UNDERESTIMATING UNCERTAINTY

Bertil Magnusson, Cyprus, May 2017

Eurachem Workshop - *Uncertainty in Qualitative and Quantitative Analyses*

Research Institutes of Sweden
Bioscience and Material Chemistry

Measure is a Treasure

- Knowledge about the sample/object
- Experience of measurements
- Statistical knowhow
- Experienceof the method

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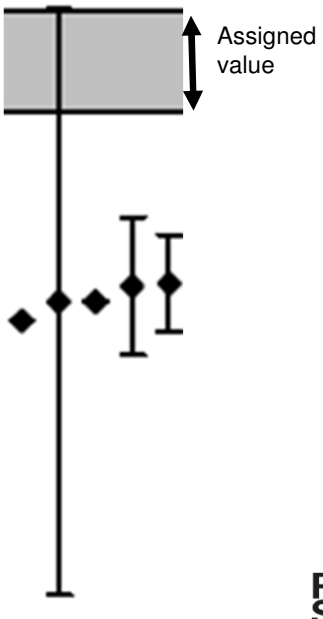
Underestimating uncertainty* – old example

Profiency testing – Pb in plastics (IMEP13) – year 2000
74 labs in total

Here five labs
2 result with no uncertainty
3 result with uncertainty
2 underestimated uncertainty

In total
24 results with no uncertainty
50 results with uncertainy
30 underestimated uncertainty

*including mistakes…



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Measurement Uncertainty (MU) estimation

According to the GUM* issued 1993

Although this Guide provides a framework for assessing uncertainty, it cannot substitute for critical thinking, intellectual honesty and professional skill.

The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement.

The quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value.

*Guide To The Expression Of Uncertainty In Measurement. ISO, Geneva (1993). Reissued as ISO Guide 98-3 (2008), available at www.bipm.org as JCGM 100:2008.

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Measurement Uncertainty (MU) estimation

We need deep knowledge and long experience about:

- Sample object
- Measurand
- Measurement Procedure

And we also need

- Clear guidance

In order to get a useful and correct uncertainty

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Summary of approaches to evaluation of MU*

Guidance summarised 2007

Specify the measurand and the procedure
Identify the sources of uncertainty

Intralaboratory

Yes — Mathematical model? — No

- Yes → Modelling approach
- No → **Single laboratory validation** & quality control approach

Interlaboratory

Procedure Performance Study — PT or procedure performance study? — **PT**

- Procedure Performance Study → Interlaboratory validation approach ISO 5725 ISO 21748
- PT → Proficiency testing approach ISO 17043 ISO 13528

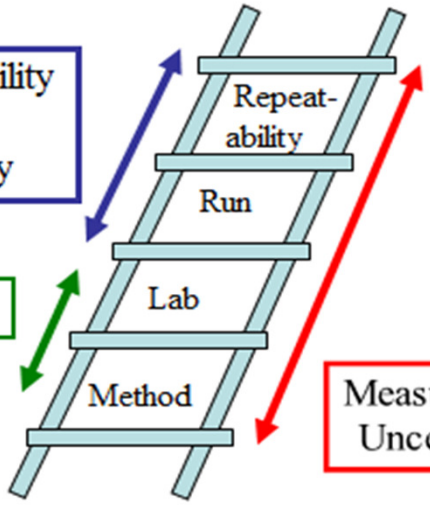
*Graph outline from: Eurolab Technical Report No. 1/2007 www.eurolab.org.

Single laboratory validation & quality control approach

Ladder of errors

u_{Rw} Reproducibility within laboratory

$u(bias)$ Bias



Repeatability – same day, person…

Run – different days, persons, instruments…

Measurement Uncertainty

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Summary of approaches to evaluation of MU*

We can compare approaches

Specify the measurand and the procedure
Identify the sources of uncertainty

Intralaboratory

Yes — Mathematical model? — No

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Interlaboratory

Procedure Performance Study — PT or procedure performance study? — PT

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Ammonia - comparison of different MU approaches – year 2010

GUM principles

Ammonium in fresh water – low levels 0.2 mg L^{-1}
According to EN-ISO 11732 - photometry

based on …

Modelling	Single- laboratory validation & QC	Interlaboratory data EN-ISO 11732	Proficiency testing
≈ 4 %	≈ 7 % - 20 % diff labs	≈ 20 %	18 – 22 %

Main problem?

