

Although this Guide provides a framework for assessing uncertainty, it cannot substitute for critical thinking, intellectual honesty and professional skill. The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement. The quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value.

GUM, 3.4.8

## Comments on CCT/08-19/rev *Uncertainties in the Realisation of the SPRT Subranges of the ITS-90*

Apart from major errors - to be highlighted here later -, the Document CCT - 08/19/rev has mistakes of lesser importance but still not acceptable in a Document published under the auspices of CCT. It is not my intention and this is not the place, for me to reveal all of them. I shall only give several examples, to illustrate the types of problems.

a) In some respects, the consistency of Document CCT with the ISO Guide [1] is doubtful. I will elaborate that on the two equations which are essential for the evaluation of uncertainty in the SPRTs calibration, that are (9.3) and (9.4).

- According to GUM [1], to estimate the value of measurand a *measurement model* needs to be defined. The measurement model should be the mathematical expression of the functional relationship between the measurand and the input quantities on which it depends (see Clause 4.1 in [1]). Instead, in equation (9.3) to calculating the triple-point resistance

$$R_{\text{H}_2\text{O,report}} = R_{\text{meas}}(t) + R_{\text{H}_2\text{O}} \frac{dW_1}{dt} (\Delta t_{\text{hyd}} + \Delta t_p + \Delta t_{\text{imp}} + \Delta t_{\text{liq}} + \Delta t_{\text{iso}} + \Delta t_{\text{ther}} + \Delta t_{\text{dyn}}),$$

the measurand, i.e.  $R_{\text{H}_2\text{O}}$ , is present not only as the *output quantity* - in the left-hand side of the equation, but also among the *input quantities* on which it depends - in the right-hand side, where this time it is treated as a constant, with no uncertainty. The correct form of the measurement model (9.3) is, obviously:

$$R_{\text{H}_2\text{O}} = \frac{R_{\text{meas}}(t)}{1 - \frac{dW_1}{dt} (\Delta t_{\text{hyd}} + \Delta t_p + \Delta t_{\text{imp}} + \Delta t_{\text{liq}} + \Delta t_{\text{iso}} + \Delta t_{\text{therm}} + \Delta t_{\text{dyn}})},$$

an expression similar to equation (5) in [2].

- In (9.4) – the equation for the calculation of the so-called ”total uncertainty”<sup>1</sup>:

<sup>1</sup> In reality, equation 9.4 does not provide the expression of the *total uncertainty*, as stated. What it gives instead is the expression of the *combined variance*. The error is not singular; it is repeated for the equations 2.2, 2.7, 2.21, 3.2, 3.7, 4.3, 4.8, 5.2, 5.6, 6.4, 6.5, 6.10, 8.3, 8.11, 8.20, 8.21, 9.4, 9.5, 9.6, 9.9, 9.11, 9.13, 9.16, 9.27, C.14, C.15, C.22, C.30.

$$\begin{aligned}
u^2(R_{\text{H}_2\text{O}}) &= \left( R_{\text{H}_2\text{O}} \frac{dW_{\text{H}_2\text{O}}}{dt} \right)^2 \\
&\left[ u^2(\Delta t_{\text{hyd}}) + u_2(\Delta t_p) + u^2(\Delta t_{\text{imp}}) + u^2(\Delta t_{\text{liq}}) + u^2(\Delta t_{\text{iso}}) + u^2(\Delta t_{\text{ther}}) + u^2(\Delta t_{\text{dyn}}) \right] \\
&+ X_{\text{H}_2\text{O}}^2 \left( u^2(R_{\text{S,cal}}) + R_{\text{S}}^2 (t_{\text{bath}} - t_{\text{cal}})^2 u^2(\beta) + u^2(R_{\text{S,ac-dc}}) + u^2(R_{\text{S,power}}) + u^2(R_{\text{S,p}}) \right) + R_{\text{S}}^2 u^2(\Delta X_{\text{INL}}) \\
&+ \frac{R_{\text{S}}^2}{(I_2^2 - I_1^2)^2} \left[ (I_2^4 + I_1^4) \left( u^2(\Delta X_{\text{DNL}}) + X^2 \beta^2 u^2(t_{\text{bath}}) \right) + I_2^4 u^2(X_{1,\text{noise}}) + I_1^4 u^2(X_{2,\text{noise}}) \right] + \\
&+ 8R_{\text{S}}^2 \Delta X_{\text{sh}}^2 \frac{I_2^4}{(I_2^2 - I_1^2)^2} \left( \frac{u^2(I)}{I^2} \right),
\end{aligned}$$

the variances of 6 quantities:  $R_{\text{S,ac-dc}}$ ,  $R_{\text{S,power}}$ ,  $R_{\text{S,p}}$ ,  $\Delta X_{\text{DNL}}$ ,  $X_{1,\text{noise}}$ , and  $X_{2,\text{noise}}$  are included, that **do not exist in the measurement model in equation (9.3)**. (Note that the model (9.3) is limited (by chance or not) to approximately the same input quantities as in Equation (3) in [2]).

