



Decision making – what more do we need than the analytical result?

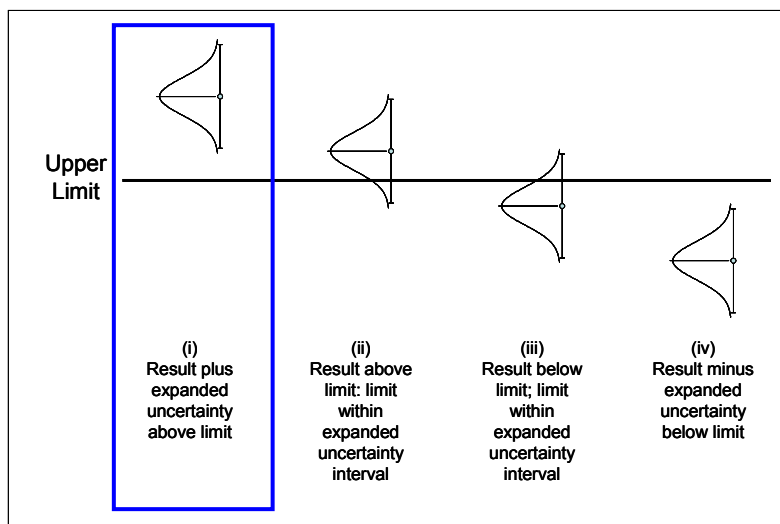
Uncertainty for compliance assessment

Eurachem Workshop
25-26 May 2010



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Result and uncertainty and limit

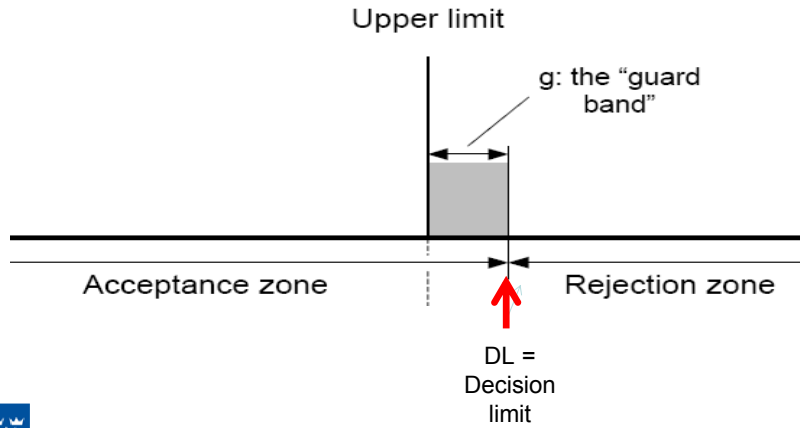


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We also need a decision limit calculated from a guard band



Lets us take an example of blood alcohol & Swedish legislation

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Example – upper permitted limit

Blood alcohol

Sample taken from a driver in Sweden and
analysed at a laboratory

Analytical Report

Concentration of ethanol in blood sample is
0,221 mg/g ± 0,013 (k=2)

**Limit is 0,200 mg/g
(20 mg/100g)
Will this driver be punished?**

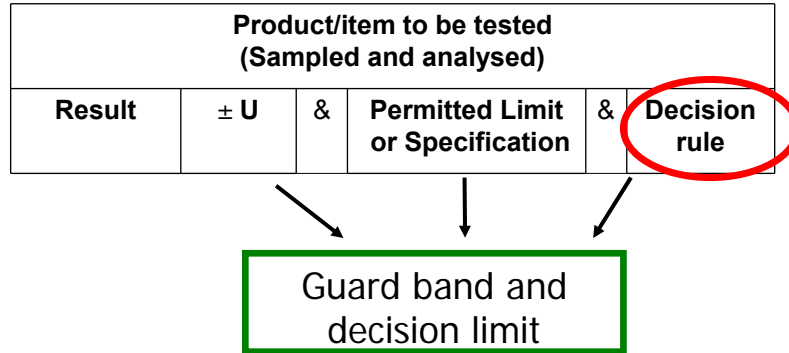


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Using a decision rule we calculate a guard band and the decision limit



