

Measurement Science in Chemistry Education at University of Tartu



<http://www.ut.ee/ams>
<http://sisu.ut.ee/measurement>

Contents

- **Applied Measurement Science**
international master's programme
- **Measurement Science in Chemistry**
international consortium
- **Estimation of measurement uncertainty
in chemical analysis** web course

Outline

- Interdisciplinary 3+2 master's degree program
 - Chemical analyses
 - Physical measurements
 - Metrology
 - Quality systems
 - Economic and legal aspects of measurements
- 120 ECTS, 2 years
- Cross-sectorial
- International: **Tuition in english**

This combination of topics is unique in Europe!

Knowledge and skills

- Measurement and analysis methods
 - Physical and chemical basis
 - Hands-on work
- Factors affecting the results
- Calculation methods
- Knowledge necessary for assessment of quality of results
- Economic and legal aspects, quality systems

Program structure

AMS

Obligatory Module (45 ECTS)

Courses: Measuring and Instrumentation, Measurement Data Processing, Lab of Physical Measurements, Practical Chemical Analysis Methods, Lab of Chemical Analysis Methods, Fundamentals of Metrology, Metrology in Chemistry, Seminar in Measurement Science, Quality Systems

Elective Module (30 ECTS, courses can be chosen from the list)

Possible courses: Materials Characterization and Testing, Structural Analysis, Measurements in Biochemistry, Measurements and the Law, Economic Aspects of Measurements, Signal Processing, Chemometrics, Environment and Measurement, Electrochemical Measurement and Analysis Methods, Nanometrology, etc

Optional Subjects

(6 ECTS, any courses can be chosen university-wide)

Practical Placement

(9 ECTS, internship placement in industry or analysis or calibration laboratories)

Master's thesis

(30 ECTS, reasearch project with a topic related to measurement science)

See www.ut.ee/ams

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Hands-on work (1)

Physical measurements

- temperature
- electrical quantities
- working environment parameters: air humidity, air flow velocity, illumination
- dimensional quantities
- light diffraction and refraction
- surface characterization (STM, AFM)



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Hands-on work (2)

Chemical measurements

- GC, GC-MS, LC-UV, LC-MS
- UV-Vis, IR, AAS and AES spectroscopy
- coulometry, voltammetry, potentiometry
- sample preparation



Hands-on work (3)

Software and data treatment

- Spreadsheet systems, MathCAD, GUM Workbench
- Basic statistics, Regression analysis, ANOVA
- Calculation of measurement results, quantification methods
- Estimation of uncertainty (ISO GUM, Nordtest)
- Calculations in validation





Practice-oriented

- Possibility to work in an accredited lab environment
 - UT Testing centre has laboratories accredited according to ISO 17025
 - Part of the Estonian NMI
- **Practical placement** in industry or field laboratory



Who can apply?

- **graduates** with Bachelor's or diploma degrees in physics, chemistry, materials science and related fields
 - no problem if studies are still in progress at the time of application
- **practitioners**
 - from analysis and measurement laboratories, industry, etc
 - personnel of accreditation, certification and inspection agencies, etc

Tuition fee, scholarships, stipends

- **Scholarships covering the tuition fee for almost all students**
 - Regular tuition fee 4430 EUR/year
- **DoRa stipends** for the best students
 - Up to 2880 EUR/year
- **Research Stipends** for hard-working students
 - Up to 2550 EUR/year
 - From research groups, normally from 2nd semester

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How many students are the "best students"?

- Example:
- There are currently 12 students studying
 - **All 12 students** have the tuition fee covered by the scholarship
 - **6 students** get some kind of stipend

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Application deadline

- **In first half of April 2014**
 - By that time just application and current study record are necessary
 - other documents can come later
 - submitting documents does not mean obligation to come!
- All necessary information:
<http://www.ut.ee/ams>

Measurement Science in Chemistry

www.msc-euromaster.eu



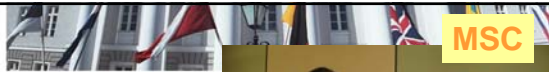
- International consortium
- 8 countries
 - Estonia, Slovenia, Bulgaria, France, Portugal, Poland, Finland, Belgium
- 10 universities





Summer school content

- Validation of chemical analysis procedures
- Basic statistics, Statistical basis of calibration
- Traceability in chemical analysis
- Alternative Approaches for the Quantification of Measurement Uncertainty
- ISO 17025, Accreditation visit to real lab
- Sampling and sample preparation in food and environmental analysis
- Customer-analyst interactions
- Importance of reliable measurements to implement EU legislation



Summer schools

- Summer **2009 Blagoevgrad** (Bulgaria)
 - 43 participants, 9 countries
- Summer **2010 Lepanina** (Estonia)
 - 39 participants, 9 countries
- Summer **2011 Poznań** (Poland)
 - 43 participants, 13 countries
- Summer **2012 Fatima** (Portugal)
 - 48 participants
- Summer **2013 Lyon** (France)
 - 34 participants