It would be interesting to know how the expressions of the sensitivity coefficients in (9.4) have been established for these quantities (i.e. the partial derivatives  $\partial R_{\text{H}_2\text{O}}/\partial R_{\text{S,power}}$ ,  $\partial R_{\text{H}_2\text{O}}/\partial R_{\text{S,ac-dc}}$ ,  $\partial R_{\text{H}_2\text{O}}/\partial R_{\text{S,p}}$ , and so on), given that the functional relationship between the output quantity  $R_{\text{H}_2\text{O}}$  and the 6 quantities is not defined.

The absence of essential measurement models in other cases presented in the Document CCT/08-19/rev has to be revealed as well. I shall bring forth, for example, the absence of the mathematical model for the standard resistance  $R_{\text{S}}$ , based on which equation (8.6) for  $u^2_{\text{total}}(R_{\text{S}})$  was determined, and the absence of the mathematical model for  $R_{\text{meas}}$ , based on which equation (8.20) for  $u^2(R_{\text{meas}})$  was determined (equation where  $R_{\text{S}}$  appears as well).

In the case of  $R_{\text{S}}$  too, I draw the attention upon the fact that, although its dependency on pressure (equation (8.5))

$$R_{\text{S}}(p) = R_{\text{S}}(p_{\text{cal}})[1 + \gamma(p - p_{\text{cal}})],$$

is identical to its dependency on temperature (equation (8.1))

$$R_{\text{S}}(t_{\text{bath}}) = R_{\text{S}}(t_{\text{cal}})[1 + \beta(t_{\text{bath}} - t_{\text{cal}})],$$

the expressions of contributory variances to the  $u^2(R_{\text{S}})$  (equation (8.6)):

$$\begin{aligned}
u^2_{\text{total}}(R_{\text{S}}) &= u^2(R_{\text{S,cal}}) + R_{\text{S}}^2 \left[ \beta^2 u^2(t_{\text{bath}}) + (t_{\text{bath}} - t_{\text{cal}})^2 u^2(\beta) \right] + u^2(R_{\text{S,ac-dc}}) \\
&+ u^2(R_{\text{S,power}}) + u^2(R_{\text{S,p}}).
\end{aligned}$$

are not similar. Thus, the contribution related to the temperature is expressed correctly by  $R_{\text{S}}^2 \left[ \beta^2 u^2(t_{\text{bath}}) + (t_{\text{bath}} - t_{\text{cal}})^2 u^2(\beta) \right]$ , while the contribution related to the pressure is expressed, without any explanation, by  $u^2(R_{\text{S,p}})$ , instead of  $R_{\text{S}}^2(p_{\text{cal}}) \left[ \gamma^2 u^2(p) + (p - p_{\text{cal}})^2 u^2(\gamma) \right]$ .

Also, to stay with this example only, the mathematical models of  $R_{\text{S,ac-dc}}$  and  $R_{\text{S,power}}$  are missing, as well as the equations for the uncertainties associated with them.

**b)** In the expressions of the variances associated with the realisation of the fixed points the same seven sources of uncertainty erroneously are considered, regardless of whether the equation refers to the triple point of water, or to the cryogenic fixed points or to the metal fixed points (see (9.4), (9.6), (9.10), (9.12), (9.14), (9.17)):

$$u^2(R_i) = \left( R_i \frac{dW_i}{dt} \right)^2 \left[ u^2(\Delta t_{\text{hyd},i}) + u^2(\Delta t_{p,i}) + u^2(\Delta t_{\text{imp},i}) + u^2(\Delta t_{\text{liq},i}) + u^2(\Delta t_{\text{iso},i}) + u^2(\Delta t_{\text{ther},i}) + u^2(\Delta t_{\text{dyn},i}) \right].$$

**c)** In Appendix A, entitled *Summary of typical ranges of fixed-point uncertainties (in  $\mu\text{K}$ )*, astonishing values are specified for some of the uncertainty components related to the impurities. For instance, the lower limit (*typical!*) of the contribution of impurities to the uncertainty of the Al fixed point is 300  $\mu\text{K}$ , while the lower limit of the "total" uncertainty (also *typical!*) is only 60  $\mu\text{K}$ !!! It is a nonsense that **the value of the typical TOTAL fixed-point uncertainty be 5 times lower than the value of the typical contribution of impurities**. (Similar cases related also to impurities: the upper limit at the Al point; the lower limit at the Ag, Sn, and In fixed points.)