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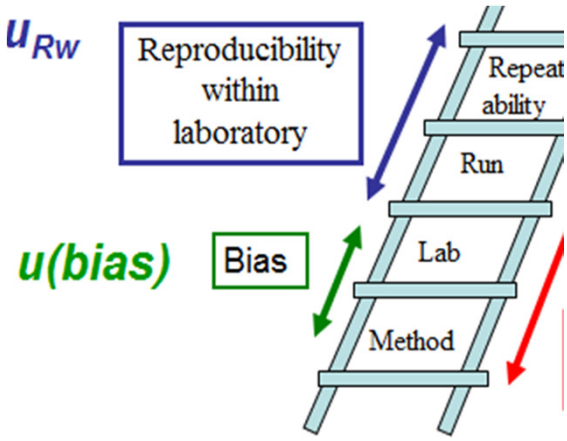
The bias issue* from year 2011

Statement from a paper titled *Dark Uncertainty* based on a meta study of interlaboratory comparisons

- Laboratories tend to underestimate the uncertainty because of its failure to account for bias
  - Some labs using only repeatability
- This is true for several national measurement institute (NMI) laboratories as well for routine test laboratories



*Thompson, M. & Ellison, S.L.R. Accred Qual Assur (2011) 16: 483

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The bias issue* from year 2011

From a paper titled *Dark Uncertainty* based on a meta study of interlaboratory comparisons

- Laboratories tend to underestimate the uncertainty

- Conclusion drawn from ratios << 1
  - u "mean" estimated from all labs uncertainty and
  - s_R is the observed SD in that round

For each interlaboratory comparison a ratio is calculated

$$Ratio = \frac{u}{S_R} \ll 1$$

*Thompson, M. & Ellison, S.L.R. Accred Qual Assur (2011) 16: 483

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The bias issue* from year 2011

Results from Key Comparison (proficiency testing) among national measurement institute (NMI)
- analytes: metals, gases, organics...

Example NMI laboratories

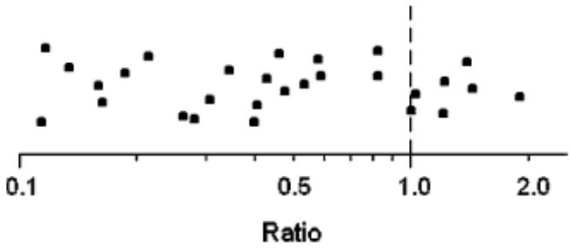

Fig. 4 Ratio of standard deviation of results expected from uncertainty estimates to that observed from results. (BIPM International Key Comparisons data)

$$Ratio = \frac{u}{S_R} \ll 1$$

Conclusion: It is common to **un**derestimate **un**certainty

*Thompson, M. & Ellison, S.L.R. Accred Qual Assur (2011) 16: 483

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Note to VIM* Definition of Measurement Uncertainty

NOTE 1 cont…***Sometimes estimated systematic effects are not corrected for but, instead, associated measurement uncertainty components are incorporated***

We can speak about u(bias)

*International Vocabulary of Metrology – Basic and General Concepts and Associated Terms
(VIM 3rd edition) JCGM 200:2012 (JCGM 200:2008 with minor corrections)

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What to do about bias?

Laboratories tend to underestimate the uncertainty – one cause is the failure to account for bias

- Shall we recommend to just increase uncertainty?
- Shall we use s_R from the standard method (ISO…) as standard uncertainty?
- Shall we try to better take into account bias?*
- e.g. Nordtest TR 537 www.nordtest.info using CRM
  Note: independent if bias is significant
  - one CRM

$$u(bias) = \sqrt{bias^2 + \left(\frac{s_{bias}}{\sqrt{n}}\right)^2 + u(CRM)^2}$$

  - several CRM

$$u(bias) = \sqrt{RMSbias^2 + u(CRM)^2}$$

B Magnusson, S L R Ellison, Treatment of uncorrected measurement bias in uncertainty estimation for chemical measurements, Anal Bioanal Chem, , (2008) 390:201-213

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Treatment of an observed bias

