Approaches to measurement uncertainty evaluation

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Eurachem/CITAC Scientific Workshop

Measurement uncertainty evaluation based on in-house validation data

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The main question of uncertainty evaluation in an analytical lab:

The uncertainty sources are more or less known

There are different data available (control charts, PT results, parallel measurements …)

How to use these data to take these uncertainty sources into account?

Different approaches offer different solutions to this question

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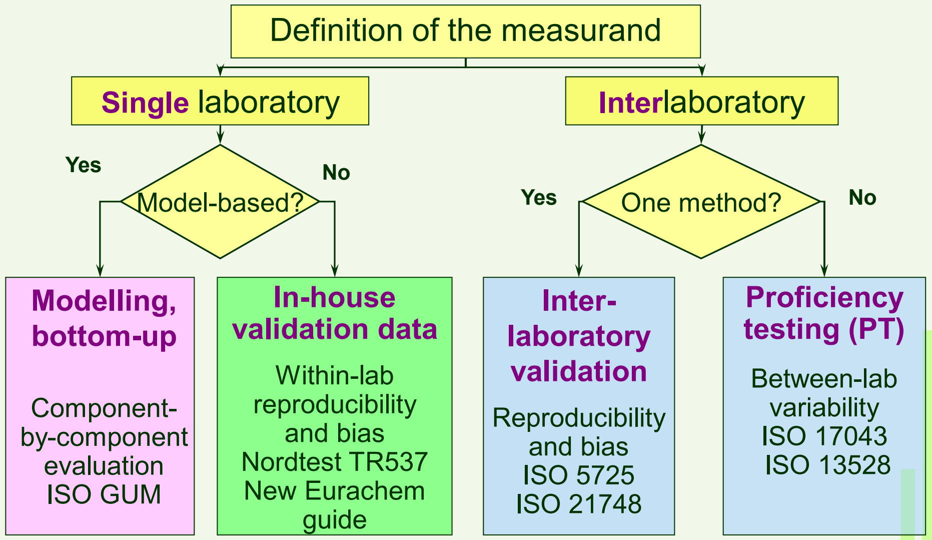
Uncertainty approaches



Eurolab Technical Report No 1/2007 Available from: http://www.eurolab.org/

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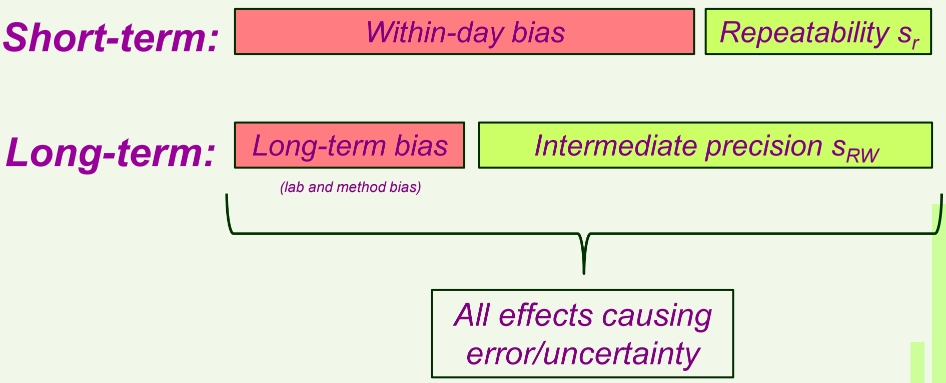
Systematic and random effects

- *Random and systematic effects can be grouped differently:*



The longer the time frame the more effects change their „status“:
systematic ⟶ random

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Modelling

Modelling

- Measurement model is built:

Output quantity → *Input quantities*

$$Y = F(X_1, X_2, \dots, X_n)$$

- Uncertainty is evaluated according to the law of propagation of uncertainty*:

Sensitivity coefficient — *Uncertainty component*

$$u_C(y) = \sqrt{\left[\frac{\partial Y}{\partial X_1}u(x_1)\right]^2 + \left[\frac{\partial Y}{\partial X_2}u(x_2)\right]^2 + \dots\dots + \left[\frac{\partial Y}{\partial X_n}u(x_n)\right]^2}$$

* Simplified equation, possible correlation is ignored

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Modelling

Modelling: aspects

- Uncertainties of input quantities are estimated
  - The model must be able to **account for all important uncertainty sources** via uncertainties of input quantities
  - One input quantity can account for several uncertainty sources
- The data of the **particular measurement done on the particular day** can be used:
  - Uncertainty of the **particular result** is obtained
- Systematic and random effects treated the same way
  - Operates in **short-term**

