

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

Uncertainty for compliance assessment

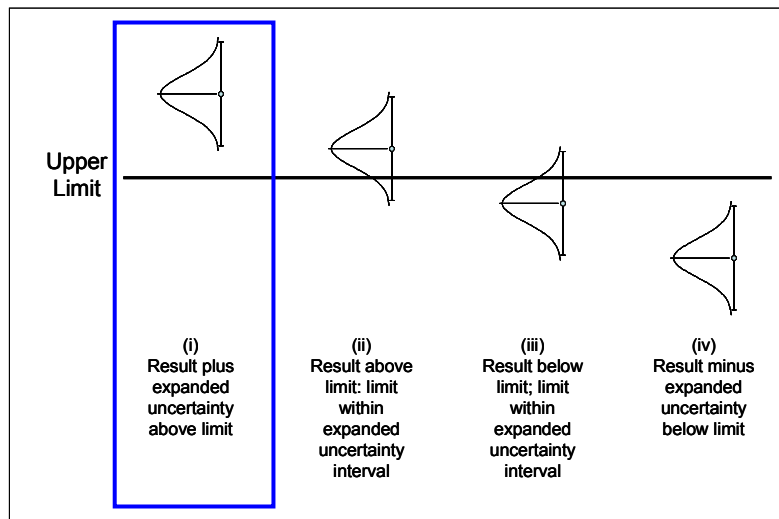
Symposium at BAM, Berlin
16 April 2008



Bertil Magnusson

SP Technical Research Institute of Sweden

Result and uncertainty and limit



Lets us take an example of blood alcohol & Swedish legislation

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Our result + uncertainty + limit

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

Analytical Report
Concentration of ethanol in blood sample is
0,220 mg/g \pm 0,013 (k=2)

Limit is 0,200 mg/g
Will this driver be punished?



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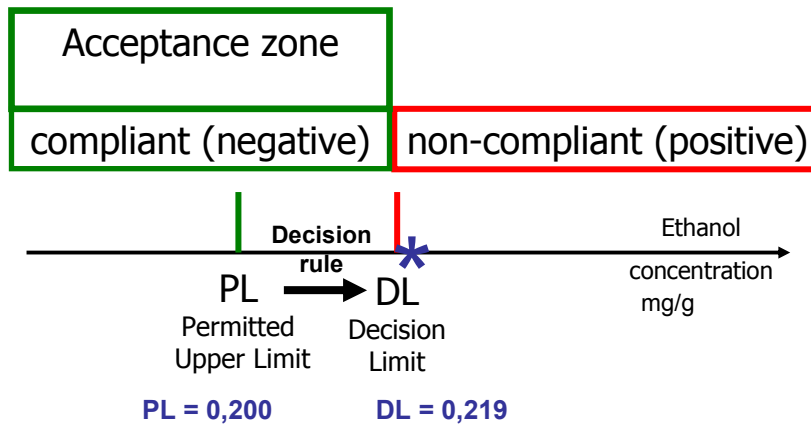
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To make a decision we need an acceptance zone

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

* Blood alcohol
Measurement result
0,220 mg/g



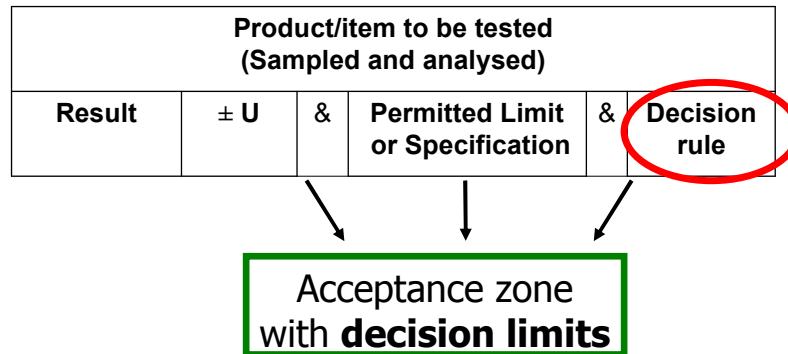
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Using a decision rule we calculate an acceptance zone