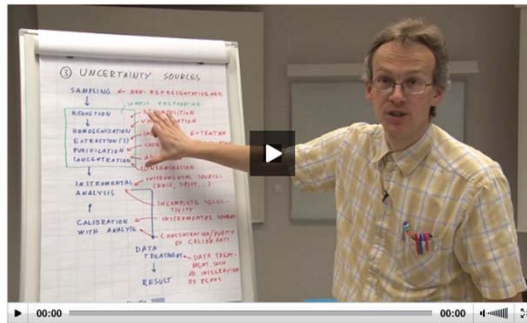
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5.3. SOURCES OF UNCERTAINTY

Course introduction

- 1. The concept of measurement uncertainty (MU)
- 2. The origin of measurement uncertainty
- 3. The basic concepts and tools
- 4. The first uncertainty quantification
- 5. Principles of measurement uncertainty estimation
 - 5.1. Measurand definition
 - 5.2. Measurement procedure
 - 5.3. Sources of uncertainty
 - Self-test 5.3
 - 5.4. Treatment of random and systematic effects
 - Self-test 5.4
- 6. Random and systematic effects revisited
- 7. Precision, trueness, accuracy
- 8. Overview of measurement uncertainty estimation approaches
- 9. The ISO GUM Modeling approach
- 10. The single-lab validation approach
- 11. Comparison of the approaches

Brief summary: The overview of possible uncertainty sources, relevant to pesticide analysis, is presented. Most of the uncertainty sources are linked to specific steps in the analysis procedure. It is stressed that sample preparation is usually the biggest contributor to measurement uncertainty. When performing chemical analysis then every care should be taken to minimize (preferably eliminate) the influence of the uncertainty sources, as far as possible. And what cannot be eliminated, has to be taken into account. It is not necessary to quantify every uncertainty source individually. Instead, it is often more practical to quantify several uncertainty sources jointly.



Measurement uncertainty sources
<http://www.uttv.ee/naita?id=17587>

<http://sisu.ut.ee/measurement/>

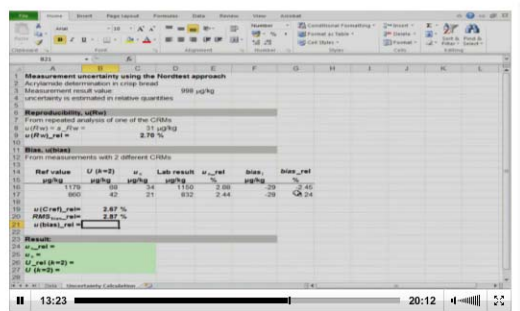


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10.5. NORDTEST APPROACH IN PRACTICE: DETERMINATION OF ACRYLAMIDE IN SNACKS BY LC-MS

Course introduction

- 1. The concept of measurement uncertainty (MU)
- 2. The origin of measurement uncertainty
- 3. The basic concepts and tools
- 4. The first uncertainty quantification
- 5. Principles of measurement uncertainty estimation
- 6. Random and systematic effects revisited
- 7. Precision, trueness, accuracy
- 8. Overview of measurement uncertainty estimation approaches
- 9. The ISO GUM Modeling approach
- 10. The single-lab validation approach
 - 10.1. Principles
 - 10.2. Uncertainty component accounting for random effects
 - Self-test 10.2
 - 10.3. Uncertainty component accounting for systematic effects
 - Self-test 10.3



Nordtest approach in practice: Determination of acrylamide in snacks by LC-MS
<http://www.uttv.ee/naita?id=18163>

Some comments on this example:

- 1. We use relative uncertainties in this example. The reason is that the concentration in these samples is quite high.
- 2. In this example we assume that the matrixes of the used CRMs – potato chips and crisp bread – are

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6. Random and systematic effects revisited
 7. Precision, trueness, accuracy
 8. Overview of measurement uncertainty estimation approaches
 9. The ISO GUM Modeling approach
 10. The single-lab validation approach
 11. Comparison of the approaches
 12. Comparing measurement results
 13. Tests and Exercises
 Please comment!

Question Results

1. Question: **Score 3 / 3**

Bioactive amines are determined by HPLC in brain dialysate. Calibration graphs are prepared daily using the same sample introduction system (cooled autosampler) as for the sample. Which of the following uncertainty causing effects are systematic **within a day**?

Response:

Uncertainty of pipetting when making the calibration solutions (different pipettes are used).

✓ **Feedback:**
 If different pipettes are used then in the long term their influence on calibration graph will be random.

Actual injection volume of the autosampler is by 5% higher than the analyst thinks.



Feedback:
 Both calibration solutions and sample solutions are injected with the same injector, therefore the actual volume of the injector does not influence the uncertainty.

The laboratory is not well air-conditioned - when the weather is cold then air temperature in the laboratory is quite low, when the weather is hot then the laboratory temperature is quite high.

✓ **Feedback:**
 In the time frame of one year the effects of some days being hot and some being cold will be random.

Baseline noise of the chromatogram.

Feedback:
 Baseline noise can never be a systematic effect.

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How can it be used?

- As a **course** for individual learning
- As a **course** taken as „virtual“ guest student at UT
 - Will be launched in spring 2014
- As a **guidance material**
- As a **collection of tests** to test your competence in MU

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Thank you for your attention!

- The Online Course of Measurement Uncertainty Estimation in Analytical Chemistry is available from:

sisu.ut.ee/measurement/

- You are always welcome to contact me:

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