Introduction to Metrology: SI unit system and measurement standards, traceability, calibration and measurement uncertainty

Experimental Design
7.2.2013

Doc. Martti Heinonen
Mars Climate Orbiter
Impact of metrology: NIST SRM case

Cholesterol Measurements

Improved Cholesterol Measurement Accuracy Saves Health Care Dollars

NIST Contributions to National Reference System for Cholesterol

- 1967 – Pure Cholesterol SRM (SRM 911)
- 1980 – Cholesterol in Serum Definitive Method
- 1981 – First Cholesterol in Human Serum SRM (SRM 909)
- 1988 – New Suite of Cholesterol in Serum SRMs at Medical Decision Points
- 1997 – New Suite of Fresh-Frozen Serum SRMs designed to address clinical analyzer commutability issues; Total-, HDL-, and LDL-Cholesterol and Triglyceride Values

Improvement in precision since 1968 has been estimated to save $100M/yr in treatment costs

DATA FROM GAO AND CAP
Outline

1. Traceability in measurements
   1.1 Basic concepts
   1.2 Why we need traceability?
   1.3 Infrastructure ensuring availability of traceable measurements

2. SI – the international system of units
   2.1 System of units: from trade to science
   2.2 Base and derived units
   2.3 Measurement standards and traceability

   3.1 Terminology
   3.2 Importance of the measurement uncertainty

4. Measurement uncertainty – part 2: Methods
   4.1 Calculating uncertainty
   4.2 Calculations step by step
   4.3 Uncertainty calculation in practice
1 Traceability in measurements

1.1 Basic concepts

1.2 Why we need traceability?

1.3 Infrastructure ensuring availability of traceable measurements
1.1 Basic concepts
Terms

QUANTITY

- Property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference (A reference can be a measurement unit, a measurement procedure, a reference material, or a combination of such.)
- Quantity can be a general quantity (e.g. length) or particular quantity (e.g. wavelength of Sodium D line)

MEASURAND

- Quantity intended to be measured

ESTIMATE (of the measurand); called also MEASURED QUANTITY VALUE

- measured value of a quantity measured value
- quantity value representing a measurement result

MEASUREMENT ERROR

- measured quantity value minus a reference quantity value
Metrology (metrologia)

metrology is:

science of measurement and its application
[1.1, 1.2]

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

Usually the concept of metrology is limited to:

- Science of measurement studying the relationship between measurands and their estimates (measured quantity values)
Uncertainty of measurement (*epävarmuus*)

A non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used.

\[ r - 2u \leq r \leq r + 2u \]

- 68% (±1σ)
- 95% (±2σ)

\( r \) = estimate = mean value
\( u \) = standard uncertainty

[1.1, 1.2]
Facts about Measurement Results

• Usually a measurement disturbs its target affecting thus the measurement result.

• A measurement result is always a combination of many factors. (reading or output signal of the measuring device is only one of them)

• We never know all the factors.

• We never know the “true value” of the factors (we can only estimate).

• The combined effect of unknown factors and inaccurate knowledge on the known factors is described quantitatively with the measurement uncertainty.

• “Absolute certainty is the privilege of uneducated minds ... or fanatics.”
Accuracy and Precision

**accuracy** (*tarkkuus*)

closeness of agreement between a measured quantity value and a true quantity value of a measurand

**precision** (*täsmällisyys*)

closeness of agreement between indications or measured quantity values obtained by replicate measurements on the same or similar objects under specified conditions

[1.1, 1.2]
Calibration (*kalibrointi*)

operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication. [1.1, 1.2]

The result of a calibration can be given as

- correction value(s) at discrete measurement point(s)
- calibration equation (curve)
- re-calculated constant(s)
- statement that the error is in given specifications.

A calibration result includes always the uncertainty.
(also the probability level should be given)

Conditions of calibration should be stated when reporting calibration results.
Adjustment (*viritys)*

set of operations carried out on a measuring system so that it provides prescribed indications corresponding to given values of a quantity to be measured [1.1, 1.2]

NOTE 1: Types of adjustment of a measuring system include zero adjustment of a measuring system, offset adjustment, and span adjustment (sometimes called gain adjustment).

NOTE 2: Adjustment of a measuring system should not be confused with calibration, which is a prerequisite for adjustment.

NOTE 3: After an adjustment of a measuring system, the measuring system must usually be recalibrated.
Traceability (jaljitettävyys)

(Metrological traceability) property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty

**Traceability chain:**
sequence of measurement standards and calibrations that is used to relate a measurement result to a reference

[1.1, 1.2]
Traceability (jäljitetävyys)

Traceability $\Rightarrow$ Evidence that your unit is of the same size as the internationally accepted one.
Measurement standard (*mittanormaali*)

- realization of a given quantity, with stated quantity value and associated measurement uncertainty, used as a reference
- Measurement standard can be an instrument, a measuring system, material measure or a reference material.

