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Teaching

Metrology and Examinology in Chemistry at the University

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ME|Chem: <http://mechem.rd.ciencias.ulisboa.pt>

Outline

1. Missions of universities
2. Terminology
3. Teaching at the Faculty of Sciences of the University of Lisbon (FCUL)
4. Teaching at the Summer School in Measurement Science in Chemistry (MSC)
5. Teaching at the Erasmus Mundus Master in Quality in Analytical Laboratories (EMQAL)
6. Final remarks

1. Missions of universities

Mission of the

Faculty of Sciences of the University of Lisbon:

To expand the limits of science and technology, transfer scientific knowledge into society, and promote research-based student education [1].

Motto:

What we do not know today, we will know tomorrow (Garcia de Orta, 1563).



1. <https://ciencias.ulisboa.pt>

1. Missions of universities

The main goal of universities [2]:

1. Carrying out scientific research studies;
 2. Producing solutions to the problems of humanity and a country;
 3. Training the human force which a country needs;
- (...)

1. Missions of universities

Some pillars of a modern society:



1. Missions of universities

Some pillars of a modern society:



2. Terminology

Metrology [1]:

2.2 (2.2)

metrology

science of **measurement** and its application

NOTE Metrology includes all theoretical and practical aspects of measurement, whatever the **measurement uncertainty** and field of application.

2. Terminology

Metrology [1]:

2.2 (2.2) metrology

science of me

NOTE Metrology
aspects of me
uncertainty and

5.13 (6.13) reference material RM

material, sufficiently homogeneous and stable with reference to specified properties, which has been established to be fit for its intended use in **measurement** or in examination of **nominal properties**

NOTE 1 Examination of a nominal property provides a nominal property value and associated uncertainty. This uncertainty is not a **measurement uncertainty**.

2. Terminology

Metrology [1]:

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material, sufficiently homogeneous and stable with reference to specified properties, which has been established to be fit for its intended use in **measurement** or in examination of **nominal properties**

NOTE 1 Examination of a nominal property provides a nominal property value and associated uncertainty. This uncertainty is not a **measurement uncertainty**.

2. Terminology

Examimology:

Science of examination and its application.

2.6 examination

process of experimentally obtaining one or more *nominal property values* (3.1) that can reasonably be attributed to a *nominal property* (2.1)

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1. JCGM, *International Vocabulary of Metrology - Basic and General Concepts and Associated Terms (VIM 3rd edition)*, JCGM 200, 2012.
 2. G. Nordin, R. Dybkaer, U. Forsum, X. Fuentes-Arderiu, F. Pontet, *Vocabulary on nominal property, examination, and related concepts for clinical laboratory sciences (IFCC-IUPAC Recomm. 2017)*, Pure Appl. Chem. 90 (2018) 913-935.

3. Teaching at FCUL - Univ. of Lisbon

Bachelor in Chemistry:

Course: Metrology in Chemistry

Optional: 3rd year (2nd semester):

ECTS: 3

Contact Lessons: 35 h (2.5 h/week);

Autonomous Work: 49 h.



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3. Teaching at FCUL - Univ. of Lisbon

Bachelor in Chemistry:

Course: *Metrology in Chemistry*

Topics:

International System of Units

Metrological infrastructure

Metrological traceability

Evaluation of the measurement uncertainty

- Bottom-up approach (principles and simple cases)
- Top-down approach based on interlaboratory data
- Top-down approach based on intralaboratory data



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3. Teaching at FCUL - Univ. of Lisbon

Bachelor in Chemistry:

Course: Metrology in Chemistry

Assessment:

20 % - Group work: Describe the socio-economic relevance and the regulation of a specific sector

80 % - Individual examination:

Part I (1.5 h): Examination without auxiliary material

Part II (1.5 h): Examination WITH auxiliary material:
Problem solving using a MS-Excel file.

2018/2019: 21 students (scores (Max. 20): 18 to 6; 2 failed)



3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Quality in Chemical Analysis

Optional: 1st year (1st semester):

ECTS: 6

Contact Lessons: 49 h (3.5 h/week);

Autonomous Work: 119 h.