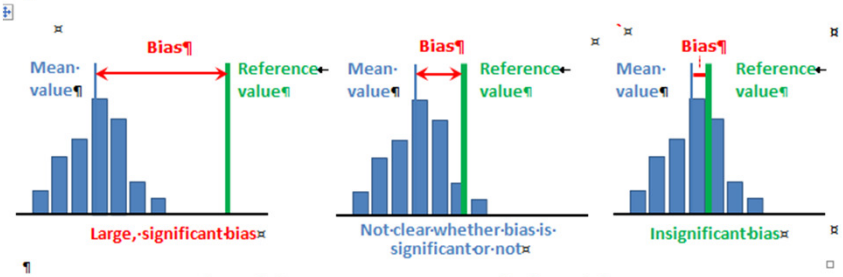
In this leaflet we discuss whether or not you should correct for an observed significant bias and the impact this may have on the measurement uncertainty (MU). How to apply the correction and how to increase the uncertainty to take account of an uncorrected bias is outside the scope of this leaflet.

Important issues for deciding on how to treat an observed significant bias are:

1. whether we understand the cause of the bias, and
2. whether its size can be reliably determined.

Further we must decide:

3. whether the bias is consistent for all test samples within the scope of the method and
4. whether any correction for bias should be multiplicative or additive, depending on whether the magnitude of the bias is constant or changes with the concentration level.



Should we correct, and should we increase the measurement uncertainty?

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New Eurachem leaflet about bias issue but no solutions!

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Measurement Uncertainty (MU) estimation

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In order to get a useful and correct uncertainty

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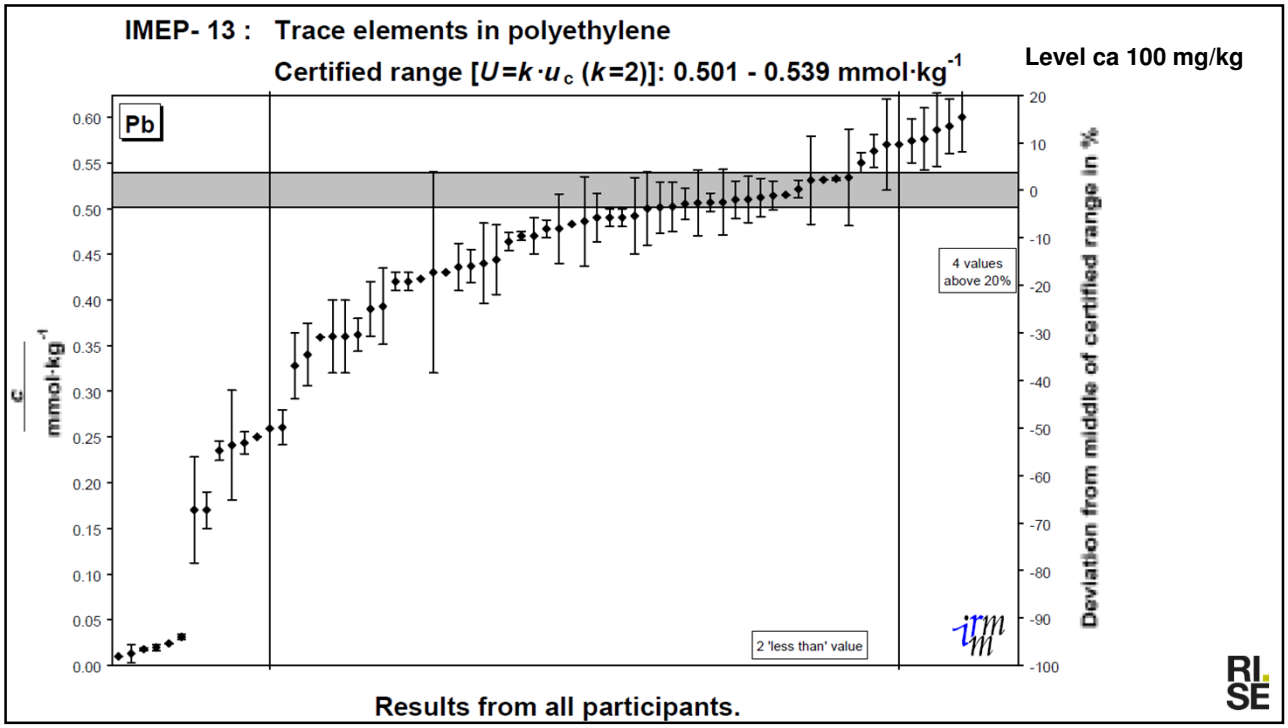

GUM says: *The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement.*

THANKS A LOT

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