



I U P A C

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY



CITAC
Cooperation on International
Traceability in Analytical Chemistry

IUPAC/CITAC Web-seminar “Metrology, Quality and Chemometrics - Correlation of Test Results and Mass Balance Influence on Conformity Assessment”

21 Jan 2021, from 14:00 to 16:00 UTC (Coordinated Universal Time)

Agenda:

Introduction

14:00-14:10 Dr. Zoltan Mester, NRC, Canada. *Opening remarks and welcoming of the IUPAC ACD President and CITAC Vice-Chair.*

14:10-14:15 Dr. Bernd Güttler, PTB, Germany. *CITAC update – Foreword by CITAC Chair.*

14:15-14:20 Dr. Michela Segal, INRIM, Italy. *CITAC as a stakeholder of the IUPAC project – Welcoming of CITAC Past Chair and the Web-seminar Moderator.*

Presentations of 20 min and 5 min discussion

(abstracts of the presentations and brief BIOs of the lecturers are attached below)

14:20-14:45 Dr. Ilya Kuselman, Independent Consultant on Metrology, Israel. *IUPAC/CITAC Guide “Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty” and correlation of test results.*

14:45-15:10 Dr. Francesca R. Pennechi, INRIM, Italy. *Influence of a mass balance constraint on risks in conformity assessment of substances and materials.*

15:10-15:35 Em. Prof. D. Brynn Hibbert, School of Chemistry, UNSW Sydney, Australia. *Metrology and the law: presenting chemical measurements to the courts.*

15:35-16:00 Dr. Angelique Botha, NMISA, South Africa. *Development of guidance for the production of high purity reference materials.*

The zoom meeting link:

<https://zoom.us/j/94875510660?pwd=VVRBMGhQRTlkVFduVHcwZUdFR0I5dz09>

Meeting ID: [948 7551 0660](https://zoom.us/j/94875510660)

Passcode: 069790

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The lectures will be recorded and published on YouTube. Links to them will be available on IUPAC webpage <https://iupac.org/event/metrology-quality-and-chemometrics/> and CITAC website www.citac.cc (Conferences & Workshops).

We invite you to participate in the event and ask to share this information with your list of contacts and social networks.

Dr. Ilya Kuselman

Webinar Chair

IUPAC/CITAC Guide “Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty” and correlation of test results

Ilya Kuselman

Independent Consultant on Metrology, Israel, ilya.kuselman@gmail.com

The Guide was developed by the IUPAC project task group consisted of Francesca R. Pennechi, INRIM, Italy; Ricardo J.N.B. da Silva, University of Lisbon, Portugal; and D. Brynn Hibbert, UNSW Sydney, Australia; chaired by me (<https://iupac.org/projects/>). The work was supported by CITAC. In this Guide, risks of a false decision on conformity of the chemical composition of a multicomponent material or object due to measurement uncertainty are defined using the Bayesian approach. Even if the conformity assessment for each particular component of a material is successful, the total probability of a false decision (total consumer's risk or producer's risk) concerning the material as a whole might still be significant. This is related to the specific batch, lot, sample, environmental compartment, or other item of material or object (specific consumer's and producer's risks), or to a population of these items (global consumer's and producer's risks). When the actual values of the components' concentrations or contents, as well as the measured values, are correlated, they are modelled by multivariate distributions. The effect of correlation on the risks is not easily predictable. Examples of the evaluation of risks are provided in the Guide for conformity assessment of denatured alcohols, total suspended particulate matter in ambient air, a cold/flu medication, and a PtRh alloy.



Dr. Ilya Kuselman, <https://orcid.org/0000-0002-5813-9051>, has been a researcher and then Head of Metrology in Chemistry Division of All-Union R&D Institute of Non-ferrous Secondary Metals, Donetsk, Ukraine, former USSR, since 1971 to 1990. In 1991 to 2014 he was a co-worker and further Director of the National Physical Laboratory of Israel. Now Ilya is Independent Consultant on Metrology. Ilya is a member of CITAC, ISO/REMCO and IUPAC Analytical Chemistry Division, Editor of CITAC News and Chair of the IUPAC Subcommittee on Metrology in Chemistry.

Influence of a mass balance constraint on risks in conformity assessment of substances and materials

Francesca Pennechi

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The IUPAC/CITAC Guide “Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty” offers a general Bayesian approach for evaluating the risks of false decisions in conformity assessment of multicomponent materials or objects. When components of such substances are linked by a mass balance constraint (i.e., the sum of their mass fractions, molar fractions or any other positive quantity ratios is 100 % or 1), test results of the components’ contents are named “compositional data”. These data are always correlated, because of the constraint. Such correlations, being named “spurious”, may influence measurement uncertainty of test results as well as risks of false decisions in conformity assessment of a substance or material. That is important in testing geological and environmental objects, products of metallurgical and food industries, etc. A special case is the evaluation of purity of substances by an indirect method based on a mass balance, and development of corresponding (pure) certified reference materials. IUPAC project 2019-012-1-500 is under development now with the aim of studying how to deal with mass balance constraint in conformity assessment. A Bayesian multivariate approach is applied to different scenarios of the data modelling, based on a Monte Carlo method that includes the mass balance constraint.