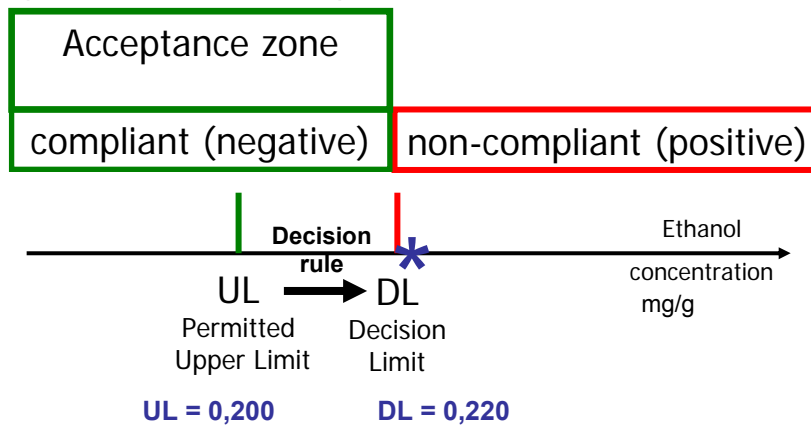
Comment: For most decision rules acceptance zone is calculated from the limit. NOT from the results – important when we have relative uncertainty



Blood alcohol - the calculated decision limit

if the measurement result lies in the acceptance zone the product is declared compliant

* Blood alcohol Measurement result 0,221 mg/g

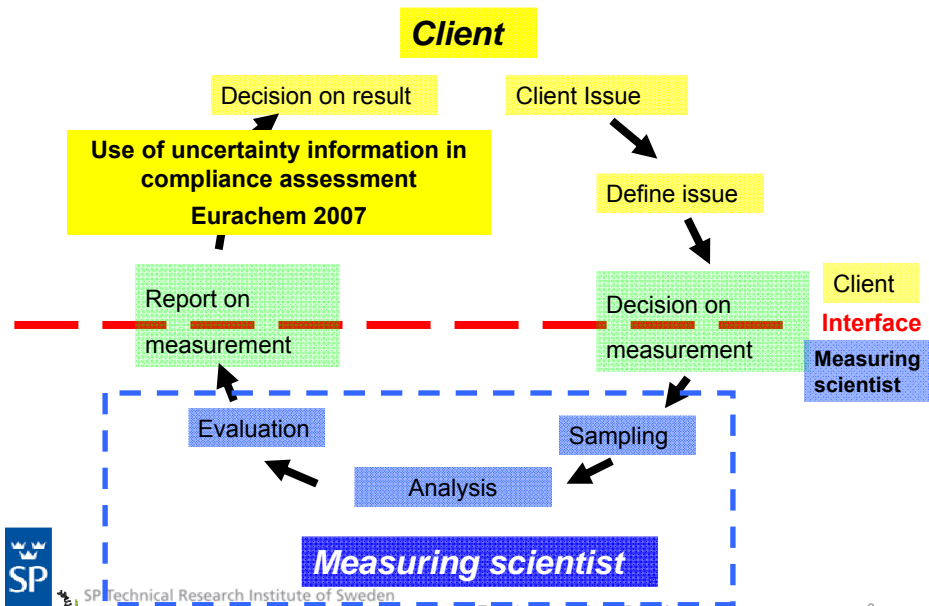


CONTENT

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- Measurement cycle
- What we need for decision making
 - Measurand
 - Decision rule
- Example of a decision rule and compliance assessment
- Blood alcohol example in detail – legal application
- Decision rule in EU directive
- Terminology in decision making
- Summary



Measurement cycle



What do we need for the decision making?

1. A measurand clearly specified
2. A specification of the **measurement object/test item** (part of measurand)
3. An analytical result
4. An uncertainty – For an expanded uncertainty the k factor and the corresponding confidence level should be stated e.g. $k = 2$ for 95 % confidence
5. A specification giving upper and/or lower limits
6. A *decision rule* - This rule can decide to *take* or *not to take* measurement uncertainty into account



Specification of measurand (VIM3*)

Measurand - **quantity** intended to be measured

NOTE 1 The specification of a measurand requires knowledge of the

- kind of quantity
- description of the state of the phenomenon, body, or substance carrying the quantity including any relevant component,
- the chemical entities involved.

