Measurement uncertainty and conformity assessment in analytical measurement – Considerations for the university curriculum

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Introduction

• Many analyses are carried out to check compliance with a specification or regulation
• Necessary to take into account the measurement uncertainty when assessing compliance

• What do we need to know?
• What do we need to understand?
Basic use of limits

Upper control limit

• Function
  – Safety regulation
  – Environmental regulation
  – Manufacturing control
  – Product specification

• Origin
  – Risk assessment
  – Epidemiology
  – Toxicology
  – Economics ...

Why is this here?

Basic use of limits

Upper control limit

(i) Result above limit
(ii) Result above limit
(iii) Result at limit
(iv) Result below limit
(v) Result below limit

Need additional information to deal with case (iii)
Basic guidance

Upper control limit

- (i) Result above limit
- (ii) Result above limit but within uncertainty
- (iii) Result at limit and within uncertainty
- (iv) Result below limit but within uncertainty
- (v) Result below limit

Need additional information to deal with cases (ii) - (iv)

Consistent decisions need rules
ISO/IEC 17025:2017

• Decision rule:
  “rule that describes how measurement uncertainty is accounted for when stating conformity with a specified requirement”

• §7.1.3: “When the customer requests a statement of conformity…the decision rule shall be clearly defined.”

Example of a decision rule

• A result equal to or above the upper limit implies non-compliance
  – result below the limit implies compliance
  
  “Simple acceptance”

• IF uncertainty is below a specified value
  – e.g. uncertainty is small compared with the limit
  • THEN the risk of making a wrong decision is acceptable
Concepts so far

• Limits
  – Function (regulation, control...)
  – Setting (how limits are decided)

• Interpretation
  – Comparison
  – “Borderline” cases
  – Measurement uncertainty
  – Expanded uncertainty
  – The idea of “decision rules”
    • Including action on borderline cases

Probability
Probability of compliance

* Strictly, for an observed value, this should be interpreted as a posterior probability

Concepts so far

• Limits
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  – Setting (how limits are decided)
• Interpretation
  – Comparison
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  – Measurement uncertainty
  – Expanded uncertainty
  – The idea of “decision rules”

• Probability distributions
• Uncertainty as a distribution
• Probability of compliance
Improving probability of compliance

Compliance probability 95%

Revised acceptance limit

A “Guard band”

Decision rules & guard bands

a) Upper limit

g: the “guard band”

e.g. U or 2u

Acceptance zone

Rejection zone

“Relaxed acceptance” (test for non-conformity)

b) Acceptance zone

Rejection zone

“Stringent acceptance” (test for conformity)
Decision rules can control probabilities of false decisions

Concepts so far

• **Limits**
  – Function (regulation, control...)
  – Setting (how limits are decided)

• **Interpretation**
  – Comparison
  – “Borderline” cases
  – Measurement uncertainty
  – Expanded uncertainty
  – The idea of “decision rules”

• **Probability distributions**

• **Uncertainty as a distribution**

• **Guard bands**
  – and effect on false acceptance

• **Probability of compliance**
False acceptance and rejection rates – Consumer and producer risk

Producer and consumer risk

Distribution of results

UPPER LIMIT

False rejection rate

Producer risk

Compliant true value

Consumer risk

False acceptance rate

NON - compliant true value
Concepts so far

- **Limits**
  - Function (regulation, control...)
  - Setting (how limits are decided)
- **Interpretation**
  - Comparison
  - “Borderline” cases
  - Measurement uncertainty
  - Expanded uncertainty
  - The idea of “decision rules”

- **Probability distributions**
- **Uncertainty as a distribution**
- **Guard bands**
- **Probability of compliance**
- **Producer & consumer risk**

Reducing risk – Test/Uncertainty ratio

- **Process distribution**
  - Compliant product
  - Non-compliant product
  - False acceptance rate for this noncompliant value
- **Non-compliant item**
Reducing risk – Test/Uncertainty ratio

\[ \text{TUR} = \frac{L_u - L_l}{U} \]