**d)** Some contradictory statements create confusion. Without going into details, here is, for instance, the existence of major inconsistencies in the statements on the DNL errors, all in the same section - Section 8.3. We find out that:

- The DNL errors (with no differentiation by the type of bridge) are typically different for different readings:

"**The errors [DNL] are typically different** for every possible reading... (emphasis mine)" (page 42).

- but the comment after equation 8.11 reads:

"In bridges using voltage or current dividers **the DNL errors [...]** are similar for every reading (emphasis mine)" (page 42).

- and then, in the same comment:

"... **the DNL errors are random for different readings** but the same over time (emphasis mine)" (page 43).

- On the other hand, in a bibliography reference<sup>2</sup> recommended for Section 8.3 (which is *White, 2003b*), we read:

"...readings made very close to each other in value [such as the readings required to assess the self-heating] will have **the same DNL error** and yield *correlated* uncertainties (emphasis mine)" (although the "DNL errors" are assumed to be *uncorrelated* throughout the entire CCT Document/08-19/rev).

**e)** The Document presents one of „the procedures meant to reduce uncertainty” – *Measure resistance ratios with the same standard resistor* (page 68). Here it is demonstrated “mathematically”, step by step, purely and simply - in fact the case is simplified down to error: if

<sup>2</sup> The list of references includes papers with minor relevance while missing key contributions as I. Lira [3] and G. Bonnier [4]. With the same concern in mind for an accurate historical perspective, I noticed, for instance, the absence of the first paper [6] on the uncertainties in SPRT calibration at the defining fixed points of ITS-90 and the absence of quoting in Section 3.1, page 15 of the first paper [5] to describe the bubble-compression test and the pressure correction for residual gas in the triple point of water cells.

we use the same standard resistor, then  $R_{S,T} = R_{S,H_2O}$  ! Hence,  $\frac{dR_{S,T}}{R_{S,T}} = \frac{dR_{S,H_2O}}{R_{S,H_2O}}$ , and the terms containing the variance  $u^2(R_{S,T})$  and  $u^2(R_{S,H_2O})$  disappear in (C.26):

$$u^2(W) = W^2 \frac{1}{R_{H_2O}^2} \left( \frac{u^2(X)}{X^2} + \frac{u^2(R_{S,T})}{R_{S,T}^2} + \frac{u^2(X_{H_2O})}{X_{H_2O}^2} + \frac{u^2(R_{S,H_2O})}{R_{S,H_2O}^2} \right).$$

The firm conclusion follows: "Now the uncertainty depends only on the uncertainty in the two bridge reading":

$$u^2(W) = W^2 \frac{1}{R_{H_2O}^2} \left( \frac{u^2(X)}{X^2} + \frac{u^2(X_{H_2O})}{X_{H_2O}^2} \right).$$

But, at the end, in brackets, the reader finds out that "**two small terms depending on the stability of the resistor**" **have not disappeared as the others**, yet no explanation is provided as to why and how this happens. It would have been illuminating to find at least the answer to the question: if using the same standard resistor means  $R_{S,T} = R_{S,H_2O}$ , what are the reasons for which the two variables,  $R_{S,T}$  and  $R_{S,H_2O}$ , are not directly simplified even from the start, in (C.24):

$$W = \frac{R}{R_{H_2O}} = \frac{R_{S,T} X}{R_{S,H_2O} X_{H_2O}} ?$$

### **Major errors in the Document CCT/08-19/rev:**

#### 1) Equation (9.6)

$$\begin{aligned} u^2(R_i) = & \left( R_i \frac{dW_i}{dt} \right)^2 \left[ u^2(\Delta t_{hyd,i}) + u^2(\Delta t_{p,i}) + u^2(\Delta t_{imp,i}) + u^2(\Delta t_{liq,i}) + u^2(\Delta t_{iso,i}) + u^2(\Delta t_{ther,i}) + u^2(\Delta t_{dyn,i}) \right] \\ & + R_S^2 u^2(\Delta X_{INL}) + \frac{R_S^2}{(I_2^2 - I_1^2)^2} \left[ (I_2^4 + I_1^4) \left( u^2(\Delta X_{DNL}) + X^2 \beta^2 u^2(t_{bath}) \right) + I_2^4 u^2(X_{1,noise}) + I_1^4 u^2(X_{2,noise}) \right] \\ & + 8 R_S^2 \Delta X_{sh,i}^2 \frac{I_2^4}{(I_2^2 - I_1^2)^2} \left( \frac{u^2(I)}{I^2} \right), \end{aligned}$$

contains a major error that triggers considerable alteration of the uncertainties associated with the realisation of the fixed points, respectively:

