CCQM KCRV WG—19 March 2008

Data Evaluation Principles
for CCQM Key Comparisons

Source
Based on the considerations of meetings of the CCQM KCRV WG at BIPM, January 2008 and the CCQM EETWG at LGC, February 2008.

Notation
- \( N \): number of participating NMIs
- \( x_i \): value submitted by \( i \)-th participating NMI \((i = 1, \ldots, N)\)
- \( u(x_i) \): standard uncertainty associated with \( x_i \) \((i = 1, \ldots, N)\), relating to measurement capability only
- \( x_{ref} \): key comparison reference value (KCRV)
- \( u(x_{ref}) \): standard uncertainty associated with \( x_{ref} \)
- \( k \): coverage factor
- \( d_i \): value component \( x_i - x_{ref} \) of the degree of equivalence (DoE) for NMI \( i \) \((i = 1, \ldots, N)\)
- \( u(d_i) \): standard uncertainty associated with \( d_i \)
- \( U(d_i) \): uncertainty component for a 95% level of confidence of the DoE for NMI \( i \) \((i = 1, \ldots, N)\)

Terminology
- result provided by NMI \( i \) \( x_i \) and \( u(x_i) \) and, where appropriate, a degrees of freedom
- DoE for NMI \( i \) \( d_i \) and \( U(d_i) \)
- NMI: metrology institute designated by the appropriate national governmental or other official authority as that responsible for national measurement standards [CIPM MRA].

Principles

1. When available an independent traceable value can be used as the KCRV \( x_{ref} \) if it is consistent with the best available results from NMIs participating in the key comparison and has credible and sufficiently small uncertainty.
   NOTE — When possible, an independent basis for the KCRV is preferable.

2. Otherwise \( x_{ref} \) and its associated uncertainty \( u(x_{ref}) \) should be calculated on the basis of the best available results from NMIs participating in the key comparison. The NMIs whose results are nominally to be used in the calculation must be agreed and documented prior to circulation of the material. Criteria for inclusion should be objective, related to prior performance and documented.

3. Only those results obtained by the application of techniques and measurement procedures that are most suitable and accurate can be used in the evaluation of the KCRV.
   NOTE — Other information, such as results from a prior pilot study for the same measurand, can be used to inform the evaluation of the KCRV.
4 Upon examination of the body of results, further exclusion of results from the calculation of $x_{\text{ref}}$ is permitted based on scientific judgment informed when appropriate by statistical considerations.

NOTE — 1. A DoE is calculated for each participant, unless it withdraws from the comparison in a manner compatible with the CIPM MRA.

NOTE — 2. In cases of an unresolved dispute concerning the exclusion of results from the calculation of a KCRV, CCQM and, if necessary, ultimately CIPM, would make a decision compatible with the CIPM MRA.

5 CCQM WGs should expect the submitted values of $x_i$ and the $u(x_i)$ to be credible, but some values, through human error or unexpected chemical or sample effects, might be discrepant.

NOTE — For small $N$, statistical tests have low power to detect discrepant values.

6 The approach used for calculating $x_{\text{ref}}$ (e.g. weighted mean, arithmetic mean) should be consistent with the assumptions applicable to the results, taking account of all available information.

NOTE — Examples of possible assumptions might be that the results were obtained independently, and that homogeneity effects are non-negligible.

7 The most efficient approach (that is giving the smallest value of $u(x_{\text{ref}})$) of those consistent with the applicable assumptions is preferred.

8 Where approaches give similar values for $x_{\text{ref}}$ and similar values for $u(x_{\text{ref}})$, the simplest estimator is preferred.

9 The principles of the *Guide to the expression of uncertainty in measurement* (GUM) should be applied in evaluating $u(x_{\text{ref}})$ and $U(d_i)$. Evaluation of $U(d_i)$ should account for correlation associated with $x_i$ and $x_{\text{ref}}$.

NOTE — The various quantities involved are regarded as being characterized by probability density functions (PDFs) based on all available knowledge of those quantities. The DoE for NMI $i$ has a value component and an uncertainty component. The value component is $d_i = x_i - x_{\text{ref}}$ and the uncertainty component is $U(d_i) = ku(d_i)$, where $k$ is a coverage factor corresponding to a 95 % level of confidence. When the weighted mean is used as a KCRV for NMI values obtained independently (and there is no independent reference value), $u^2(d_i) = u^2(x_i) - u^2(x_{\text{ref}})$. When $x_{\text{ref}}$ is determined from a method that is independent of the submitted NMI results, the correlation associated with $x_i$ and $x_{\text{ref}}$ is zero, and $u^2(d_i) = u^2(x_i) + u^2(x_{\text{ref}})$. There will be counterparts of these expressions for other estimators, although it will not always be possible to provide explicit formulae.

10 $u(x_{\text{ref}})$ is the standard uncertainty associated with $x_{\text{ref}}$, rather than a measure of dispersion of the $x_i$ such as the standard deviation of the $x_i$.

NOTE — For results provided independently by $N$ NMIs, $u(x_{\text{ref}})$ would generally reduce with $N$.

11 Homogeneity effects should be taken into account by the coordinating NMI when determining a KCRV and its associated uncertainty. Homogeneity effects should be characterized by the coordinating NMI before distributing samples.

NOTE — 1. Homogeneity effects should be expressed in terms of a standard uncertainty $u_{wb}$ for within-bottle effects and a standard uncertainty $u_{bb}$ for between-bottle effects.

NOTE — 2. A similar statement applies to some other effects such as stability.

12 CCQM WGs should carry out calculations in terms of the $u(x_i)$ rather than expanded uncertainties. In terms of reporting or presenting results, the use of expanded uncertainties is useful for comparison and other purposes. CCQM WGs should supply results for the KCDB in the requisite format.

NOTE — Guidance on the requisite format is available from the curator of the KCDB.

13 Each participating NMI should provide an uncertainty budget relating to all uncertainty components that are appropriate to its measurement. A template should be used for KCs when all participating NMIs use the same measurement procedure.