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3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Quality in Chemical Analysis

Topics:

International System of Units

Metrological infrastructure

Measurement procedure validation

Internal and external quality control

Evaluation of the measurement uncertainty

- Bottom-up approach
- Top-down approach based on interlaboratory data
- Top-down approach based on intralaboratory data



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3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Quality in Chemical Analysis

Assessment:

20 % - Group work: Describe the socio-economic relevance and the regulation of specific sector including measurement requirements

80 % - Individual examination:

Part I (1.5 h): Examination without auxiliary material

Part II (1.5 h): Examination WITH auxiliary material:
Problem solving using a MS-Excel file.

2019/2020: 25 students (scores: 19 to 2; 3 failed)



3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Metrology and Examinology in Chemistry

Optional: 1st year (2nd semester):

ECTS: 6

Contact Lessons: 49 h (3.5 h/week);

Autonomous Work: 119 h.



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3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Metrology and Examinology in Chemistry

Topics:

Theory - Metrology:

- Numerical uncertainty combination: Kragten and MCM;
- Bayesian uncertainty evaluation: MCMC;
- Using uncertainty in conformity assessment;

Theory - Examinology:

- Evaluation of the uncertainty of an examination;

Practice - Evaluation of the MU of a specific test:

- Evaluation planning, experimental work, data processing and preparation for publication.



3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Metrology and Examinology in Chemistry

Assessment:

100 % - Performance during the practicals and uncertainty evaluation report.

2017/2018: 2 students - Tutorial mode
(scores: 19)

Publication:

D. Ferreira, M. Barros, C. Oliveira, R. Bettencourt da Silva, *Quantification of the uncertainty of the visual detection of the end-point of a titration: determination of total hardness in water*, Microchemical Journal 146 (2019) 856-863



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3. Teaching at FCUL - Univ. of Lisbon



Publication:

D. Ferreira, et al. *Quantification of the uncertainty of the visual detection of the end-point of a titration: determination of total hardness in water*, *Microchem. J.* 146 (2019) 856-863.

- Bottom-up evaluation of the uncertainty of a titration.
- End-point detection uncertainty quantified by difference (...).
- Three uncertainty combination methods were compared.

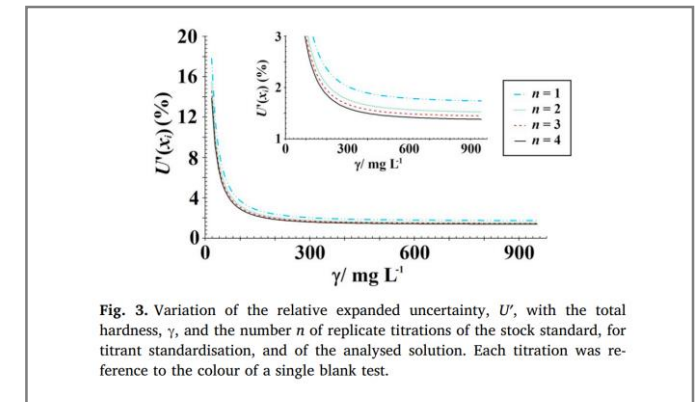
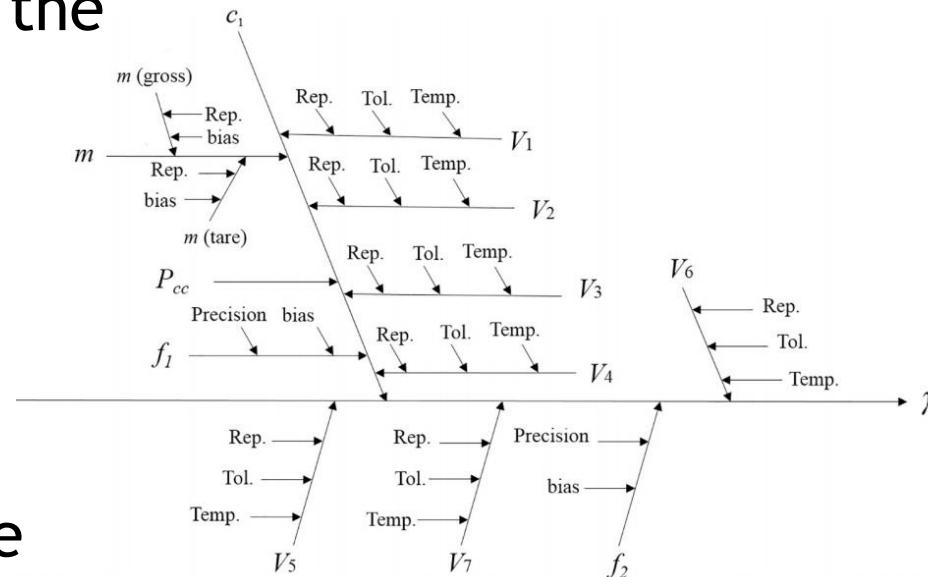