**a) their values are increased by up to 4.3 times, for temperatures above 0 °C**

or

**b) their values are decreased by up to 118 times, for temperatures below 0 °C.**

The error emerges from the wrong definition of the sensitivity coefficient of the SPRT at a temperature  $t$ ,  $\left( \frac{dR_i}{dt} \right)$ . It is easy to demonstrate that, although (9.6) is used to calculate the

measurement uncertainty of the SPRT resistance at the fixed point  $i$ , the variation  $\left( \frac{dW_i}{dt} \right)$  should be multiplied by  $R_{H_2O}$ , and not by  $R_i$ , because:

$$\left. \frac{dR_i}{dt} \right|_{t_{90}=t_i} = R_{\text{H}_2\text{O}} \left. \frac{dR_i}{R_{\text{H}_2\text{O}} dt} \right|_{t_{90}=t_i} = R_{\text{H}_2\text{O}} \left. \frac{dW_i}{dt} \right|_{t_{90}=t_i}, \quad (1)$$

where  $W_i = \frac{R_i}{R_{\text{H}_2\text{O}}}$ .

The use of factor  $\left( R_i \frac{dW_i}{dt} \right)$  in (9.6) leads to a value of uncertainty  $W_i$  times greater for  $t > 0$  °C and  $\left( \frac{1}{W_i} \right)$  times smaller for  $t < 0$  °C:

$$R_i \left. \frac{dW_i}{dt} \right|_{t_{90}=t_i} = R_i \left. \frac{dR_i}{R_{\text{H}_2\text{O}} dt} \right|_{t_{90}=t_i} = W_i \left. \frac{dR_i}{dt} \right|_{t_{90}=t_i}. \quad (2)$$

I have to stress that the error is not accidental and it is not limited to (9.6), but it is repeated in all of the subsequent equations, (9.10), (9.12), (9.14), (9.17), (9.23), and (9.25). Moreover, the **increase or reduction of the uncertainties associated with the realisation of each fixed point  $i$  in the calibration subrange propagates by interpolation into the value of the uncertainty of each intermediate temperature,  $u(T_{90})$ .**

As a result of this error, the Document CCT/08-19/rev has turned from a guide for a most correct uncertainty assessment into a instrument for „harmonisation” and uniformisation of the substantial increase or of the huge reduction of the measurement uncertainty and, implicitly, of the Calibration and Measurement Capabilities of NMIs.

**2) The measurement uncertainty related to the variations in the observations of the measurand obtained under repeatability conditions, that is  $u(X) = s(\bar{X})$ , is completely absent from the Document CCT/08-19/rev.** See, for instance, the expression of ”the total uncertainty of the zero-current water-triple-point resistance”, (9.4), where this component of uncertainty is absent, just as it is absent from all equations.

The omission may very well be deliberate, given the statement in Section 5.3:

*The observed variations in the liquidus point (non-repeatability) are attributable to a combination of thermal effects<sup>3</sup> (Section 5.1) and impurity effects (Section 2.3), so **no additional uncertainty should be added** (emphasis mine).*

This statement may be correlated with an earlier position of MSL, put in a similar form (the *strain in SPRT* was nominated instead of *thermal effects*), on the occasion of a WG 3 meeting in 2003 [15]:

*The non-repeatability of fixed points for example arises from identifiable physical causes including impurities and strain in SPRT for example. **To include a term for repeatability is to count these terms twice** (emphasis mine).*

<sup>3</sup> Between 1997 and 2001, in the CCT-K3 Report, p. 321 [7], MSL considered that ”immersion curves [i.e. evaluating the ”thermal effects”] are unnecessary since they have demonstrated to their satisfaction that the SPRT readings in the various cells are independent of furnace temperature variations”.

Hence, MSL considered in 2003 that to include a term for repeatability would be "to double-count" some uncertainty components that would have the same physical causes as the observed variability – such as *impurities* and *strain in SPRT*.

Unexpected statements! I find it absurd to discard the standard uncertainty associated with the readings of the bridge,  $u(X)$  when calculating the combined standard uncertainty of the measurement result, as long as the input quantity  $X$  ( $\bar{X}$ , to be exact) is present in the equation that provides the measurement result, and it is the very essential part of this result. The fundamental principle for evaluating uncertainty established in GUM [1] is that the mathematical model of the measurement should serve both operations:

- the determination of the measurement result *by simply replacing into the model* the estimate for each input quantity, and
- the calculation of the uncertainty of the measurement result by combining the uncertainties associated with the estimated values of the input quantities, *the manner of combination being prescribed by the model*.

