LAB QUALITY INTERNATIONAL

Eurachem
A focus for analytical chemistry in Europe

The use of Decision Rules

Presentation at

A two-day training course

ACCREDITATION OF ANALYTICAL, MICROBIOLOGICAL AND MEDICAL LABORATORIES - ISO/IEC 17025:2017 AND ISO 15189:2012

20 - 21 February 2020 in Nicosia, Cyprus

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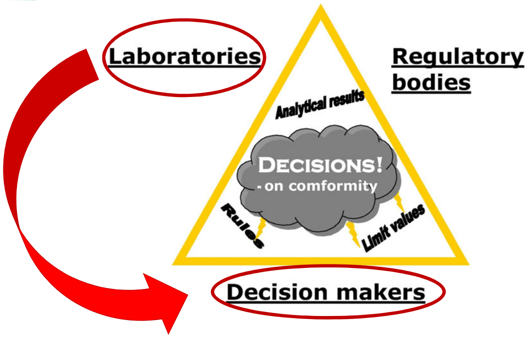
Analytical results for decisions!



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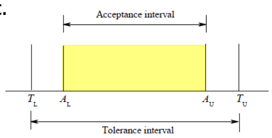
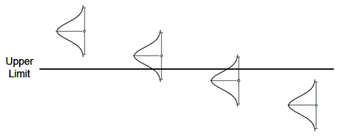
Testing for Conformity Assessment

- Laboratories often do testing as part of a conformity assessment
  - Measuring whether a parameter is within tolerance limits
  - Testing whether content of a sample is in accordance with specifications ...etc.
- Conformity vs. Non-Conformity
  - Compliance vs. Non-Compliance
  - Acceptance vs. Rejection
  - Pass vs. Fail
- Decisions not alway straightforward





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2017 version of ISO/IEC 17025 requirement

- In paragraph 7.1 on agreements with client:
  - *When the customer requests a statement of conformity to a specification or standard for the test or calibration (e.g. pass/fail, in-tolerance/out-of-tolerance), the specification or standard and the decision rule shall be clearly defined. Unless inherent in the requested specification or standard, the decision rule selected shall be communicated to, and agreed with, the customer.* [7.1.3]
- ..and in paragraph 7.8 on reporting of results:
  - *When a statement of conformity to a specification or standard is provided, the laboratory shall document the decision rule employed, taking into account the level of risk (such as false accept and false reject and statistical assumptions) associated with the decision rule employed, and apply the decision rule.* [7.8.6.1]

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Risk of making wrong decisions

- Many deciscions made on the basis of some tests and measurements
- BUT tests & measurements do not provide a 100% sure basis for making the correct decison
  - Tests/measurements only (!) made on a sample from the material/items for which the decision must be made.
  - There is a measurement uncertainty to the result of the test /measurement
  - The decision may be biased if somebody have a special interest in the outcome of the decision
- There will always be a RISK of making a wrong decision

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Errors and risks

- **Errors** are always made during measurements and tests
  - Systematic errors ⇨ Biased results (…to be dealt with!)
  - Random errors ⇨ Measurement uncertainty
- These errors leads to **the risk of making errors** when the results are used as **basis for decisions**

… even <u>two types</u> of errors:

- **<u>Type I</u>**: Deciding that something is NOT OK – when it really is OK. - given the probability (risk): **α**
- **<u>Type II</u>** : Deciding something is OK – when it really was NOT - given the probability (risk): **β**

	Decision	
Actual situation	Accept H_0	Reject H_0
H_0 (True)	Correct decision	**Type I Error**
H_0 (False)	**Type II Error**	Correct decision

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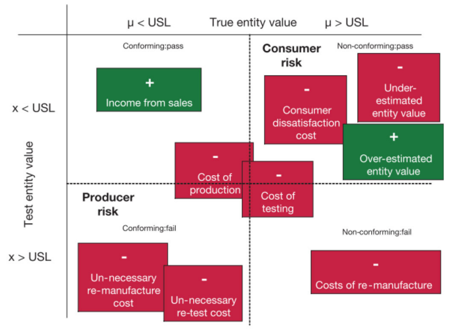
Consequenses of taking a risk