Fig. 3. Variation of the relative expanded uncertainty, U' , with the total hardness, γ , and the number n of replicate titrations of the stock standard, for titrant standardisation, and of the analysed solution. Each titration was reference to the colour of a single blank test.

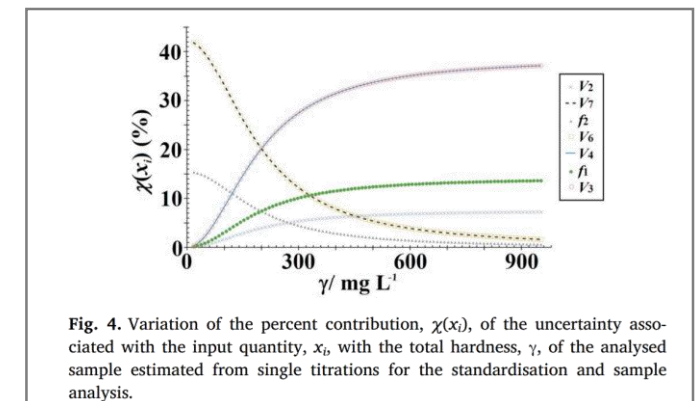


Fig. 4. Variation of the percent contribution, $\chi(x_i)$, of the uncertainty associated with the input quantity, x_i , with the total hardness, γ , of the analysed sample estimated from single titrations for the standardisation and sample analysis.

3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Forensic Chemical Analysis
(Examinology in chemistry: 21 %)

Optional: 1st year (2nd semester):

ECTS: 21% of 6

Contact Lessons: 10.5 h;

Autonomous Work: 25.5 h.



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3. Teaching at FCUL - Univ. of Lisbon

Master in Chemistry:

Course: Forensic Chemical Analysis
(Examinology in chemistry: 21 %)

Topics:

Evaluation of the uncertainty of an examination;

Evaluation of the uncertainty of compound identification by
GC-MS:

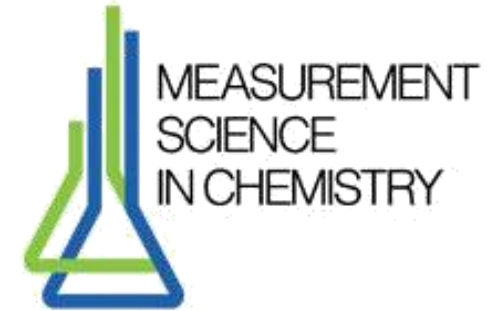
- Identification procedure validation;
- Identification quality control;
- Identification uncertainty evaluation.



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4. Teaching at MSC | Summer School

International Summer School on Analytical Science,
Metrology and Accreditation
(<http://www.msc-euromaster.eu>)



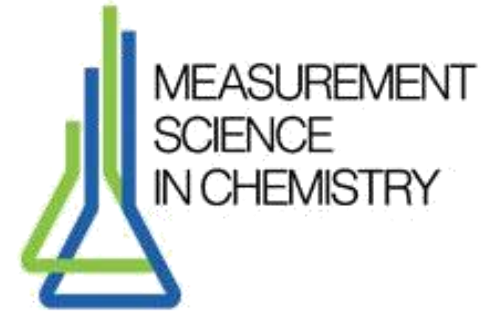
Past editions (two weeks duration):

2008 Slovenia; 2009 Bulgaria; 2010 Estonia; 2011 Poland;
2012 Portugal; 2013 France; 2014 Morocco; 2015 Poland;
2016 Belgium; 2017 Lithuania; 2018 Estonia; 2019 France;
2020 Online (on-going)



4. Teaching at MSC | Summer School

International Summer School on Analytical Science,
Metrology and Accreditation
(<http://www.msc-euromaster.eu>)