Of course, the authors of GUM [1] could not have missed the "double-counting" problem invoked by MSL. But their solutions are precisely contrary to those in the Document. As such, Clause 4.3.10 of the *Guide* [1] gives the analysis a particular effect whose uncertainty is obtained from a Type B evaluation:

*4.3.10 It is important not to "double-count" uncertainty components. If a component of uncertainty arising from a particular effect is obtained from a Type B evaluation, it should be included as an independent component of uncertainty in the calculation of the combined standard uncertainty of the measurement result only to the extent that the effect does not contribute to the observed variability of the observations. This is because the uncertainty due to that portion of the effect that contributes to the observed variability is already included in the component of uncertainty obtained from the statistical analysis of the observations.*

Therefore, according to GUM, if that effect does contribute to the observed variability of the observations, it is not the Type A uncertainty that should be eliminated, but, on the contrary, the Type B uncertainty.

Leaving aside the statements in GUM and giving credit to the allegations in Section 5.3 of the Document CCT - "the observed variations in the liquidus point (non-repeatability) are attributable to a combination of thermal effects and impurity effects" -, I have performed a "quantitative verification". I compared the value of  $u_A$  for "freeze-to-freeze repeatability" [7], against the resultant of the Type B standard uncertainties related to the incriminated "thermal effects" and "impurity effects", which will be denoted here  $u_{B,2\text{effects}}$ . To perform this verification, I used the data in the comparison CCT-K3 [7].

The calculus contradicts the theory enounced in Section 5.3. It is for 8 out of the 107 values analysed that the equation  $u_A = u_{B,2\text{effects}}$  is valid; the rest of the values are equally distributed in two groups: one group where the ratio  $u_A : u_{B,2\text{effects}}$  is subunitary ( $u_A < u_{B,2\text{effects}}$ ) and a second group where the ratio  $u_A : u_{B,2\text{effects}}$  is superunitary ( $u_A > u_{B,2\text{effects}}$ ), even up to the value 17 (NIST, Sn point). (In absolute value, the "freeze-to-freeze repeatability" varies within the Comparison [7] from 0.32 mK at the Ar point (VSL), to 0.89 mK at the Zn point (MSL) or to 1.1 mK at the Al point (NRLM)).

There is no place here to give these results an interpretation beyond the objective set. I shall only add that a similar comparison between  $u_A$  and the combined value of all uncertainties obtained from a Type B evaluation - the *total* Type B uncertainty - showed that  $u_A$  is up to 7 times greater

for more than a quarter (27 %) of the 107 values of CCT-K3<sup>4</sup>. For instance: NIST at Hg: 7; VSL at Ar: 6; NIST at Sn: 6 etc. Therefore, to exclude  $u_A$  would mean to reduce the fixed point uncertainty,  $u_c(W)$ , by up to 7 times: NIST - from 0,07 mK to 0,01 mK, at Hg point and from 0,12 mK to 0,02 mK at Sn point; VSL - from 0,32 mK to 0,05 mK at Ar point etc.

One thing is beyond doubt and imperative: the uncertainty associated with the readings of the bridge,  $u(X)$ , must be included in the Document CCT/08-19/rev! It is simply amazing for me to see this essential component of uncertainty in SPRT calibration omitted, deliberately or not.

I wonder whether there has been any user of the Document CCT/08-19/rev for the past 4 years since its release? If yes, what were the consequences?

3) The Document CCT/08-19/rev introduces the uncertainty of the resistance ratio due to oxidation, which is given by (6.4):

$$u^2(W_{\text{ox}}) = (1-Z)^2 W(t)^2 \frac{u^2(R_{\text{H}_2\text{O,ox}})}{R_{\text{H}_2\text{O}}^2} + u^2\left((1-Z)^2 W(t)^2\right) \frac{\Delta R_{\text{H}_2\text{O,ox}}}{R_{\text{H}_2\text{O}}^2},$$

”where  $u(R_{\text{H}_2\text{O,ox}})$  is the uncertainty of the water triple point resistance due to oxidation”. The uncertainty  $u(R_{\text{H}_2\text{O,ox}})$ , says the Document (p.29), ”can be estimated<sup>5</sup> from the range of water-triple-point resistances observed during calibration”.