[1,2]
Characteristics of Unbroken Traceability

For each calibration of the chain:

- **Uncertainty estimation**
- **Documented and generally acknowledged procedures, documented results**
- **Competence**
- **Calibration is valid for the application.** (interval of calibrations, conditions etc.)
Traceability Tower

- The tower is collapsed if any part of it is missing or incomplete

  i.e.

  there is no traceability unless all levels include all the characteristics of traceability

- At any level the measurement uncertainty can’t be smaller than levels below.
Typical problems in traceability

No calibration

Calibration interval too long

No evidence on the traceability in calibration

Calibration was carried out in conditions too different from the application

Calibration results have not been used

Calibration covers only a part of the measuring system

There is no evidence on the traceability of the reference materials

Incomplete traceability chain = no traceability
1.2 Why we need traceability?
Traceability – why?

• Modern industrial production is not possible if subcontractors have different scales

• Scientific technical research can not necessarily be repeated if it is done without traceably calibrated instruments

• Traceability is the answer to the questions:
  • From where can I find a reliable measurement standard?
  • How can I convince others of the reliability of my measurement standard?
Traceability – why?

Examples:

• Pharmaceutics
• Telecommunication
• Aviation
• Space technology
• Safety: Nuclear power plant
1.3 Infrastructure ensuring availability of traceable measurements
Metrology Infrastructure

• for ensuring global availability of traceable measurements

• foundation: The Metre Convention – a diplomatic treaty first signed in 1875 by representatives of 17 nations

• three levels:
  • Global
  • Regional
  • National
Global:

Finnish members:
- 1953-1971 Yrjö Väisälä
- 1992-1998 Olli Lounasmaa

MIKES is a member of:
- CC for Length
- CC for Electricity and Magnetism
- CC for Thermometry
- CC for Photometry and Radiometry

Consultative Committees (CCs)
Ten CCs normally chaired by a member of CIPM; to advise the CIPM; act on technical matters and take important role in CIPM MRA; comprise representatives of NMIs and other experts.

International Bureau of Weights and Measures (BIPM)
International centre for metrology
Laboratories and offices at Sèvres

Metre Convention 1875
Diplomatic treaty
Governments of Member States
International organizations

Associate States and Economies of the CGPM
General Conference on Weights and Measures (CGPM)
meets every four years and consists of delegates from Member States.

International Committee for Weights and Measures (CIPM)
consists of eighteen individuals elected by the CGPM
It is charged with supervision of the BIPM and affairs of the Metre Convention
The CIPM meets annually at the BIPM

CIPM MRA
National metrology institutes (NMIs)
Regional:
National:

- Electricity
- Acoustics
- Time
- Frequency
- Temperature
- Gas flow
- Humidity
- Pressure
- Mass
- Force
- Torque
- Length

MIKES

Water quality
SYKE

Optics
Aalto University

Air quality
FMI

Ionising radiation
STUK

Acceleration of free fall
FGI

Length in geodesy
Impact of metrology: Finnish numbers

Approximate amount of traceable calibration and testing certificates issued annually and traceable instruments/measurements

- ~ 2000
- ~ 20,000
- ~ 2,000,000
- ~ 2,000,000,000 (00?)
CIPM MRA objectives:

- to establish the degree of equivalence of measurement standards maintained by NMIs;
- to provide for the mutual recognition of calibration and measurement certificates issued by NMIs; thereby to
- to provide governments and other parties with a secure technical foundation for wider agreements related to international trade, commerce and regulatory affairs

MRA has been signed by 67 NMIs from 45 states and 20 associate states

MRA includes database of NMIs reviewed calibration services with corresponding uncertainties (CMCs)

MIKES has several 100s of different CMC entries

Reconnaissance mutuelle
des étalons nationaux de mesure
et des certificats d’étalonnage et de mesurageémis par les laboratoires nationaux de métrologie
Paris, le 14 octobre 1999

Mutual recognition
of national measurement standards
and of calibration and measurement certificates
issued by national metrology institutes
Paris, 14 October 1999

Comité international des poids et mesures

Bureau international des poids et mesures
Organisation intergouvernementale de la Convention du Mètre