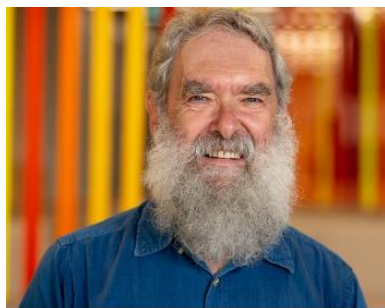
Dr. Francesca Pennechi, <https://orcid.org/0000-0003-1328-3858>, holds a European PhD in “Metrology”. She is a senior researcher at the INRIM Division of Applied Metrology and Engineering. Francesca is Chair of the UNI/CT 016/GL 69 and Co-chair of the ENBIS Special Interest Group on Measurement Uncertainty. She is a member of ISO/TC 69/SC 6/WG 7, CITAC, Eurachem/CITAC Measurement Uncertainty and Traceability Working Group, IUPAC Subcommittee on Metrology in Chemistry and Steering Committee of the European Metrology Network for Mathematics and Statistics.

Metrology and the law: presenting chemical measurements to the courts

D. Brynn Hibbert

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In Australia, an expert is bound to help the court no matter who is paying. Expert conferences are encouraged so that complex science can be presented to allow the ‘trier of fact’ to make a properly informed decision. In particular, for example, the issue is often one of conformity assessment – is the driver over the legal limit for alcohol? Three examples from the author’s case book will show how reliable measurements have been crucial to providing justice. First, a racing horse is not allowed to have more than 100 ng/mL of cobalt in its urine. In a landmark case the court accepted a statistical distribution of cobalt mass concentrations that allowed calculation of the probability of an ‘ordinary horse’ having a mass concentration greater than the legal threshold. Second, illegal ‘meth labs’ are found in most countries. While the identity of the product (‘ice’ or N-methylamphetamine hydrochloride) is often not in dispute, the amount of drug synthesised determines the length of the custodial sentence. Measurement of purities, and thus mass of drug, requires proof that the sample analysed was representative of the item seized. Estimation of potential yields from seized precursors also has a bearing on indictable amounts. Finally, in a recent cold-case murder, the author successfully argued against the admissibility of lead isotope analysis results that matched bullets in a body to bullets in a box of bullets in the possession of one of the accused. Was the method properly validated? And does the chemical match actually prove the body bullets came from the box?



Brynn Hibbert, <https://orcid.org/0000-0001-9210-2941>, is an Emeritus, Professor of Analytical Chemistry at UNSW Sydney. He is a go-to expert witness in the courts on matters chemical, particularly on drugs of abuse (in society and sports), although he has been known to do the occasional murder. As a past president of the Analytical Division of IUPAC he is the editor of a new edition of the Orange Book and is involved in the revision of the on-line Gold Book.

Development of guidance for the production of high purity reference materials

Angelique Botha

National Metrology Institute of South Africa (NMISA), South Africa, abotha@nmisa.org

The ISO Committee for Reference Materials (ISO/REMCO) has actively been updating its guidance documents over the past eight years. Since the conversion of the third edition of ISO Guide 34 to the international standard ISO 17034 to address the conformity assessment of reference material producers, the work of the committee has focused on the revision of ISO Guide 35 and the development of up-to-date guidance for the users of reference materials.

In 2014, a guidance document, ISO Guide 80, for the in-house preparation of quality control materials was published by the committee. The third edition of ISO Guide 33 ‘Reference materials – Good practice in using reference materials’ was published early in 2015. While the previous edition focused on the use of certified reference materials, the new one relates to all types of reference materials and their uses.

The prospects for the future work of the committee include the development of more field specific guidance. At the beginning of 2018 a proposal was approved for the development of a guidance document for the production of qualitative reference materials (ISO Guide 85). Two new proposals (ISO Guide 86 and ISO Guide 87) were also approved for the development of harmonized guidance for the preparation of high purity reference materials for small organic molecules as well as metals and metalloids, respectively.



Dr. Angelique Botha, <https://orcid.org/0000-0003-3987-359X>, is Chief Metrologist in inorganic analysis at NMISA. Her research activities focus on the production of matrix reference materials for trace elements in food and environmental samples. She is currently Chair of ISO/REMCO. Angelique is also active in several working groups of the Consultative Committee for Amount of Substance: Metrology in Chemistry and Biology (CCQM) of the International Committee for Weights and Measures (CIPM), as well as in CITAC.