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

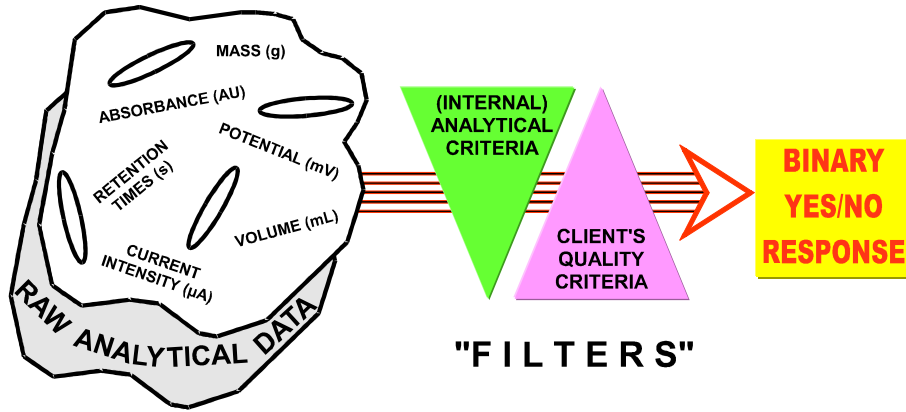


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 - Decision rule
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- Blood alcohol example in detail
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- Terminology in decision making
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Assessing compliance*



*Courtesy QUANAL project by Valcarcel et al

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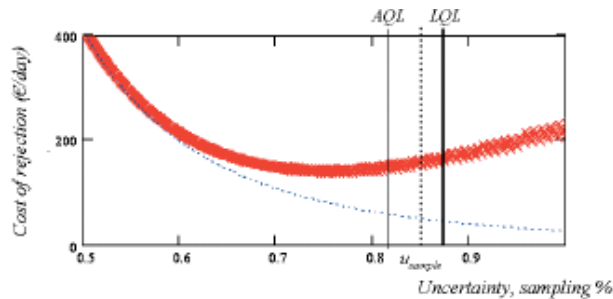
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Risk and consequences of wrong decision

The risk is normally taken into account in the decision rule.
Not part of this guide!

Poster at this workshop by Leslie Pendril, SP
Optimised uncertainties and risk costs in sampling by
variable and attribute

