Use of uncertainty information in compliance assessment

In this leaflet we present the Eurachem/CITAC guide on how to assess compliance with a specification or a regulation.

Introduction
When test results are used to assess compliance i.e. to decide whether specifications or regulations are met, the measurement uncertainty of the test results has to be taken into account. Assessment of compliance for cases i and iv in Figure 1 is clear – the measurement results including the uncertainty interval are clearly below or above the limit value. For cases ii and iii the decision is not clear since the uncertainty interval overlaps the limit value. The Eurachem/CITAC guide [1] gives guidance on cases ii and iii.

Fig 1 Test results with expanded uncertainty in relation to an upper limit

We need acceptance & rejection zones
In order to judge whether the results in cases ii and iii comply with the limit value we need a decision rule, based on the risks associated with making a wrong decision. This decision rule enables a guard band, g to be calculated (see Figure 2) which defines an acceptance zone and a rejection zone. If the measurement result is within the acceptance zone the specifications are met and we can assess compliance. If the measurement result is in the rejection zone we can assess non compliance. The intersection between these two zones is called the decision limit, see Figure 2. The guard band is chosen so that for a measurement in the acceptance zone the probability of false acceptance/rejection is less than or equal to a defined confidence value α.

Information needed for decision making
The following information is needed to reach a decision
• A measurand clearly specified
• An analytical result
• An uncertainty – For an expanded uncertainty the k factor and the corresponding confidence level should be stated e.g. k = 2 for 95 % confidence
• A specification giving upper and/or lower limits
• A decision rule

Based on the uncertainty and the decision rule the guard band is calculated. Based on the specification and the decision rule, the decision limit and the acceptance and rejection zones are calculated – see Figure 2.

Three examples
Example 1 – case ii in Figure 1 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.
• 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
Example 1 cont.
- Decision rule - \( \text{The decision limit is the mass fraction where it can be decided with a confidence level of approximately } 95\%\ (\alpha = 0.05) \) that the batch has a mass fraction below the upper limit.

- The guard band is calculated as \( 1.65u = 0.165 \text{ mg/kg} \) - (case 1 in the guide [1] with \( k \) 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 above are in the rejection zone – see Figure 2. The sludge sample meets the compliance requirements.

Example 2 – case iii in Figure 1 - 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. Here 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.

- 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 – \( U = 0.013 \text{ mg/g}, k = 2 \) (95\%). Standard uncertainty, \( u = 0.0065 \text{ mg/g} \) [1]. This uncertainty includes both sampling and analytical uncertainty.
- Regulation – Upper permitted limit 0.200 mg/g
- Decision rule - \( \text{The decision limit is the mass fraction above which it can be decided with a confidence level of approximately } 99.9\%\ (\alpha = 0.001) \) that the permitted limit has been truly exceeded.

- The guard band is calculated as \( 3.10u = 0.020 \text{ mg/g} \) - (case 1b in the guide [1] with \( k \) value 3.10 for one tailed \( t \) value at 95\% confidence). The decision limit will be \( 0.200 + 0.020 = 0.220 \text{ mg/g} \). 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 above are in the rejection zone – see Figure 3.

Example 3 – case ii in Figure 1 - with a lower and an 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.

- Measurand – Mass fraction of nickel, Ni in a batch of steel delivered to a customer
- Analytical result - mass fraction (Ni) = 16.1 %
- Uncertainty – \( U = 0.2 \% \text{ weight \% Ni}, k = 2 \) (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 %.
- Decision rule – \( \text{The decision limit is the mass fraction where it can be decided with a confidence level of approximately } 95\%\ (\alpha = 0.05) \) that the batch has a mass fraction above the lower limit and below the upper limit.

- Each guard band is calculated as \( 1.65u = 0.17 \% \) (case 1b in the guide [1] with \( k \) value 1.65 for one tailed \( t \) value at 95\% confidence). Decision limits will be 16.17 \% and 17.83 \%. All values between these values are in the acceptance zone – see Figure 4.

Fig 3 - A guard band (g), a decision limit and an acceptance and a rejection zone based on a upper specification and a decision rule stating a high confidence of correct rejection

Fig 4 - Guard bands (g), decision limits and an acceptance and two rejection zones estimated from a specification with lower and upper limit and a decision rule stating a high confidence of correct acceptance

\[1\] Eurachem/CITAC Guide Use of uncertainty in compliance assessment, 2007 [www.eurachem.org]