MIKES

MH 2013
2 SI – the international system of units

2.1 System of units: from trade to science
2.2 Base and derived units
2.3 Unit realisations and measurement standards
2.1 A system of units: from trade to science
SI – system for characterizing physical and chemical phenomena

speed: \[ v = \frac{\Delta x}{\Delta t} \]

force: \[ F = ma = m \frac{\Delta x}{(\Delta t)^2} \]

energy: \[ E = F \Delta x = m \frac{(\Delta x)^2}{(\Delta t)^2} \]

power: \[ P = \frac{F}{\Delta t} = \frac{m(\Delta x)^2}{(\Delta t)^3} \]

pressure: \[ p = \frac{F}{A} = \frac{m \Delta x}{(\Delta t)^2 l^2} \]

density: \[ \rho = \frac{m}{V} = \frac{m}{l^3} \]
SI – system for characterizing physical and chemical phenomena

for real gas: \[ p_g V = n_g RT_g (p, T) \]

rotating speed: \[ \omega = \frac{n}{\Delta t} \]

thermal expansion: \[ \Delta l = l \alpha \Delta T \]

frequency: \[ f = \frac{n}{\Delta t} = \frac{1}{\tau} \]

resistance: \[ R = \frac{U}{I} \]

Electr. power: \[ P = U \cdot I \]

illuminance: \[ E_v = \frac{F}{A} = \frac{I_v \Omega}{A} \]

\[ \text{C}_{12}\text{H}_{26}(l) + \frac{37}{2} \text{O}_2(g) \rightarrow 12 \text{CO}_2(g) + 13 \text{H}_2\text{O}(g) \]
2.2 Base and derived units
SI system – properties

- based on a set of 7 base units
  - by convention these are assumed to be independent
- other units are formed as products of powers from base units (derived units)
- some derived units have special names like Newton
- system is coherent i.e.
  - equations between the numerical values of quantities take exactly the same form as the equations between the quantities themselves
- decimal system is used
## SI system – Base units

<table>
<thead>
<tr>
<th>Base quantity</th>
<th>SI base unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Symbol</td>
</tr>
<tr>
<td>length</td>
<td>$l, x, r$, etc.</td>
</tr>
<tr>
<td>mass</td>
<td>$m$</td>
</tr>
<tr>
<td>time, duration</td>
<td>$t$</td>
</tr>
<tr>
<td>electric current</td>
<td>$I, i$</td>
</tr>
<tr>
<td>thermodynamic temperature</td>
<td>$T$</td>
</tr>
<tr>
<td>amount of substance</td>
<td>$n$</td>
</tr>
<tr>
<td>luminous intensity</td>
<td>$I_v$</td>
</tr>
</tbody>
</table>

[2.1]
Definitions of base units

- **Kilogram:**
  The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram.

- **Metre:**
  The metre is the length of the path travelled by light in vacuum during a time interval of $1/299\ 792\ 458$ of a second.

- **Second:**
  The second is the duration of $9\ 192\ 631\ 770$ periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium 133 atom.
Definitions of base units

- **Kelvin:**
  The kelvin, unit of thermodynamic temperature, is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.

- **Mole:**
  The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon 12.
  
  When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.
Definitions of base units

- **Ampere:**
The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 metre apart in vacuum, would produce between these conductors a force equal to $2 \times 10^{-7}$ newton per metre of length.
  - NOTE 1: Direct realisation of the SI ampere is very difficult in practice
  - NOTE 2: $N = \text{kg} \cdot \text{m} \cdot \text{s}^{-2} \Rightarrow$ Depends on the prototype of kg

- **Candela:**
The candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency $540 \times 10^{12}$ hertz and that has a radiant intensity in that direction of $1/683$ watt per steradian.
Need for redefining SI base units

• Drawbacks of the current SI are:
  • Kilogram is defined with an artefact
  • The definition of kelvin is based on material properties
  • The definition of ampere limits the achievable accuracy and is not currently use (quantum standards of ohm and voltage are used instead through the Ohm’s law)
  • Because of these, drift, non-uniqueness and limitations in accuracy cannot completely be prevented.
SI base units in future

Ground state hyperfine splitting frequency of the caesium 133 atom

\[ f_{\text{hfs}}^{(133\text{Cs})} \]

Speed of light in vacuum

Planck constant

Avogadro constant

Elementary charge

Boltzmann constant

Luminous efficacy

MH 2013
## SI system – Derived units

<table>
<thead>
<tr>
<th>Derived quantity</th>
<th>SI coherent derived unit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Name</strong></td>
<td><strong>Symbol</strong></td>
</tr>
<tr>
<td>area</td>
<td>( A )</td>
</tr>
<tr>
<td>volume</td>
<td>( V )</td>
</tr>
<tr>
<td>speed, velocity</td>
<td>( v )</td>
</tr>
<tr>
<td>acceleration</td>
<td>( a )</td>
</tr>
<tr>
<td>wavenumber</td>
<td>( \sigma, \bar{v} )</td>
</tr>
<tr>
<td>density, mass density</td>
<td>( \rho )</td>
</tr>
<tr>
<td>surface density</td>
<td>( \rho_A )</td>
</tr>
<tr>
<td>specific volume</td>
<td>( u )</td>
</tr>
<tr>
<td>current density</td>
<td>( j )</td>
</tr>
<tr>
<td>magnetic field strength</td>
<td>( H )</td>
</tr>
<tr>
<td>concentration</td>
<td>( c )</td>
</tr>
</tbody>
</table>

(a) In the field of clinical chemistry this quantity is also called substance concentration.