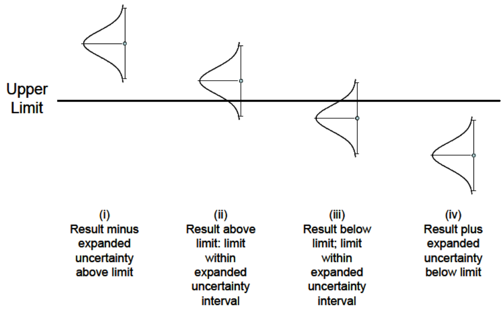


- Buyer's / Seller's risk (consequences from Seller's point of view)

LAB QUALITY INTERNATIONAL (Ref.: EUROLAB Techn. Rep. No. 01/2017, *Decision rules applied to conformity assessment*)

The "dilemma"

- The content of a pollutant must not exceed an upper limit



- What to decide in situation II and III ?

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The "dilemma"

- In case (ii) there is a high probability that the value of the measurand is above the limit, but the limit is nonetheless within the expanded uncertainty interval.
- Depending on the circumstances,
  - and **particularly on the risks associated with making a wrong decision**,
  - the probability of an incorrect decision may be or may not be sufficiently small to justify a decision of non-compliance.
- Similarly, in case (iii) in relation to justifying compliance.
- **Without further information**, which has to be based on the risks associated with making a wrong decision**, it is not possible to use these two results to make a decision on compliance.**

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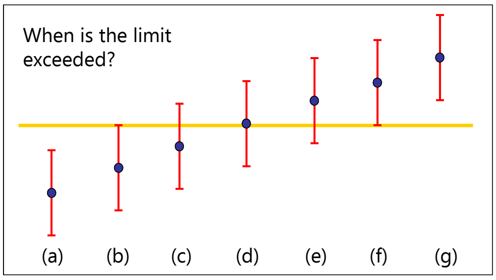
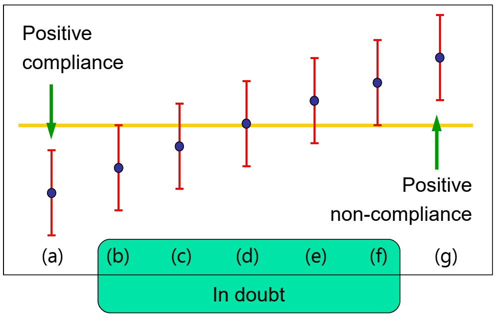
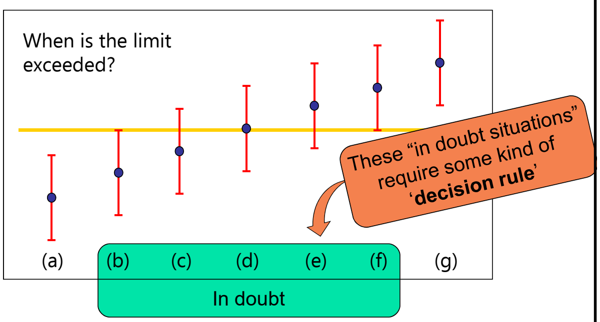
MU influences the interpretation of a result



Typical (simple) guidance



How does Measurement Uncertainty affect interpretation?



Decision rules

- The key to the assessment of compliance is the concept of "**Decision rules**".
  - These rules give a prescription for the acceptance or rejection of a product based on the
    - measurement result,
    - its uncertainty and
    - the specification limit or limits,

    …taking into account the acceptable level of the probability of making a wrong decision.
- And it has become a requirement in the 2017 version of ISO/IEC 17025!

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What do we need for a decision ?

1. A **measurand** clearly specified
   A specification of the **measurement object/test item** (part of measurand)
2. A **test result**
   (normally assuming normal distribution of test results)
3. A **measurement uncertainty**
   For an expanded uncertainty the *k* factor and the corresponding confidence level should be stated e.g. *k* = 2 for 95 % confidence
4. A **specification** giving **upper and/or lower limits**
5. A **decision rule**
   This rule can decide to *take* or *not to take* measurement uncertainty into account
   - AND it can include the **risk** of making a wrong decision, which the involved parts are willing to take

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Decision rule

- Definitions
  - Documented rule that describes how measurement uncertainty will be accounted for with regard to accepting or rejecting an item, given a specified requirement and the result of a measurement
    [Re. ISO Guide 98-4 = JCGM 106]
  - A documented rule that describes how measurement uncertainty will be allocated with regard to accepting or rejecting a product according to its specification and the result of a measurement.
    [Re. Eurachem Guide on Compliance assessment]
  - Rule that describes how measurement uncertainty is accounted for when stating conformity with a specified requirement
    [Re. ISO/IEC 17025:2017]