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Modelling

Systematic and random effects

Modelling typically operates here

Short-term: Within-day bias | Repeatability s_r

Long-term: Long-term bias (lab and method bias) | Intermediate precision s_{RW}

All effects causing error/uncertainty

The longer the time frame the more effects change their „status“: systematic ⟶ random

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Modelling

Modelling: advantages and limitations

Advantages

- Investigative
  - Uncertainty budget
  - **Contributions of uncertainty sources**
- Educative
- Helpful for improving measurement method
- (Mathematically correct)

Limitations

- All importnt uncertainty sources must be
  - Identified
  - **Quantified**
- Extra experiments may be required
- **Danger to underestimate uncertainty**

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In-house validation data approach

In-house validation data

Effects contributing to uncertainty

Random | Systematic

- The two groups of uncertainty contributions are quantified separately and then combined:

$$u_c = \sqrt{u_1^{\,2} + u_2^{\,2}}$$

Uncertainty arising from random effects

Uncertainty accounting for *possible* bias (recovery below 1)

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In-house validation data approach

In-house validation data

- Notations of the upcoming Eurachem guide*:

$$u_c\langle \mathrm{II} \rangle = q\sqrt{s'^2_{\mathrm{I}}\langle \mathrm{II} \rangle + u'^2_{\bar{R}}}$$

Uncertainty arising from random effects

Uncertainty accounting for *possible* bias (recovery below 1)

* The two uncertainty components are relative. Multiplication with *q* (the value of the measured quantity) is for converting relative uncertainty to absolute.

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In-house validation data: aspects

In-house validation data

- Uncertainties are quantified **in large batches**
  - Uncertainties of individual input quantities are not estimated
- The data of the particular measurement done on the **particular day is not used**:
  - **Average uncertainty** of the **method** is obtained
- As many short-term systematic effects as possible are quantified as long-term random effects
  - Operates in **long-term**

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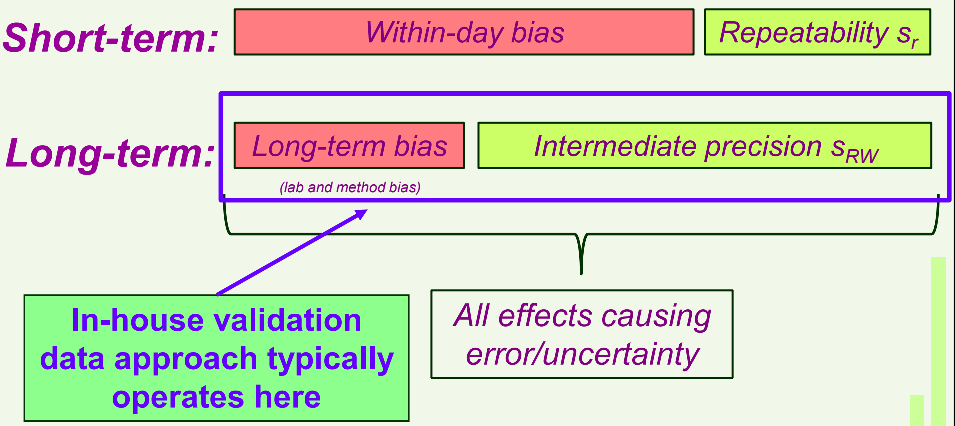
Systematic and random effects

In-house validation data



The longer the time frame the more effects change their „status“: systematic ⟶ random

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In-house validation data

In-house validation: advantages and limitations

Advantages

- Exiting data can be used
  - **Less extra work**
- Low danger to underestimate uncertainty
  - **Realistic uncertainty estimates**

Limitations

- Less insight than with modelling
  - Lower educational value
- Occasionally overestimated uncertainty
- Mathematically less rigorous

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Interlaboratory

Interlaboratory approaches

- The main uncertainty sources can be taken into account via the between-lab reproducibility

Main equation:

$$u_c = s_R$$

s_R is between-lab reproducibility

These approaches completely ignore the situation at a yor laboratory

Should be used only with highly standardised methods

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Uncertainty by different approaches

- Modelling
  - Uncertainty of an **individual result** of a measurement can be obtained
- In-house validation data
  - Typical uncertainty of results obtained using a **method in the laboratory**
- Interlaboratory approaches
  - Uncertainty of results obtained using the same **method in different laboratories**

These uncertainties have different meanings

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Choosing the approach

- If you have
  - Competence and time
  - Data on all important influencing quantities
    - Use the Modeling approach
- If you have
  - Validation and quality control data and results of participation in ILC-s or CRM analysis
    - Use the in-house validation approach
- Interlab approaches should be used only with highly standardised methods

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Thank you for your attention!

Happy to answer your questions!

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