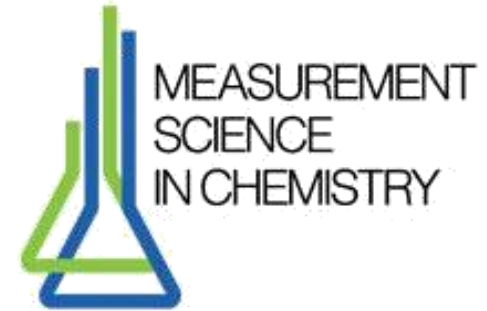
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4. Teaching at MSC | Summer School

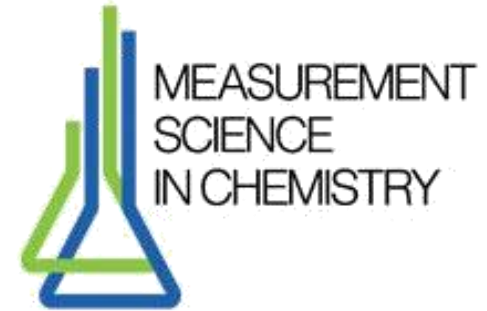
International Summer School on Analytical Science,
Metrology and Accreditation
(<http://www.msc-euromaster.eu>)



Content: Covers broad range of topics related to quality assurance, ISO/IEC-17025, metrology and accreditation: Traceability, uncertainty, compliance assessment, validation, use of CRMs, internal and external quality assurance, interlaboratory comparisons and auditing.

4. Teaching at MSC | Summer School

International Summer School on Analytical Science,
Metrology and Accreditation
(<http://www.msc-euromaster.eu>)

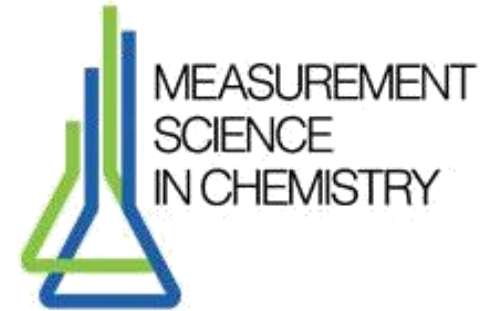


Teaching methodology:

- Classical lectures;
- Individual and group assignments: Analytical game;
- Assessment: Analytical game & Individual examination.

4. Teaching at MSC | Summer School

International Summer School on Analytical Science,
Metrology and Accreditation
(<http://www.msc-euromaster.eu>)



13th edition 2020:

On-going in on-line format:

Number students: 35 students from four continents

Analytical game (13th edition): Synthetic data distributed instead of asking students to produce their own data (...)

5. Teaching at Erasmus Mundus EMQAL

Erasmus Mundus Master in Quality in
Analytical Laboratories
(<http://www.emqal.org/>)



Partner institutions:

- University of Algarve (Portugal)  **UAlg**
UNIVERSIDADE DO ALGARVE
- University of Barcelona (Spain)  **UNIVERSITAT DE BARCELONA**
- University of Bergen (Norway)  **UNIVERSITY OF BERGEN**
- University of Cadiz (Spain)  **UCA** | **Universidad de Cádiz**
- Gdansk University of Technology (Poland)  **GDANSK UNIVERSITY OF TECHNOLOGY**

5. Teaching at Erasmus Mundus EMQAL

Erasmus Mundus Master in Quality in
Analytical Laboratories
(<http://www.emqal.org/>)

Past editions:
2009 - 2019

The next edition is postponed until January 2021



5. Teaching at Erasmus Mundus EMQAL

Erasmus Mundus Master in Quality in
Analytical Laboratories
(<http://www.emqal.org/>)

EMQAL is a high-level integrated international study programme of 120 ECTS leading to a Joint Master's Degree.

EMQAL is specialize in:

- Quality management
- Analytical methods
- Data analysis



5. Teaching at Erasmus Mundus EMQAL

Erasmus Mundus Master in Quality in
Analytical Laboratories
(<http://www.emqal.org/>)



Structure:

One year of classes

One year of research project (Research Master Thesis)

Study in at least two European universities

All classes are taught in English by experts from around the world

6. Final remarks

- Competencies in Metrology and Examinology in chemistry (ME|Chem) have high employability
- Students easily understand the relevance of these topics
- Most students enjoy the development and implementation of algorithms in excel
- Some students continue their studies in ME|Chem
- We need analysts with this expertise



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