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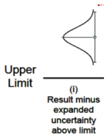
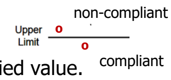
Simple decision rules

- Decision rules may be very simple:
  - A result implies non-compliance with an upper limit if the measured value exceeds the limit by the expanded uncertainty.
  - A result equal to or above the upper limit implies non-compliance and a result below the limit implies compliance -provided that uncertainty is below a specified value. This is normally used where the **uncertainty** is so **small compared with the limit** that the risk of making a wrong decision is acceptable.
  - BUT to use such a rule without specifying the maximum permitted value of the uncertainty would mean that **the probability (risk) of making a wrong decision would not be known**.





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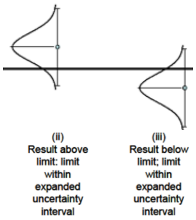
More complicated rules

- What about situation II and III?



- Depending on the actual situation the rules may include - e.g.
  - A request for additional measurement(s)
  - A manufactured (and tested) product must be compared with an alternative specification to decide on possible sale at a different price.

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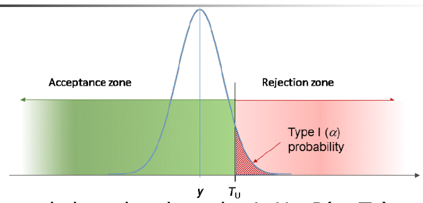
Use of the statistical distribution



- Decision rule based on hypothesis H_0: $P(y \leq T_U) \geq (1-\alpha)$
  - where α is the acceptable risk for false rejection
- A comformance probability P_C is calculated based on the normal cumulative distribution (Φ):

$$P_C = P(\eta \leq T_U) = \Phi((T_U - y)/u(y))$$

(where η is a variable describing possible values of a measurand Y)

NOTE: Φ in Excel: NORM.DIST(T_U; y; u(y); TRUE)

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Use of the statistical distribution - Example 1

- Consider a measurement estimate y = 2,7 mm with a standard uncertainty of u(y) = 0,2 mm, a single tolerance upper limit of T_U = 3,0 mm, and a specification of conformity (1 - α) of 0,95 (95 %), thus assuming a type I error α = 0,05 (5 %).
- Normal distribution assumed.
- Decision rule:
  Acceptance if the hypothesis H_0: P(y≤3,0 mm)≥0,95 is true.
- Calculation of P_C :

$$P_C = \Phi((3{,}0-2{,}7)/0{,}2) = \Phi(1{,}5) \Leftrightarrow$$

$$P_C = 0{,}933 \approx 93{,}3\%$$

(NORM.DIST(3,0; 2,7; 0,2; 0,2; TRUE) - or look up 0,15 in cum. norm. distr. table)

- As 93,3% < 95% the H_0 is rejected and the **the sample is declared Non-compliant** with the tolerance.
  - Having a risk of α = 6,7% of false rejection

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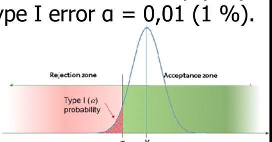
Use of the statistical distribution - Example 2

- Consider a measurement estimate y = 0,012 g with a standard uncertainty of u(y) = 0,001 g, a single tolerance lower limit of T_L = 0,010 g, and a specification of conformity (1-α) of 0,99 (99 %) thus assuming a type I error α = 0,01 (1 %).
- Decision rule:
  Acceptance if the hypothesis H_0:
  P(y≥0,010g)≥0,99 is true.



- Calculation of P_C :
  P_C = 1- Φ((0,01-0,012)/0,001) = Φ((0,012-0,01)/0,001) = Φ(2,0)
  ⇔ P_C = 0,977 ≈ 97,7%
- As 97,7% < 99% the H_0 is rejected and the the sample is **declared Non-compliant** with the tolerance.
  - Having a risk of α = 2,3% of false rejection
    (..and only 1% was acceptable; conforming if 5% had been acceptable)

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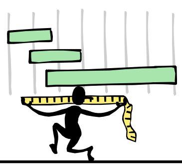
Use of Acceptance/Rejection Zones