(b) These are dimensionless quantities, or quantities of dimension one, and the symbol “1” for the unit (the number “one”) is generally omitted in specifying the values of dimensionless quantities.
## SI system – Derived units with special names

<table>
<thead>
<tr>
<th>Derived quantity</th>
<th>Name</th>
<th>Symbol</th>
<th>Expressed in terms of other SI units</th>
<th>Expressed in terms of SI base units</th>
</tr>
</thead>
<tbody>
<tr>
<td>plane angle</td>
<td>radian (^{(b)})</td>
<td>rad</td>
<td>1 (^{(b)})</td>
<td>m/m</td>
</tr>
<tr>
<td>solid angle</td>
<td>steradian (^{(b)})</td>
<td>sr (^{(c)})</td>
<td>1 (^{(b)})</td>
<td>(m^2/m^2)</td>
</tr>
<tr>
<td>frequency</td>
<td>hertz (^{(d)})</td>
<td>Hz</td>
<td></td>
<td>s(^{-1})</td>
</tr>
<tr>
<td>force</td>
<td>newton</td>
<td>N</td>
<td></td>
<td>m kg s(^{-2})</td>
</tr>
<tr>
<td>pressure, stress</td>
<td>pascal</td>
<td>Pa</td>
<td>N/m(^2)</td>
<td>m(^{-1}) kg s(^{-2})</td>
</tr>
<tr>
<td>energy, work, amount of heat</td>
<td>joule</td>
<td>J</td>
<td>N m</td>
<td>m(^2) kg s(^{-2})</td>
</tr>
<tr>
<td>power, radiant flux</td>
<td>watt</td>
<td>W</td>
<td>J/s</td>
<td>m(^2) kg s(^{-3})</td>
</tr>
<tr>
<td>electric charge, amount of electricity</td>
<td>coulomb</td>
<td>C</td>
<td></td>
<td>s A</td>
</tr>
<tr>
<td>electric potential difference,</td>
<td>volt</td>
<td>V</td>
<td>W/A</td>
<td>m(^2) kg s(^{-3}) A(^{-1})</td>
</tr>
<tr>
<td>electromotive force</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>capacitance</td>
<td>farad</td>
<td>F</td>
<td>C/V</td>
<td>m(^{-2}) kg(^{-1}) s(^4) A(^2)</td>
</tr>
<tr>
<td>electric resistance</td>
<td>ohm</td>
<td>Ω</td>
<td>V/A</td>
<td>m(^2) kg s(^{-3}) A(^{-2})</td>
</tr>
<tr>
<td>electric conductance</td>
<td>siemens</td>
<td>S</td>
<td>A/V</td>
<td>m(^{-2}) kg(^{-1}) s(^3) A(^2) ([2.1])</td>
</tr>
</tbody>
</table>
## SI system – Derived units with special names 2

<table>
<thead>
<tr>
<th>Derived quantity</th>
<th>Name</th>
<th>Symbol</th>
<th>Expressed in terms of other SI units</th>
<th>Expressed in terms of SI base units</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnetic flux</td>
<td>weber</td>
<td>Wb</td>
<td>V s</td>
<td>m² kg s⁻² A⁻¹</td>
</tr>
<tr>
<td>magnetic flux density</td>
<td>tesla</td>
<td>T</td>
<td>Wb/m²</td>
<td>kg s⁻² A⁻¹</td>
</tr>
<tr>
<td>inductance</td>
<td>henry</td>
<td>H</td>
<td>Wb/A</td>
<td>m² kg s⁻² A⁻²</td>
</tr>
<tr>
<td>Celsius temperature</td>
<td>degree Celsius</td>
<td>°C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>luminous flux</td>
<td>lumen</td>
<td>lm</td>
<td>cd sr (c)</td>
<td>cd</td>
</tr>
<tr>
<td>illuminance</td>
<td>lux</td>
<td>lx</td>
<td>lm/m²</td>
<td>m⁻² cd s⁻¹</td>
</tr>
<tr>
<td>activity referred to a radionuclide (f)</td>
<td>becquerel (d)</td>
<td>Bq</td>
<td></td>
<td></td>
</tr>
<tr>
<td>absorbed dose, specific energy (impacted), kerman</td>
<td>gray</td>
<td>Gy</td>
<td>J/kg</td>
<td>m² s⁻²</td>
</tr>
<tr>
<td>dose equivalent, ambient dose equivalent, directional dose equivalent, personal dose equivalent</td>
<td>sievert (g)</td>
<td>Sv</td>
<td>J/kg</td>
<td>m² s⁻²</td>
</tr>
<tr>
<td>catalytic activity</td>
<td>katal</td>
<td>kat</td>
<td></td>
<td>s⁻¹ mol</td>
</tr>
</tbody>
</table>

---

[2.1]
Realisation of a derived unit

• The realisation forms a link between the measurements of a derived quantity and the SI base units.