← **Measurement object/test item**

Example of a measurand specification

mass fraction of total Cd in mg/kg in a
certain soil batch
reported on dry mass basis (105 °C 2h)



Example of a decision rule

Appendix B Example 1

Decision rule

The batch will be considered to be non-compliant if the probability of the value of the concentration being greater than 200 ng/g exceeds 95%

1. A specification of the measurand
2. A specification of the measurement object/test item
- Batch**
3. An analytical result - Single value, mean value, each single value?
4. An uncertainty - Normally an expanded uncertainty at 95% confidence level
5. A specification giving upper and/or lower permitted limits
- Upper limit 200 ng/g**
6. A decision rule how to take measurement uncertainty into account
- Non-compliant if probability for out of specification is higher than 95%**



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95 % probability versus 95 % confidence interval

Upper permitted limit

Then decision limit at:

95 % result + 1,6 u

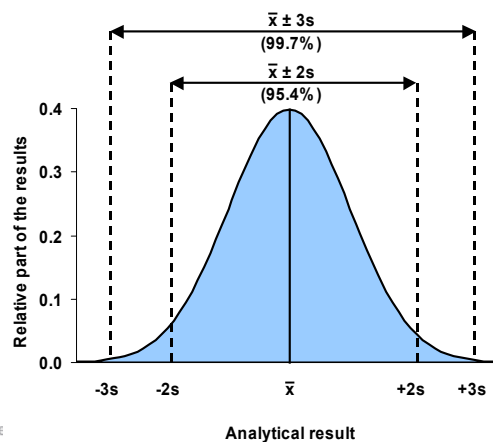
99,9 % result + 3,09 u

where u is the standard uncertainty

Measurement result

Confidence interval

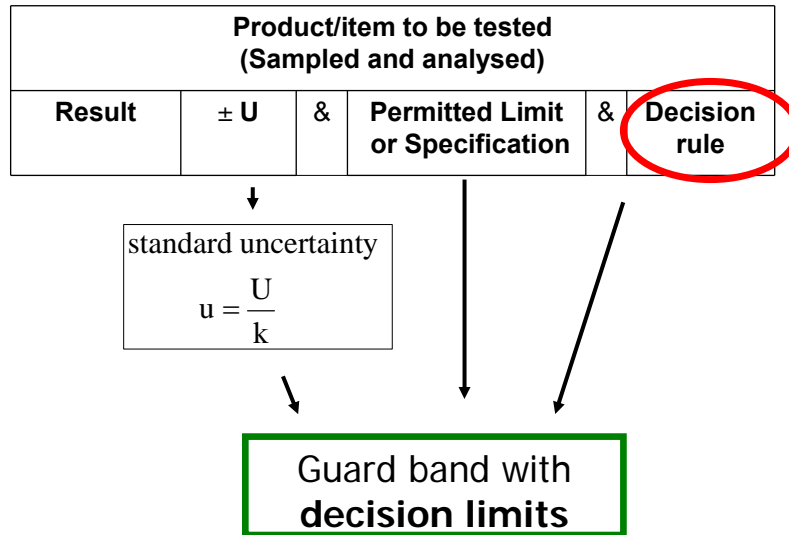
95 % result \pm 2 u



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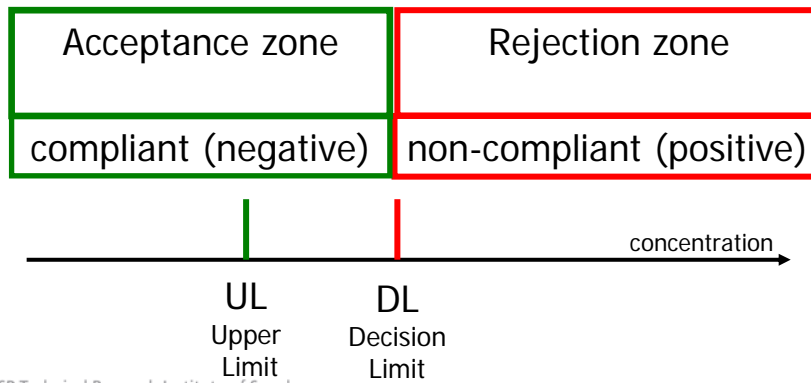
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From these input we calculate a decision limit

