ACD in relation to Project type and generation.

The Workshop may also seed discussions about specific project ideas and stimulate discussions on the formation of Task Groups and the scoping of projects, but probably these would be follow-on activities. The emphasis will be on "emerging issues". There is no wish to have an analysis of the maturity of a specific field.

The presentations (10 minutes each followed by a 10-min. discussion) are going to include:

- Emerging issues in separations science applied to analytical chemistry, *presented by Roger Smith, discussion led by Jan Åke Jönsson*

- Challenges for analytical atomic spectrometry", presented by Walter Lund, discussion led by Ryszard Lobinski

- Molecular spectroscopy - emerging opportunities for the analytical chemist, *presented by David Moore, discussion led by Ryszard Lobinski*

- Critical evaluations: future challenges and opportunities, *presented by Heinz Gamsjaeger, discussion led by David Shaw*
- Emerging issues in bioanalytical chemistry, *presented by Ryszard Lobinski, discussion led by Walter Lund*
- Metrology and quality assurance: challenges for the analytical chemist, *presented by Ales Fajgelj, discussion led by Brynn Hibbert*
- Emerging needs of developing countries, *presented by Nelson Torto, discussion led by Jan Åke Jönsson*
- Challenges for nuclear methods in radioanalytical (and radiopharmaceutical) chemistry, *presented by Mauro Bonardi, discussion led by Zhifang Chai*

The workshop will be held on **Saturday, August 13rd** the morning and is open to all GA delegates interested. We invite and encouraged members of other Divisions to participate. This is an excellent opportunity to think about new interdivisional projects!

> [Link to GA info](#)

## **New projects of the Analytical Chemistry Division**

### ***- Comparable pH Measurements by Metrological Traceability***

This is a joint project of our Division, Physical and Biophysical Chemistry Division (I), and Chemistry and the Environment Division (VI), with support of the Committee on Chemistry and Industry. The project is planned for three years and will be carried out in two parts pertaining to pH measurements in complex matrices:

- Part I: pH Measurements in water quality monitoring and assessment
- Part II: pH Measurements of clinical, biochemical, and environmental relevance

The project is considered as a follow-up of "The Measurement of pH. Definitions, Standards, and Procedures (IUPAC Recommendations 2002)," *Pure Appl. Chem.* **74**, 2169-2200 (2002) and responds to a number of issues raised during a workshop on the "Importance of Traceable pH Measurements in Science and Technology" held at PTB/Braunschweig, Germany, in September 2001. The workshop, which was organized and promoted by members of this project's task group, attracted a wide range of participants and revealed priorities and strong interest from the concerned community for continuing action. They were:

- implementation of traceability chains for pH values in routine measurements in order to achieve target uncertainties for specific applications
- development of educational and quality control tools for reference and testing laboratories under the observation of chemical and metrological principles
- improvement of the comparability and the assessment of pH values

The task group, which consists of worldwide experts in the field, aims to impact the scientific community due to both the relevance of the subject and the multiple scientific aspects involved in pH measurement and assessment. For more information contact the Task Group Chairman Maria Filomena Camões: [fcamoes@fc.ul.pt](mailto:fcamoes@fc.ul.pt).

> link to [project 2004-005-2-500](#)

### **- Guidelines for Potentiometric Measurements in Suspensions**

This project aims to define and interpret the suspension effect on the basis of recent experiments. It will take into account the enormous amount of theoretical and experimental work accomplished in 75 years since the term was first introduced—a period in which no consensus was achieved. On the basis of the recommended definition and interpretation, the significance of potentiometric measurements in suspensions performed in different ways will be explained.

The suspension effect relates to the difference of the galvanic cell voltage measured with the electrodes (i) in the equilibrium solution of the suspension and (ii) in its sediment. It will be argued that the suspension effect should be regarded as the sum of two effects that occur when the electrodes are immersed in a suspension. These are (i) the transition of the indicator electrode from a reversible potential to an irreversible mixed potential, and (ii) a systematic error of measurement caused by the outflow of the solution from the reference electrode salt bridge into the suspension.