• Characteristics of the realisation:
  • Based on the definition of the quantity
  • Measurements in terms of SI units (base or derived but not of the same quantity) with traceability to national/international measurement standards
  • Full uncertainty analysis
  • Comparisons to other realisations of the same quantity

• National Standards Laboratories maintain realisations (or secondary standards) for a set of derived quantities
Realisation of the pascal

- Unit with a special name: 1 Pa = 1 m\(^{-1}\) kg s\(^{-2}\)

**Definition of pressure:**

\[ p = \frac{F}{A} \]

**Realisation of the unit:**

- Force lifting the piston \( F_1 \):
  \[ F_1 = pA \]
- Force lowering the piston \( F_2 \):
  \[ F_2 = mg \]

**In equilibrium:**

\[ F_1 = F_2 \Rightarrow p = \frac{mg}{A} \]
Realisation of the unit of the dew-point temperature (K or °C)

• Same unit as of the temperature but different meaning:

Dew-point temperature \( (t_d) \):
The temperature at which the gas would be saturated with respect to a plane surface of pure liquid water or solid ice at the same gas pressure.

A saturator-based primary humidity standard
Air or other gas is saturated with respect to plane water or ice surface:
\[ \Rightarrow \text{dew-point temperature} \ (t_d) = \text{air/gas temperature in the saturator} \ (t_s) \]

Saturated air/gas passes through internally polished stainless steel tubing:
\[ t_d \approx t_s < t_{\text{tubing}} \]
\[ RH < 100\% \]

The air or gas enters a measurement chamber.
Humidity in the chamber is determined by the temperatures and pressures of the saturator and the chamber:
\[ t_d = t_s + \Delta t_{\text{dp}} < t_{\text{chamber}} \]
\[ RH = RH(t_d, t_{\text{chamber}}) \]
2.3 Measurement standards and traceability
Traceability in chemical measurements

**SI unit: mole**

The mole was added to SI in 1971.

**Chemical primary methods**

- Isotope Dilution Mass Spectrometry
- Gravimetry
- Titrimetry
- Coulometry
- Freezing Point Depression (Differential Scanning Calorimetry)

**Certified reference materials**


**Validated measurement methods and reference materials in laboratories**

MH 2013
Traceability to altitude measurements in a military aircraft

- MIKES Primary Mass and Length Standards
- MIKES Primary Pressure Standard
- K013 pressure reference standard
  - ±10 Pa ~ ±0.9 m
- K013 pressure working standard
  - ±20 Pa ~ ±1.7 m
- The pressure simulator of the brigade
  - ±30 Pa ~ ±2.6 m
- Altimeter
  - ±10 m
3 Measurement uncertainty – part 1: Introduction

3.1 Terminology

3.2 Importance of the measurement uncertainty
3.1 Terminology
Terms

MEASUREMENT REPEATABILITY
• measurement precision under a set of repeatability (similar) conditions of measurement

MEASUREMENT REPRODUCIBILITY
• measurement precision under reproducibility (changed) conditions of measurement

RANDOM ERROR
• Component of measurement error that in replicate measurements varies in an unpredictable manner

SYSTEMATIC ERROR
• Component of measurement error that in replicate measurements remains constant or varies in a predictable manner
3.2 Importance of the measurement uncertainty
Measurement result and its uncertainty

- Estimated quality of a result is expressed as the uncertainty
- The uncertainty is an essential part of a measurement result:
  
  Measurement result = Estimate ± uncertainty

- The uncertainty gives the limits of the range in which the “true” value of the measurand is estimated to be at a given probability.
- Too often the uncertainty is not presented explicitly with the estimate
  ⇒ confusion, incorrect conclusions, non-equal users etc.
- If the uncertainty is not taken into account, incorrect conclusions are drawn and the number of unsatisfactory products increases.
- When you know the uncertainty in a measurement, then you can judge its fitness for purpose.
Importance of uncertainty of measurements

• Measurements are never absolutely accurate, but there is always some uncertainty in the measured values.

• Measurement result without uncertainty estimate is meaningless.

• Estimation of measurement uncertainties is one of the most important parts of practical metrology.