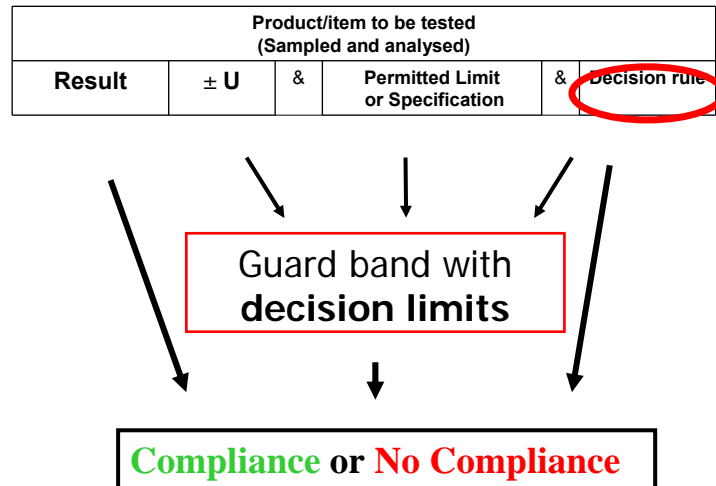


Acceptance zone and rejection zone

Case: An upper permitted limit –
 concentration should not be greater than



Compliance – No compliance



Assessing compliance from measurement results

Example with blood alcohol where we want to be sure to **only** punish those that truly has **exceeded** the limit

Measurement procedure: *Ethanol in blood by Head-Space GC*

Quality routine: *Two independent results – different analysts using different instrument - Max range 0,003 mg/kg*



Input for decision making

A specification of the measurand including measurement object	Concentration (massfraction) of total EtOH in a blood sample delivered to the laboratory
Test item	A blood sample from a person
An analytical result (mean value of 2 independent results)	C (EtOH)= 0,221 mg/g
An uncertainty	U = 0,013 mg/g, k=2 (95 %) Upper permitted limit 0,200 mg/g
A specification	<i>The decision limit is the concentration above which it can be decided with a statistical certainty of 99.9 % (alfa =0,001) that the permitted limit has been truly exceeded</i>
A decision rule.	

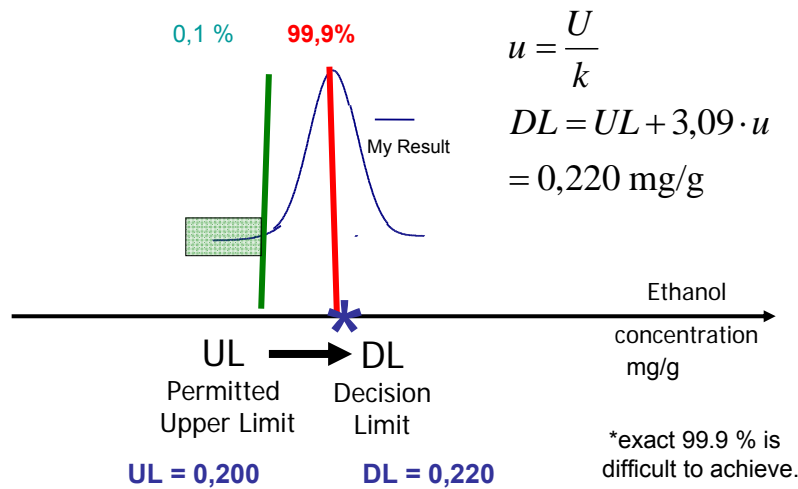


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Decision rule - the decision limit is the concentration above which it can be decided with a statistical certainty of 99.9 % that the permitted limit has been truly exceeded.



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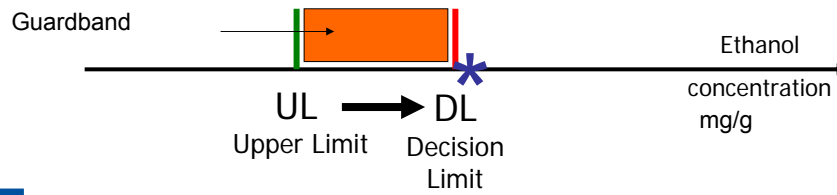
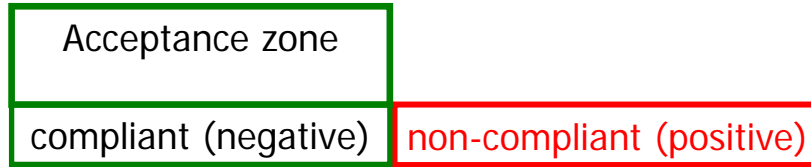
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Result over decision limit → Non-compliant

if the measurement result lies
in the acceptance zone
the product is declared compliant