Due to the irreversible mixed potential of the indicator electrode, which cannot be eliminated in suspension measurements, no thermodynamically exact data can be obtained. Guidelines will be presented for potentiometric methods applied to suspensions and the significance of these measurements will be interpreted and illustrated.

For more information and comments, contact the Task Group Chairman Srečko F. Oman: [irena.lipar@uni-lj.si](mailto:irena.lipar@uni-lj.si).

> link to [project 2004-016-2-500](#)

### **- Uncertainty Estimation and Figures of Merit for Multivariate Calibration**

With the ever-increasing sophistication of analytical instruments, multivariate calibration methods are continually evolving, each with its own underlying assumptions and statistical properties. The main purpose of these methods is to produce valid predictions from highly unselective data (e.g., the quantification from near-infrared spectra). A wide variety of multivariate methods have been developed, broadly classified in terms of the tensorial order of the instrumental data. Important conceptual differences exist between first-order methods employing vector data, and second-order methods using matrix data, particularly since the latter make possible the quantification in the presence of unknown interferences. This is also reflected in the approaches followed for the estimation of figures of merit.

While univariate calibration leads to relatively simple models, and the associated uncertainty estimation and figures of merit are thoroughly covered in several official documents, multivariate calibration does not enjoy a similar status in this regard. Uncertainty estimation and figures of merit for multivariate calibration methods have become subjects of active research, especially in the field of chemometrics.

This work is intended as an introduction to multivariate calibration from a chemometrics perspective and as a review of the various proposals to generalizing the well-established univariate methodology to the multivariate domain.

Uncertainty and figures of merit are subjects of interest to IUPAC's Analytical Chemistry Division, as established within the general aims of the Division, and also in the terms of reference of its Interdivisional Working Party on Harmonization of Quality Assurance.

For more information and comments contact the Task Group Chairman Alejandro C. Olivieri: [aolivier@fbioyf.unr.edu.ar](mailto:aolivier@fbioyf.unr.edu.ar).

> link to [project 2004-041-1-500](#)

## IUPAC Vice President on the ACD move to the project system

Prof. Bryan R. Henry, IUPAC Vice-President has recently published a [Critical Assessment report](#) on the efficiency of handling the move to the project system. Here are the excerpts concerning our Division:

*Analytical Chemistry Division (V): The Analytical Chemistry Division has handled the move to the project system very efficiently. The Division Committee takes on the responsibility for generating projects, and the Division President serves as the project coordinator. In generating projects, they use young observers, both as a source of projects, and in an attempt to introduce new blood. They also use conferences and the corresponding IUPAC representatives in generating projects. They hold workshops at their Division meeting and at the General Assembly, and one goal of such workshops is project generation.*

*They have procedures for active guidance in bringing a project to a stage where it can compete for funding. This nurturing process clearly benefits the quality of the resultant projects. An [example proposal is posted online](#), and they make extensive use of [Chemistry International](#) (CI) to advertise existing projects. In fact, communication within this Division is very good. They publish a [Divisional newsletter](#). A project reporting form is required every six months. This monitoring system works very well. The officers carry out an in-depth review of all projects at their officers meeting, which precedes the Divisional meeting. Projects are also reviewed at the Divisional meeting. For most projects, one Task Group meeting is adequate. Under the project system, the average duration to carry out a given scientific investigation has decreased. They find [ICTNS](#) to be very helpful, particularly with regard to Gold Book entries. They believe that interdivisional cooperation is working well. An important issue for the Division is that IUPAC maintains access to the computer capability to maintain their project-generated databases such as the [Stability Constants Database](#). The Division believes that the project system is more flexible, and they have no desire to return to commissions.*

Full text can be found at [www.iupac.org/news/archives/2005/vpca\\_henry.html](http://www.iupac.org/news/archives/2005/vpca_henry.html)

[Ryszard Lobinski](#)  
[ryszard.lobinski@univ-pau.fr](mailto:ryszard.lobinski@univ-pau.fr)