- On the basis of the Decision rules we can determine …
  - An "**Acceptance zone**"
  - If the result lies here, the sample/product is declared **compliant**

  and
  - A "**Rejection zone**"
  - If the result lies here it is declared **non-compliant.**



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Use of "Guard Bands"

- Decision rule for non-compliance or rejection with **low risk of false rejection** (high confidence of correct rejection).
- A rejection zone can be defined as starting from the specification limit L plus an amount g - the **Guard band**. (see figure, case a)
- The value of g is chosen so that for a measurement result greater than or equal to L+ g the **probability of false rejection** is less than or equal to **α – the accepted risk**;
- The Guard Band, g, can also be chosen to provide **low risk of false acceptance** (case b)

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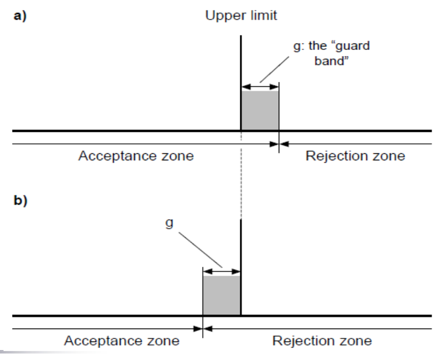
Guard bands!!



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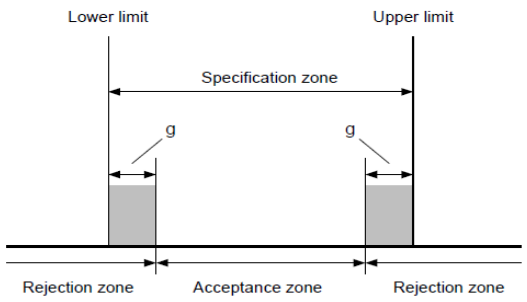
Double Guard bands!!



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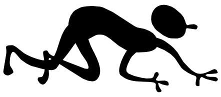
Establishing the Guard Band

- In general, g will be **a multiplum of the standard uncertainty u.**
  - For the case where the distribution of the likely values of the measurand is approximately normal, a value of 1.64u will give a risk, α, of 5% and a value of 2.33u implies a risk, α, of 1%.
  - I.e. the "one-tailed" t-factor on 5% or 1% level
- In some cases the decision rule may state the value of the multiplum to be used.
- In specific cases the guard band will **depend upon the acceptable risk-value α** and the **knowledge about the distribution** of the likely values of the measurand



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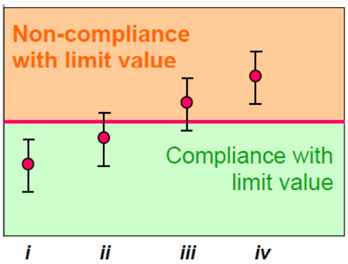
Use of Guard Bands - Examples

- Based on the "classical picture":



- Test results with expanded uncertainty in relation to an upper limit

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Use of Guard Bands - Example 1

- Case *ii* in the figure with an upper limit
  - and a decision rule focusing on **correct acceptance**
  - Sludge from water purification plants can be used for soil improvement. One of the toxic metals that can be a problem is cadmium. The upper limit on the total cadmium in sludge is set to 2 mg/kg.
- The following requirements for decision in place:
  - **Measurand:** Mass fraction of cadmium, Cd, in a consignment delivered to a customer
  - **Analytical result:** Mass fraction (Cd) = 1.82 mg/kg
  - **Uncertainty:** U = 0.20 mg/kg, k=2 (95 %).
    Standard uncertainty, u = 0.10 mg/kg. The uncertainty includes both sampling and analytical uncertainty
  - **Specification:** Upper permitted limit 2.0 mg/kg

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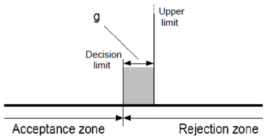
Example 1 (cont'd)

- **Decision rule:** *The decision limit is the mass fraction where it can be decided with a confidence level of approximately 95 % (α=0.05) that the batch has a mass fraction below the upper limit.*
- **The guard band** is calculated as 1.65·*u* = 0.165 mg/kg (*k* value 1.65 for one tailed t value at 95 % confidence).
  The decision limit will be 2 – 0.165 =1.84 mg/kg.
  All values below this value are in the acceptance zone.
  All values equal to or over are in the rejection zone



The sludge sample meets the compliance requirements.