Unfortunately, the wording<sup>6</sup> ”the range of water-triple-point resistances observed during calibration” is ambiguous, and the two examples in Sections 9.9 and 9.10, where  $u(R_{\text{H}_2\text{O,ox}})$  is considered, do not clarify but aggravate the confusion, as they contradict each other. The estimate of  $u(R_{\text{H}_2\text{O,ox}})$  ”from the range of water-triple-point resistances observed during calibration” could mean that  $u(R_{\text{H}_2\text{O,ox}})$  is calculated from the range of all  $R_{\text{H}_2\text{O}}$  values determined during calibration and, therefore,  $u(R_{\text{H}_2\text{O,ox}})$  will have the same value at all fixed points in the subrange, as in (9.16). Alternatively, it could mean that it is calculated from the  $R_{\text{H}_2\text{O}}$  values determined during calibration at each fixed point, in which case  $u(R_{\text{H}_2\text{O,ox},i})$  will have different values for the different fixed points, as in (9.13).

<sup>4</sup> CCT, the world highest authority in thermometry, in its Key Comparison 3 performed between 1997 and 2001, did not use mathematical models for evaluating the measurement uncertainty: the Type A or Type B standard uncertainties were simply combined using summation in quadrature, with no sensitivity coefficients, and the correlations between the input quantities were ignored. I would point out that, during the same period, in Romania, in the Thermometry Laboratory of the National Institute of Metrology, GUM guidelines (measurement modelling, the law of propagation of uncertainty, the correlations issue, etc.) had been gradually implemented and mathematical models of the measurement for evaluating the uncertainty had been developed. Two methods for the calculation of the propagated uncertainties at intermediate temperatures in the water – zinc subrange from the measurement uncertainties at the fixed points were published in 1993 [13]. The sensitivity coefficients  $\partial W/\partial W(\text{Sn})$  and  $\partial W/\partial W(\text{Zn})$  were calculated by computer assisted symbolic processing. Although advanced and rigorous, the methods did not sort out the major problem of the propagation of measurement uncertainty, which is the problem of the covariance associated with the  $W_{\text{Sn}}$  and  $W_{\text{Zn}}$  ratios. The first mathematical model of the measurement for the calibration of the SPRTs at the fixed points of ITS-90, that I have developed in a study of the National Institute of Metrology in June 1998, was published in the *Metrologie* 2, 2000 [14]. In 1998, no measurement model for the calibration of SPRTs at the fixed points had been presented in a paper of international circulation. A confirmation of the validity of the model came from the one put forward in the 2001 Technical Protocol of EUROMET-T.K3, by BNM-INM/CNAM. In 2001, I have elaborated [2, 9] a new measurement model of an SPRT calibration at the defining fixed points, and a new method for evaluating the uncertainties propagated at intermediate temperatures [8].

<sup>5</sup> There is no guidance in the Document for how to evaluate  $u(R_{\text{H}_2\text{O,ox}})$  ”from the range of water-triple-point resistances observed during calibration”.

<sup>6</sup> The Document should not be a charade or a contest where we try to guess „what the authors meant to say” (and what they did not mean to say). It should comply with general standards for scientific writing, moreover as the authors meant it to be a guide. Therefore, the symbols used, the models involved, the calculation methods, should be as explicit as possible. The role of the Document should be to clarify, and not to stir confusion.

Regardless of how many of the  $R_{\text{H}_2\text{O}}$  values are used to calculate  $u(R_{\text{H}_2\text{O,ox}})$ , one thing is certain: **the increases in the triple-point resistance due to oxidation,  $\Delta R_{\text{H}_2\text{O,ox}}$  and the measured resistances at the triple point of water,  $R_{\text{H}_2\text{O}}$  are correlated. Unfortunately, their covariances are ignored** in the Document.

Moreover, **to include a component due to oxidation in the calculus of the uncertainty  $u(W)$  is to double-count one part of the uncertainty of the water triple point resistance.** This is because the oxidation contributes to the variability of the observations.

4) A CCT Document "for assessing the uncertainty in calibrations and temperature measurements employing SPRTs", intended even to be as a guide for the "users of the ITS-90", should have first presented and analysed the three general cases, including all of the possible sources of uncertainty in Sections 2-8 for low, medium, and, respectively, high temperatures. More than that, since the authors declare "the interests of promoting harmonisation and ensuring consistency with the ISO Guide", the Document CCT/08-19/rev should have covered all steps for evaluating the uncertainty of the measurement result as presented in Section 8 in GUM [1], where defining a proper measurement model is of critical importance for the evaluation of uncertainty.

These general models should clearly define the functional relationship between the measurand and all input quantities upon which it depends. Subsequent analyses on specific cases could then be made. In their turn, the users would be able to fine-tune the general models down to their laboratory measurement conditions, without difficulty.

Unfortunately, the Document CCT/08-19/rev does not meet these expectations. Instead of mathematical models that are as complete as possible and instead of methodologies that follow the GUM rules, the examples in the Document are extremely restrictive, as they issue from simplifying assumptions or from approximations.