• A proper uncertainty budget indicates what parts of the measurement should be developed to decrease the overall uncertainty most effectively.
Certified range \([U=k\cdot u_c \ (k=2)]:\ 1.226 - 1.294 \text{ mmol}\cdot\text{kg}^{-1}\)

Results from all participants.

9 values below -50%  
3 values above 50%

Certified range [\(U=k\cdot u_c \ (k=2)\): 1.226 - 1.294 mmol·kg\(^{-1}\)]

Results from all participants.

\[\text{Cd}\]

3 values above 50%  
9 values below -50%

[\(\text{Deviation from middle of certified range in } \%\)]

\([\text{Mittaustulosten epävarmuus, MIKES 26.6.2005}]\)
4 Measurement uncertainty – part 2: Methods

4.1 Calculating uncertainty
4.2 Calculations step by step
4.3 Uncertainty calculation in practice
4.1 Calculating uncertainty
Calculating a measurement result

- A measurement result is calculated from input data. In addition to the measurement values, the data often include information from earlier measurements, specifications, calibration certificates etc.

- The calculation method is described with an equation (or a set of equations) called measurement model (mathematical model).

- The model is used for both calculation of the estimate and the uncertainty of the results.

- The model should include all factors (input quantities) affecting significantly the estimate and/or the uncertainty.

- The model is never complete; approximations are needed.
6 steps to evaluating uncertainty

1) Measurement model:
   List essential input quantities (i.e. parameters $x_i$ having a significant effect on the result) and build up a mathematical model (function) showing how they are related to the final result: $y = f(x_1, \ldots, x_i)$

2) Standard uncertainty:
   Estimate the standard uncertainty of each input quantity ($x_i$)

3) Using the model in uncertainty calculations:
   Determine the uncertainty due to standard uncertainty of each input quantity ($x_i$).

4) Correlation:
   Determine correlation between the input quantities (if relevant)

5) Calculate the combined standard uncertainty

6) Calculate the expanded uncertainty.
4.2 Calculations step by step

Step 1: Measurement model
Step 2: Standard uncertainty
  Type A evaluation of standard uncertainty
  Type B evaluation of standard uncertainty
Step 3: Using the model in uncertainty calculations
Step 4: Correlation
Step 5: Combining the uncertainty components
Step 6: Expanded uncertainty
Step 1: Measurement model

Equation which describes the measurement:

Measurand \( Y = f(X_1, X_2, \ldots, X_n) \)

Input quantities \( X_i \)

- The model should include:
  - Measurement results, corrections, reference values, influence quantities...
  - The magnitude of a correction can be zero but it can still have uncertainty
  - The values and uncertainties of the input quantities should be determined

Measurement result \( (y) \) is:

\[
y = f(x_1, x_2, \ldots, x_n)
\]

- \( x_i \) is the value (estimate) of the input quantity \( X_i \)

Example:

\[
t_x = t_{\text{ind}} + \delta t_{\text{Cal}} + \delta t_D + \delta t_{\text{resol}} + \delta t_G
\]
Step 2: Standard uncertainty

- All uncertainty components should be comparable ⇒ standard uncertainty $u_i$
- The variance of the sum of non-correlating random variables is the sum of their variances
- Standard uncertainty is the square root of variance
- All uncertainty components should be expressed as standard uncertainties
- For normal distribution standard uncertainty corresponds to about 68% confidence level
Two methods for estimating the standard uncertainty of an input quantity

- **Type A:**
  - Evaluated from a number of observations (usually > 10)

- **Tyyppi B:**
  - Evaluated from a single (or a small number of) data value(s)
  - Often taken from data reported earlier or by others
Type A evaluation of standard uncertainty

- Uncertainty is evaluated by statistical analysis of a series of observations \( q_i \)
  - The spread of the results is assumed to be random
  - An estimate for the value of the quantity is the arithmetic mean \( \bar{q} \)
  - An estimate for the variance of the probability distribution is \( s(x)^2 \):

\[
\bar{q} = \frac{1}{n} \sum_{i=1}^{n} q_i
\]

\[
s^2(q) = \frac{1}{n-1} \sum_{i=1}^{n} (q_i - \bar{q})^2
\]

\[
s^2(\bar{q}) = \frac{s^2(q)}{n}
\]

- An estimate for the variance of the mean \( s^2(\bar{q}) \) (the experimental variance of the mean) is:
- The standard uncertainty of \( q \) equals the experimental standard deviation of the mean:

\[
u(q) = s(q) = \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} (q_i - \bar{q})^2}
\]

If type A measurement uncertainty is based on few measurements the estimation of \( u(x) \) is not reliable and normal distribution can not be assumed.
(unless other information on the distribution is available)
Type B evaluation of standard uncertainty