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Use of Guard Bands - Example 2

- Case *iii in the figure with* an upper limit
  - and a decision rule focusing on **correct rejection**
  - In law it is important not to punish an innocent person. The decision limit can be set to reduce the chance of this happening. This is an example from measurement of blood alcohol (EtOH) in a sample taken from a driver in Sweden who tested positive in a screening test.
- The following requirements for decision in place:
  - **Measurand:** Mass fraction of total EtOH in a blood sample as delivered to the laboratory
  - **Analytical result:** Mass fraction (EtOH) = 0.221 mg/g
  - **Uncertainty:** U = 0.013 mg/g, k=2 (95 %).
    Standard uncertainty, u, 0.0065. This uncertainty includes both sampling and analytical uncertainty.

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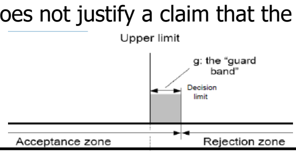
Example 2 (cont'd)

- **Regulation:** Upper permitted limit 0.200 mg/g
- **Decision rule:** *The decision limit is the mass fraction above which it can be decided with a confidence level of approximately 99.9 % (α=0.001) that the permitted limit has been truly exceeded.*
- **The guard band** is calculated as 3.10u = 0.020 mg/g - (*k* value 3.10 for one tailed t-value at 99.9 % confidence).
  The decision limit will be 0.200 + 0.020 = 0.220 mg/g.
  All values below this value are in the acceptance zone (i.e. acceptance that the result does not justify a claim that the limit has been exceeded).
  All values equal to or over are in the rejection zone



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Use of Guard Bands - Example 3

- ✓ Case ii in the figure
  - with a lower and upper limit and a decision rule focusing on **correct acceptance**
  - In steel production, the nickel content for a type of stainless steel must be in the range from 16.0 to 18.0 % w/w.
- ✓ The following requirements for decision in place:
  - **Measurand:** Mass fraction of nickel, Ni in a batch of steel delivered to a customer
  - **Analytical result:** Mass fraction (Ni)= 16.1 %
  - **Uncertainty:** U = 0.2 % weight % Ni, k=2 (95 %). Standard uncertainty, u, 0.1 %. This uncertainty includes both sampling and analytical uncertainty.
  - **Specification:** Lower permitted limit 16.0 %. Upper permitted limit 18.0 %.

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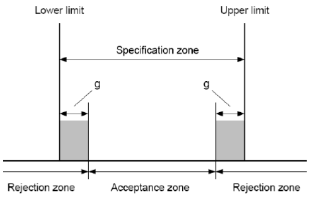
Example 3 (cont'd)

- ✓ **Decision rule:** *The decision limit is the mass fraction where it can be decided with a confidence level of approximately 95 % (α=0.05) that the batch has a mass fraction above the lower limit and below the upper limit.*
- ✓ **Each guard band** is calculated as $1.65 \cdot u = 0.17$ % (k value 1.65 for one tailed test at 95 % confidence). Decision limits will be 16.17 % and 17.83 %. All values between these values are in the acceptance zone



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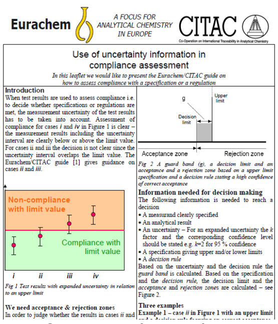
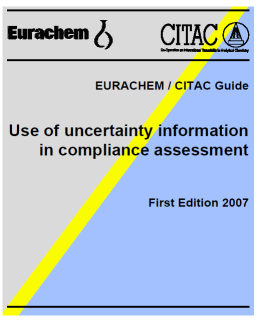
Eurachem guidance

- ✓ Leaflet:



.... referring to the guide ⇨

- ✓ Guide:



...under revision

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References

- ISO/IEC Guide 98-4, "*Uncertainty of measurement - Part 4: Role of measurement uncertainty in conformity assessment*", 1st ed., 2012 (= JCGM 106:2012)
- EUROLAB Technical Report No. 01/ 2017, "*Decision rules applied to conformity assessment*"
- Eurachem Leaflet, "*Use of uncertainty information in compliance assessment*" (2007)
- Eurachem Guide, "*Use of uncertainty information in compliance assessment*", 1st ed., 2007 (Under revision 2020)

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