Here is an example: the equation for the calculation of the variance associated with a measured zero-current resistance (8.20):

$$\begin{aligned}
 u^2(R_{\text{meas}}) = & X^2 \left( u^2(R_{\text{S,cal}}) + R_S^2 (t_{\text{bath}} - t_{\text{cal}})^2 u^2(\beta) + u^2(R_{\text{S,ac-dc}}) + u^2(R_{\text{S,power}}) + u^2(R_{\text{S,p}}) \right) + \frac{I_2^4 + I_1^4}{(I_2^2 - I_1^2)^2} R_S^2 X^2 \beta^2 u^2(t_{\text{bath}}) \\
 & + R_S^2 u^2(X_{\text{INL}}) + \frac{R_S^2}{(I_2^2 - I_1^2)^2} \left[ (I_1^4 + I_2^4) u^2(X_{\text{DNL}}) + I_2^4 u^2(X_{1,\text{noise}}) + I_1^4 u^2(X_{2,\text{noise}}) \right] \\
 & + 4R_S^2 \Delta X_{\text{sh}}^2 \frac{I_2^4}{(I_2^2 - I_1^2)^2} \left( \frac{u^2(I_1)}{I_1^2} + \frac{u^2(I_2)}{I_2^2} \right),
 \end{aligned}$$

which is one of the most important equations in the Document CCT/08-19/rev.

Equation (8.20) stands for the law of propagation of uncertainty applied to a **mathematical model missing from the Document** and on which we can only speculate based on the scarce information that is provided. The equation is based on a series of assumptions, many of which are not stated explicitly:

- a)  $t_{\text{bath1}} - t_{\text{cal}} = t_{\text{bath2}} - t_{\text{cal}} = t_{\text{bath}} - t_{\text{cal}}$  i.e.  $t_{\text{bath1}} = t_{\text{bath2}} = t_{\text{bath}}$ ,
- b)  $R_{\text{S,power1}} = R_{\text{S,power2}} = R_{\text{S,power}}$ ,
- c)  $R_{\text{S,ac-dc1}} = R_{\text{S,ac-dc2}} = R_{\text{S,ac-dc}}$ ,
- d)  $R_{\text{S,p1}} = R_{\text{S,p2}} = R_{\text{S,p}}$ , i.e.  $p_1 = p_2 = p$  (see Equation (8.5)),
- e)  $X_1 = X_2 = X$ ,
- f)  $R_S(t_{\text{cal}}) = R_S$ ,



- g)  $\beta(t_{\text{bath1}} - t_{\text{cal}}) \ll 1$  and  $\beta(t_{\text{bath2}} - t_{\text{cal}}) \ll 1$ ,
- h)  $X_{1,\text{INL}} = X_{2,\text{INL}} = X_{\text{INL}}$ ,
- i)  $u(X_{1,\text{DNL}}) = u(X_{2,\text{DNL}}) = u(X_{\text{DNL}})$ ,
- j)  $X_{1,\text{DNL}}$  and  $X_{2,\text{DNL}}$  are uncorrelated,
- k)  $X_{1,\text{noise}}$  and  $X_{2,\text{noise}}$  are uncorrelated,
- l)  $I_1$  and  $I_2$  are uncorrelated,
- m)  $t_{\text{bath1}}$  and  $t_{\text{bath2}}$  are uncorrelated,
- n)  $u(t_{\text{bath1}}) = u(t_{\text{bath2}}) = u(t_{\text{bath}})$ .

(Indexes 1 and 2 refer to the two measurements made using the currents  $I_1$  and  $I_2$ , respectively).

Thus, for all input quantities with the exception of  $X_{\text{noise}}$  and  $I$ , the assumption was made that their estimates or their uncertainties **are equal** for both of the measurements made using the currents  $I_1$  and  $I_2$ .

Even more, the assumptions are used selectively to deduct (8.20). For instance, hypothesis e) is considered only for the calculation of the term in  $u^2(t_{\text{bath}})$ . Moreover, for the calculation of the term in  $u^2(t_{\text{bath}})$ , approximation a) on the equality of temperatures is not valid, only the equality between their uncertainties stands true (assumption n)). Finally, the approximation f) is used only in the second and the sixth term on the first line of 8.20, where  $R_S$  no longer stands for the standard resistance after the corrections have been applied (see equations (8.1) – (8.6)), but it stands for the standard resistance at the calibration temperature (previously symbolised as  $R_S(t_{\text{cal}})$  or  $R_{S,\text{cal}}$ ).

Also, it is worth repeating that the equation lacks the Type A uncertainties associated with the bridge readings,  $u(X_1)$  and  $u(X_2)$ , respectively.