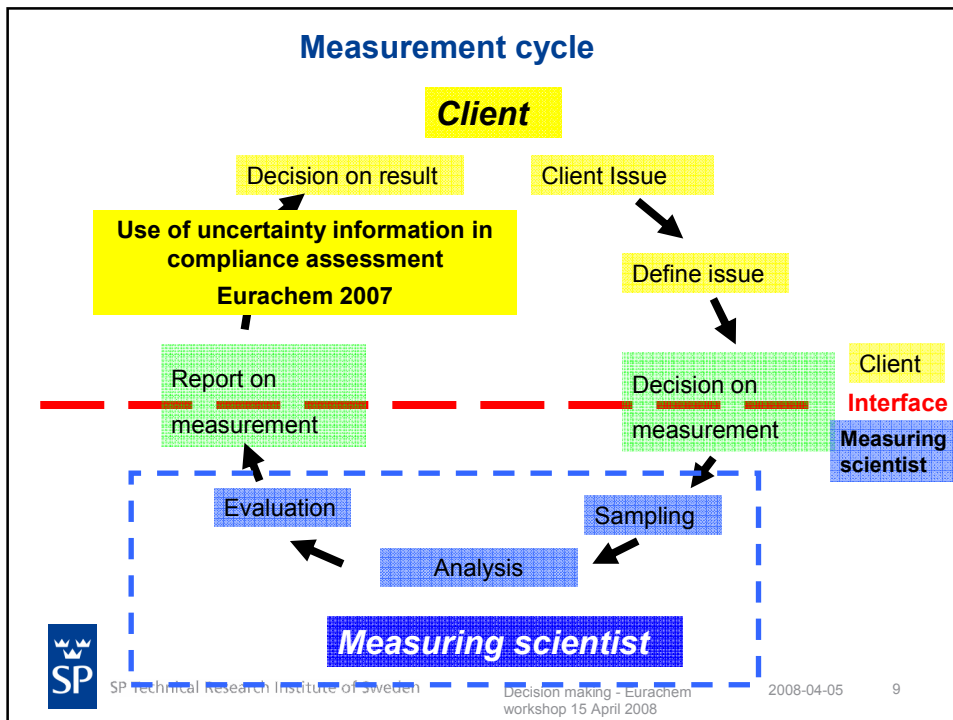


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What do we need for the decision making?

1. An analytical result
2. An uncertainty - the confidence level and the corresponding k-factor should be stated. e.g. k=2 for approximate 95 %
3. A specification of the **measurand**
4. A specification of the **measurement object/test item** (part of measurand)
5. A specification giving upper and/or lower permitted 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**

VIM2 quantity subject to measurement'.

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)



*ISO Guide 99 (2007) International Vocabulary of Metrology – Basic and General Concepts and Associated Terms VIM 3rd edition, ISO, Geneva

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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. An analytical result - Single value, mean value, each single value?
2. An uncertainty - Normally an expanded uncertainty at 95% confidence level
3. A specification of the measurand
4. A specification of the measurement object/test item
Batch
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

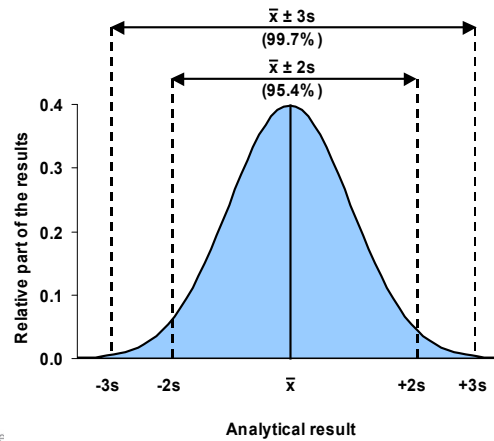
99,9 % result + 3,09 u

where u is the standard uncertainty

Measurement result

Confidence interval

95 % result $\pm 2 u$



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From these input we calculate an acceptance zone

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

standard uncertainty

$$u = \frac{U}{k}$$

Acceptance zone
with **decision limits**



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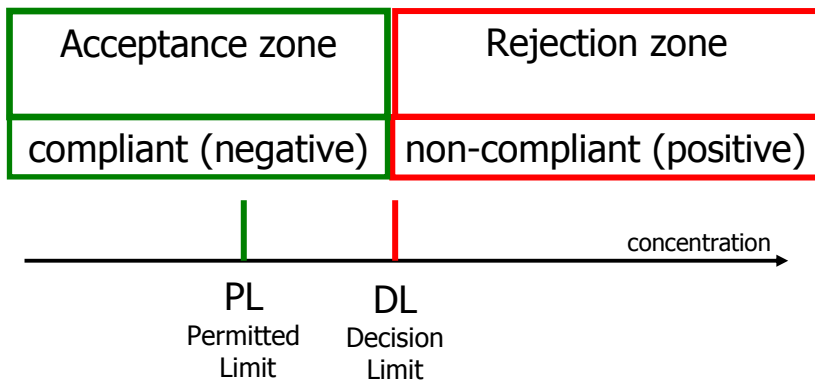
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Acceptance zone and rejection zone