* Blood alcohol
Measurement result
0,221 mg/g



UL = 0,200

DL = 0,220



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Example where we can find decision rules

Commission Decision

of 12/08/2002

implementing Council Directive 96/23/EC
concerning the performance of analytical methods
and the interpretation of results

(notified under document number C(2002) 3044)

For food sector



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The EU directive talks about alfa error – false positive
With upper limit - non-compliant is a positive result

Test result	Women	
	Non-pregnant	Pregnant
Negative	True negative	False negative
Positive	False positive	True positive

↑
 α error

α error = probability that women is non-pregnant, even though a positive measurement result is obtained (FP)



A decision rule giving you a decision limit

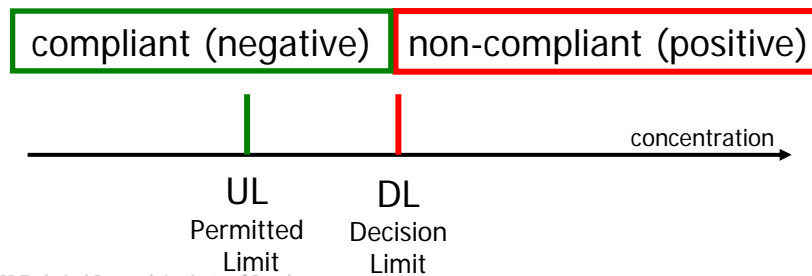
- If a permitted (higher) limit has been established for a substance,
the decision limit is the concentration above which it can be decided with a statistical certainty of $(1-\alpha)$ that the permitted limit has been truly exceeded.
- Permitted limit = maximum residue limit, maximum level or other maximum tolerance
- Decision limit, DL (also $CC\alpha$) = limit at (and above) which it can be concluded with an error probability $(1-\alpha)$ that the sample is non-compliant (positive result)



Example of assessing compliance/no compliance

The result of an analysis shall be considered non-compliant if the **decision limit** of the confirmatory method for the analyte is exceeded.

Decision rule →



Terminology

decision rule: 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.

acceptance zone: the set of values of a characteristic, for a specified measurement process and decision rule, that results in product acceptance when a measurement result is within this zone.

rejection zone: the set of values of a characteristic, for a specified measurement process and decision rule, that will give non-compliance when a measurement result is within this zone.

guard band: the magnitude of the offset from the specification limit to the acceptance or rejection zone boundary

Alpha error (α) = probability that tested sample is compliant, even though a non-compliant measurement is obtained (FP)



Summary

What do we need for the decision making?

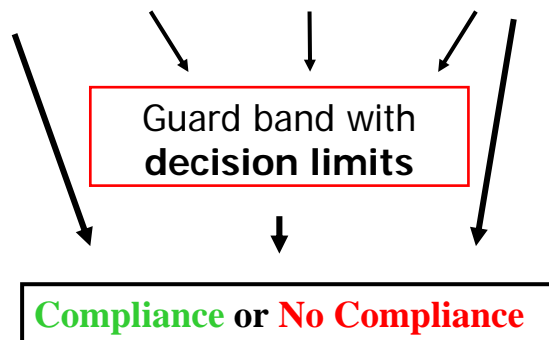
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Summary

From these input we can decide on compliance!

Product/item to be tested (Sampled and analysed)				
Result	$\pm U$	&	Permitted Limit or Specification	& Decision rule



Workshop – example 1

The limit set in a regulation is $100\mu\text{g/g}$. the decision rule states that the sample is non compliant with the regulation if the measured value exceeds the limit by more than $2u$, where u is the standard uncertainty.

Which of the following measured values show compliance, non-compliance or require further information in order to make a decision?

- (a) $103\mu\text{g/g}$ $u = 1.2\mu\text{g/g}$
 - (b) $102\mu\text{g/g}$ expanded uncertainty $U = 1.5\mu\text{g/g}$
 - (c) $103\mu\text{g/g}$ expanded uncertainty $U = 4.6\mu\text{g/g}$
- based on a 95% level of confidence with 8 degrees of freedom