TUR ≥ 3 recommended

Concepts so far

• **Limits**
  – Function (regulation, control...)
  – Setting (how limits are decided)

• **Interpretation**
  – Comparison
  – “Borderline” cases
  – Measurement uncertainty
  – Expanded uncertainty
  – The idea of “decision rules”

• **Probability distributions**

• **Uncertainty as a distribution**

• **(Conditional) Probability of compliance**

• **Guard bands**

• **Producer & consumer risk**

• **The process distribution**

• **Test uncertainty ratio (TUR)**
Calculating Consumer and Producer risk

Principle of risk calculation - consumer risk

Process distribution

Compliant product

Non-compliant product

Result distributions for non-compliant product

False acceptance rate for this true value*

*Also sometimes called a “specific risk”
**Principle of risk calculation - consumer risk**

- **Compliant product**
  - Process distribution
  - $f(x_i)$
  - $P_{a,i}$

- **Non-compliant product**

'Global' consumer risk is the sum of 'specific' consumer risks $P_{a,i}$ (acceptance rates) over all possible noncompliant values, multiplied by their likelihood of occurrence $f(x_i)$.

In integral form:

$$\int_{-\infty}^{L_l} P_{a,i} f(x_i) dx + \int_{L_l}^{\infty} P_{a,i} f(x_i) dx$$
Consumer risk for a good process

Process distribution

Compliant product

\[ f(x_i) \]

\[ P_{a,i} \]

\[ \int_{-\infty}^{L_l} P_{a,i} f(x_i) dx + \int_{L_u}^{\infty} P_{a,i} f(x_i) dx \]

In integral form:

A narrow process distribution delivers smaller risks of false acceptance
Concepts so far

• Limits
  – Function (regulation, control...)
  – Setting (how limits are decided)
• Interpretation
  – Comparison
  – “Borderline” cases
  – Measurement uncertainty
  – Expanded uncertainty
  – The idea of “decision rules”
• Probability distributions
• Uncertainty as a distribution
• Guard bands
• Probability of compliance
• Producer & consumer risk
• Specific risk
• The process distribution
• Test uncertainty ratio (TUR)
• Integration to obtain ‘global’ risks

Additional technical problems

• Multiple observations in compliance assessment
  – Replicate measurements on sampled items
  – Repeated results for borderline or failed product
  – Decision can be on an average, all results, or a proportion, within acceptable limits
• Multivariate conformity assessment
  – Products are subject to multiple requirements
  – Measurements may be correlated
• Non-normality
  – Of process or uncertainty distributions
Non-normal processes

• Example*: Total suspended particulate matter in air near a quarry
  – 220 observations
  – Line shows lognormal distribution

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EURAMET Project EMUE, Example A.1.2.3

Concepts for conformity assessment with uncertainty

• Limits
  – Function (regulation, control...)
  – Setting (how limits are decided)

• Interpretation
  – Comparison
  – “Borderline” cases
  – Measurement uncertainty
  – Expanded uncertainty as an interval
  – The idea of “decision rules”
  – Using replicate or repeated results

• Probability distributions
• Uncertainty as a distribution
• Guard bands
• Test uncertainty ratio (TUR)
• The process distribution

Useful

• Probability of compliance
• Producer & consumer risk
• Specific risk
• Integration for ‘global’ risks
• Non-normality
• Multivariate conformity

Basic

Advanced
Summary

• Conformity assessment with measurement uncertainty can be a complex topic

• A basic understanding of limits, decision rules and measurement uncertainty (as an interval) is essential

• A comprehensive understanding is likely to require extended statistical training or qualifications

Further reading

• Use of uncertainty information in compliance assessment (Eurachem/CITAC Guide)
  – www.eurachem.org

• ILAC G8: Guidelines on Decision Rules and Statements of Conformity
  – ilac.org/publications-and-resources/ilac-guidance-series/

• JCGM 106:2012 Evaluation of measurement data – The role of measurement uncertainty in conformity assessment