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



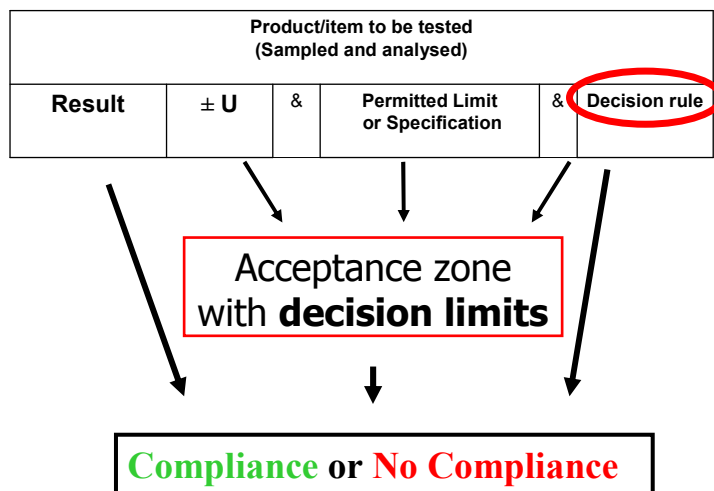
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Compliance – No compliance



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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

An analytical result

$C(\text{EtOH}) = 0,220 \text{ mg/g}$

An uncertainty

$U = 0,013 \text{ mg/g}, k=2 (95 \%)$

A specification of the
**measurand including
measurement object**

Concentration (massfraction) of
total EtOH in a blood sample
delivered to the laboratory

A specification

Upper permitted limit 0,200 mg/g

A **decision rule.**

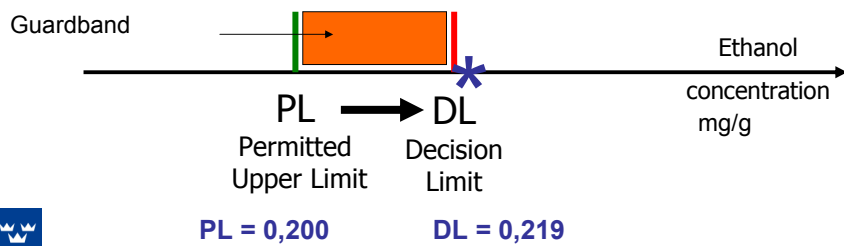
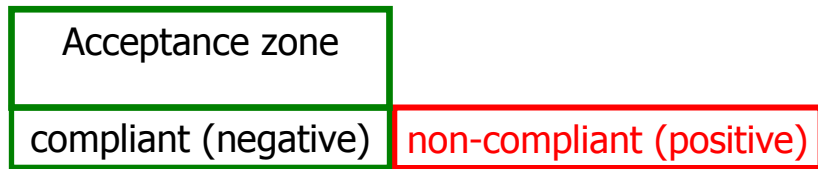
*The decision limit is the
concentration above which it can
be decided with a statistical
certainty of 99.9 % ($\alpha = 0,001$)
that the permitted limit has been
truly exceeded*



Result over decision limit → non-compliant

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

* Blood alcohol
Measurement result
0,220 mg/g

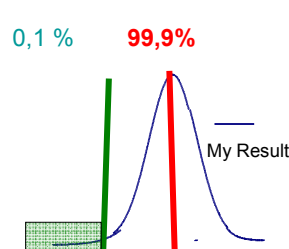


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Probability at results is over limit is > 99,9%



$$u = \frac{U}{k}$$

$$DL = PL + 3,09 \cdot u$$

$$= 0,219 \text{ mg/g}$$



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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



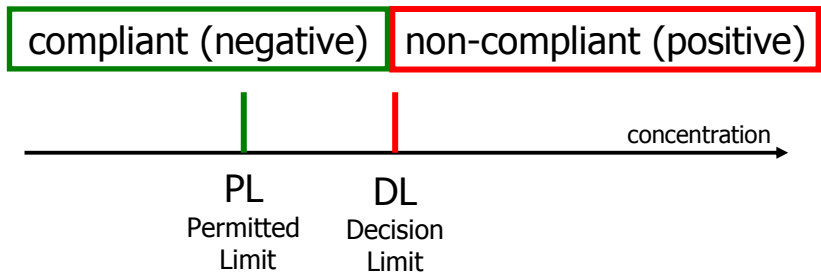
A decision rule giving you a decision limit

- Decision rule
- 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

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



What is a positive result? 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)



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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2. An uncertainty - the confidence level and the corresponding k-factor should be stated. e.g. k=2 for approximate 95 %
3. A specification of the **measurand**
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Summary

From these input we can decide on compliance!