- To be applied for estimates of input quantities that has not been obtained from repeated measurements

- Typical examples:
  - uncertainties of values and drifts of reference standards
  - uncertainties of environmental quantities
  - uncertainties from specifications of instrument
  - uncertainties from literature values
  - uncertainty due to the method or calculation
  - uncertainty due to staff
  - uncertainties from calibration certificates
Rectangular distribution

- All values in the range $x_i - a$ … $x_i + a$ have equal probability
- Standard uncertainty $u(x_i) = \frac{a}{\sqrt{3}} \approx 0.577a$
- Examples: specifications, resolution
- Applied if only limiting values are known
• Example: convolution of two rectangular distribution

• Standard uncertainty:

\[ u(x_i) = \frac{a}{\sqrt{6}} \approx 0.408 \, a \]
U-shape distribution

- Example: sinusoidal variation between limits ± a

- Standard uncertainty:
  \[ u(x_i) = \frac{a}{\sqrt{2}} \approx 0.707 \ a \]
Step 3: Using the model in uncertainty calculations

- The contribution of \( u(x_i) \) to the uncertainty of \( y \) is determined by the sensitivity coefficient \( c_i \).

- The sensitivity coefficient can be determined:
  - from partial derivative of \( f(X_1, X_2, \ldots, X_n) \) with \( X_i \)
    i.e. \( c_i = \frac{\partial f}{\partial X_i} \) (at \( x_1, x_2, \ldots, x_n \))
  - by numerical methods \( c_i = \frac{\Delta y}{\Delta x_i} \)
  - experimentally by changing \( x_i \) by \( \Delta x_i \) and determining \( \Delta y \);
    \( c_i = \frac{\Delta y}{\Delta x_i} \)

- The contribution of \( u(x_i) \) to the uncertainty of \( y \) is:
  \( u_i(y) = c_i u(x_i) \)
Step4: Correlation

The covariance \( u(x_i, x_j) \) of two random variables is a measure of their mutual dependence.

If \( X_i = F(Q_l) \) and \( X_j = G(Q_l) \) depend on the same quantities \( Q_l \) (\( l=1..n \)) then

\[
    u(x_i, x_j) = \sum_i \frac{\partial F}{\partial q_l} \frac{\partial G}{\partial q_l} u^2(q_i)
\]

- Correlation coefficient :
  \[
  r(x_i, x_j) = \frac{u(x_i, x_j)}{u(x_i)u(x_j)}
  \]

The covariance can increase or decrease uncertainty.

If the correlation coefficient is \( r=1 \) the components will be added in a linear way.
Step 5: Combining the uncertainty components

- Uncorrelated input quantities:

\[ u_c(y) = \sqrt{\sum_{i=1}^{N} u_i^2(y_i)} = \sqrt{\sum_{i=1}^{N} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i)} \]

- Correlated input quantities:

\[ u_c(y) = \sqrt{\sum_{i=1}^{N} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j)} \]

\( u_c(y) = \text{combined standard uncertainty}; \quad u(x_i, x_j) = \text{covariance} \)
Step 6: Expanded uncertainty

Often the result of the measurement is reported with a higher level of confidence than given by the standard uncertainty.

- Expanded uncertainty $U$ is the standard uncertainty multiplied by a coverage factor $k$:

$$U = ku_c(y)$$

- In calibration it is recommended to report 95 % level of confidence.
- For normal distribution this corresponds to $k=2$ (approximately).

<table>
<thead>
<tr>
<th>Coverage probability $p$</th>
<th>Coverage factor $k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>68,27 %</td>
<td>1,00</td>
</tr>
<tr>
<td>90 %</td>
<td>1,65</td>
</tr>
<tr>
<td>95 %</td>
<td>1,96</td>
</tr>
<tr>
<td>95,45%</td>
<td>2,00</td>
</tr>
<tr>
<td>99 %</td>
<td>2,58</td>
</tr>
<tr>
<td>99,73%</td>
<td>3,00</td>
</tr>
</tbody>
</table>
Measurement result is approximately normally distributed if
- it is a combination of several random variables (independent of distribution)
- none of the (non-normally distributed) components is dominating.
Degrees of freedom and the coverage factor

• For a combined standard uncertainty, we can calculate the effective number of degrees of freedom ($\nu_{\text{eff}}$):

$$\nu_{\text{eff}} = \frac{\sum_{i=1}^{N} u_i^4(x_i)}{u(y)^4}$$

• The figure shows that we need a coverage factor larger than 2 to obtain 95 % confidence level if the number of degrees of freedom is small.
4.2 Uncertainty calculation in practice
Example: Measurement of SO$_2$ content

