

 Setting standards
 in analytical science

ISO/TS 21748: A new guide to uncertainty estimation using interlaboratory study data

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LGC


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Overview

- Reproducibility and uncertainty estimation
- Introduction to ISO TS 21748

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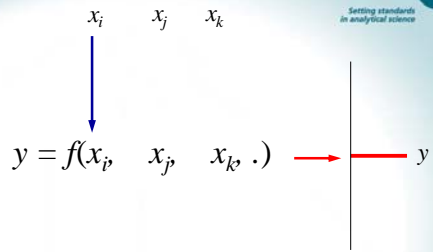
What is Measurement Uncertainty?

"A parameter, associated with the result of a measurement, that characterises the dispersion of the values that could reasonably be attributed to the measurand"
(ISO Guide)

The number after the \pm

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Models and Uncertainty



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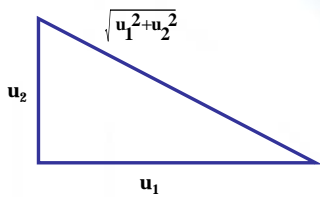
ISO Guide approach



- Specify the measurand
 - including complete equation
- Quantify significant uncertainties in all parameters
 - A: from statistics of repeated experiment
 - B: by any other means (theory, certificates, judgement...)
- Express as standard deviation
- Combine according to stated principles

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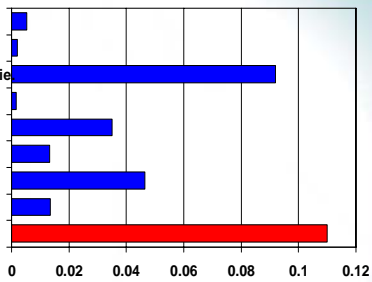
Combining uncertainties (ISO)



- *Standard deviations*
- *Established error propagation theory*

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Oxidant conc.
Extent Oxid⁴ie



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A simpler model



- The best available estimate of precision
 - *An effect varied representatively during a precision experiment requires no further study*
- The best available estimate of bias *and its uncertainty*
- Other significant effects evaluated
 - By experiment, or from standing data

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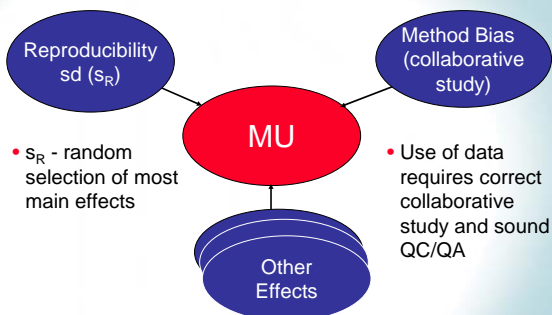
Collaboratively trialed methods



- Collaboratively trialed method
 - bias and precision verified in-house
- Assessed against collaborative study estimates
 - ISO/TS 21748
 - demonstrate method bias and repeatability are under control

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Collaborative trial data



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Process for evaluating uncertainty according to ISO/TS 21748



- Obtain repeatability, reproducibility and bias estimates from collaborative study
- Establish whether laboratory bias is within that expected on the basis of the collaborative study
- Establish whether laboratory precision is within that expected on the basis of the collaborative study
- Where laboratory bias and precision are under control, combine effects appropriately to form a combined uncertainty estimate

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TS21748 uncertainty budget



$$u_c^2(y) = \hat{s}_R^2 + u^2(\hat{}) + \sum_{i=k,n} c_i^2 u^2(x_i)$$

- Combined uncertainty
 - Adjusted reproducibility estimate
 - Uncertainty associated with method bias
 - Effects not covered, e.g. sampling uncertainty

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Demonstrating acceptable laboratory bias



- Study of CRMs
 - Simple test for significant bias
 - Ideally with small bias check uncertainty
- Comparison with known test method
 - Typically paired tests on several materials
- Comparison with other laboratories
 - Proficiency testing or other collaborative study

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Including trueness data in an uncertainty estimate

$$u_c^2(y) = \hat{s}_R^2 + u^2(\hat{}) + \sum_{i=k,n} c_i^2 u^2(x_i)$$

- Combined uncertainty
- Adjusted reproducibility estimate
- **Uncertainty associated with method bias**
 - Effects not covered, e.g. sampling uncertainty

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Demonstrating acceptable laboratory precision

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Including reproducibility data

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$$u_c^2(y) = \hat{s}_R^2 + u^2(\hat{\cdot}) + \sum_{i=k,n} c_i^2 u^2(x_i)$$

- Combined uncertainty
- **Adjusted reproducibility estimate**
 - Uncertainty associated with method bias
 - Effects not covered, e.g. sampling uncertainty

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Other effects

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- Simple "worst case" calculations can often show an effect is negligible
- Formal uncertainty calculations often show negligible components
- Typical criteria:
 - $u < u_{\max}/3$ (<6% effect on combined uncertainty)
 - $u < u_{\max}/5$ (<2% effect on combined uncertainty)
 - ISO/TS 21748 effects $< 0.2S_R$

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Numerical calculation

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Calculated result y

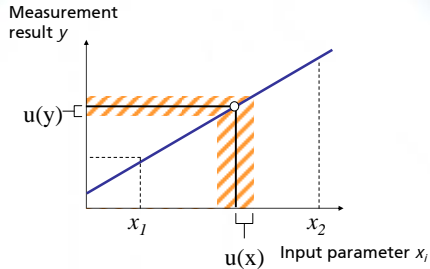
$y(x+u(x))$
 $y(x)$

x $x+u(x)$

$u(y) \approx y(x+u(x)) - y(x)$

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Other effects: A simple uncertainty experiment



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