- An analyzer with electrical current signal output was used for measuring SO$_2$ content in exhaust gas.
- The signal was measured with a DMM and the total error in the current measurement was estimated to be within ±0,1 mA.
- The arithmetic mean of the 15 recorded DMM readings is 9,59 mA and the corresponding standard deviation is 0,49 mA.
- An accredited laboratory has determined the calibration function for the analyzer:
  \[ f_c (I_m) = -7,64 \text{ mg/m}^3 + 3,25 \frac{\text{mg/m}^3}{\text{mA}} \cdot I_m \]
  The reported expanded uncertainty \((k=2)\) is 6 mg/m$^3$
- When comparing two last calibrations, we can conclude that the drift of the analyzer is less than 5 mg/m$^3$/year (calibr. interval is 1 year)
Example: Measurement of SO₂ content - continuing

- The measurement result is calculated as follows:

\[ C_{SO2} = f_c(I_m + \delta I_m) + \delta f_c + \delta_{Drift} \]

\[ = -7.64 \text{ mg/m}^3 + 3.25 \frac{\text{mg/m}^3}{\text{mA}} \cdot (I_m + \delta I_m) + \delta f_c + \delta_{Drift} \]

- The variables can be assumed independent on each other; therefore we can calculate the uncertainty:

\[ u(C_{SO2}) = \sqrt{[c_1 u(I_m)]^2 + [c_2 u(\delta I_m)]^2 + [c_3 u(\delta f_c)]^2 + [c_4 u(\delta_{Drift})]^2} \]
Example: Measurement of SO$_2$ content - continuing

- The sensitivity coefficients are:

\[
c_1 = \frac{\partial C_{SO_2}}{\partial I_m} = 3.25 \text{ mg/m}^3 \text{ mA}^{-1}
\]

\[
c_2 = \frac{\partial C_{SO_2}}{\partial \delta I_m} = c_1
\]

\[
c_3 = \frac{\partial C_{SO_2}}{\partial \delta f_c} = c_4 = \frac{\partial C_{SO_2}}{\partial \delta_{Drift}} = 1
\]

- Thus:

\[
u(C_{SO_2}) = \sqrt{c_1^2 [u^2 (I_m) + u^2 (\delta I_m)] + u^2 (\delta f_c) + u^2 (\delta_{Drift})}
\]
Example: Measurement of SO$_2$ content - continuing

- Standard uncertainties of the components:

  \[ u(I_m) = 0.49 \text{ mA} \text{ type A, normal distribution} \]

  \[ u(\delta I_m) = \frac{0.1 \text{ mA}}{\sqrt{3}} = 0.06 \text{ mA} \text{ type B, rectangular distribution} \]

  \[ u(\delta f_c) = \frac{6 \text{ mg/m}^3}{2} = 3 \text{ mg/m}^3 \text{ type B, normal distribution} \]

  \[ u(\delta_{Drift}) = \frac{5 \text{ mg/m}^3}{\sqrt{3}} = 2.9 \text{ mg/m}^3 \text{ type B, rectangular distribution} \]
Example: Measurement of SO$_2$ content - continuing

• Estimate for the SO$_2$ content:

\[
C_{SO_2} = -7,64 \text{ mg/m}^3 + 3,25 \frac{\text{mg/m}^3}{\text{mA}} \cdot (9,59 \text{ mA} + 0 \text{ mA}) + 0 \text{ mg/m}^3 + 0 \text{ mg/m}^3
\]

\[
= 23,5 \text{ mg/m}^3
\]

• and its combined standard uncertainty:

\[
\begin{aligned}
& \begin{aligned}
& u(C_{SO_2}) = \sqrt{\left(3,25 \frac{\text{mg/m}^3}{\text{mA}}\right)^2 \left[0,49 \text{ mA}^2 + 0,06 \text{ mA}^2\right] + (3 \text{ mg/m}^3)^2 + (2,9 \text{ mg/m}^3)^2}
\end{aligned}
\end{aligned}
\]

\[
= 4,5 \text{ mg/m}^3
\]
Example: Measurement of $\text{SO}_2$ content - continuing

• Thus the expanded uncertainty at about 95 % confidence level ($k = 2$) is:

$$U = k \times u = 2 \times 4,5 \text{ mg/m}^3 = 9,0 \text{ mg/m}^3$$

• As a conclusion, the measurement result is:

$$C_{\text{SO}_2} = (24 \pm 9) \text{ mg/m}^3$$
References and literature


Literature about estimating uncertainty:

- UKAS M3003, The Expression of Uncertainty and Confidence in Measurement
- S. A. Bell, A beginner’s guide to uncertainty in measurement, Measurement Good Practice Guide No. 11, (Issue 2), National Physical Laboratory 2001, 41 p. (www.npl.co.uk)

MIKES has published several guides in Finnish on the uncertainty estimations in different fields.