The series of approximations continues in the equation of the variance associated with a resistance ratio, that is (8.21):

$$u^2(W_{\text{meas}}) = \frac{(1+W^2)}{X_{\text{H2O}}^2} \left[ u^2(X_{\text{INL}}) + \frac{(I_2^4 + I_1^4)}{(I_2^2 - I_1^2)^2} (X^2 \beta^2 u^2(t_{\text{bath}}) + u^2(X_{\text{DNL}}) + u^2(X_{\text{noise}})) \right] + \frac{(\Delta X_{\text{sh}} - W \Delta X_{\text{sh,H2O}})^2}{X_{\text{H2O}}^2} \frac{8I_2^4}{(I_2^2 - I_1^2)^2} \left( \frac{u^2(I)}{I^2} \right),$$

which brings us to the incredible situation where **the estimates/uncertainties of all input quantities to  $R_i$  are considered equal with the corresponding ones for  $R_{\text{H2O}}$** :

- a)  $t_{\text{bath1}/i} = t_{\text{bath2}/i} = t_{\text{bath1}/\text{H2O}} = t_{\text{bath2}/\text{H2O}} = t_{\text{bath}}$ ,
- b)  $R_{S,p1/i} = R_{S,p2/i} = R_{S,p1/\text{H2O}} = R_{S,p2/\text{H2O}} = R_{S,p}$ , i.e.  $p_{1/i} = p_{2/i} = p_{1/\text{H2O}} = p_{2/\text{H2O}} = p$ ,
- c)  $R_{S,\text{power1}/i} = R_{S,\text{power2}/i} = R_{S,\text{power1}/\text{H2O}} = R_{S,\text{power2}/\text{H2O}} = R_{S,\text{power}}$ ,
- d)  $R_{S,\text{ac-dc1}/i} = R_{S,\text{ac-dc2}/i} = R_{S,\text{ac-dc1}/\text{H2O}} = R_{S,\text{ac-dc2}/\text{H2O}} = R_{S,\text{ac-dc}}$ ,
- e)  $X_{1,\text{INL}/i} = X_{2,\text{INL}/i} = X_{\text{INL}/i}$  and  $X_{1,\text{INL}/\text{H2O}} = X_{2,\text{INL}/\text{H2O}} = X_{\text{INL}/\text{H2O}}$ ,
- f)  $u(X_{\text{INL}/i}) = u(X_{\text{INL}/\text{H2O}}) = u(X_{\text{INL}})$ ,

g) the authors "have ignored the correlation in the two INL terms (which is likely if  $W$  is close to 1)",

- h)  $X_{1/i} = X_{2/i} = X_{1/\text{H2O}} = X_{2/\text{H2O}} = X$ ,

- i)  $u(X_{1,DNL/i}) = u(X_{2,DNL/i}) = u(X_{1,DNL/H_2O}) = u(X_{DNL,2/H_2O}) = u(X_{DNL})$ ,
- j)  $u(X_{1,noise/i}) = u(X_{2,noise/i}) = u(X_{1,noise/H_2O}) = u(X_{2,noise/H_2O}) = u(X_{noise})$ ,
- k)  $\frac{u(I_{1/i})}{I_{1/i}} = \frac{u(I_{2/i})}{I_{2/i}} = \frac{u(I_{1/H_2O})}{I_{1/H_2O}} = \frac{u(I_{2/H_2O})}{I_{2/H_2O}} = \frac{u(I)}{I}$ ,
- l)  $X_{1,DNL/i}$ ,  $X_{2,DNL/i}$ ,  $X_{1,DNL/H_2O}$  and  $X_{2,DNL/H_2O}$  are uncorrelated,
- m)  $X_{1,noise/i}$ ,  $X_{2,noise/i}$ ,  $X_{1,noise/H_2O}$  and  $X_{2,noise/H_2O}$  are uncorrelated,
- n)  $I_{1/i}$ ,  $I_{2/i}$ ,  $I_{1/H_2O}$  and  $I_{2/H_2O}$  are uncorrelated,
- o)  $R_{S/i}(t_{cal}) = R_{S/H_2O}(t_{cal}) = R_S(t_{cal})$ ,  $\beta_i = \beta_{H_2O} = \beta$  and  $\gamma_i = \gamma_{H_2O} = \gamma$  (the resistance measurements are made with the same standard resistor),
- p)  $R_S(t_{cal}) = R_S$ ,
- q)  $\beta(t_{bath1/i} - t_{cal}) \ll 1$ ,  $\beta(t_{bath2/i} - t_{cal}) \ll 1$ ,  $\beta(t_{bath1/H_2O} - t_{cal}) \ll 1$  and  $\beta(t_{bath2/H_2O} - t_{cal}) \ll 1$ ,
- r)  $t_{bath1/i}$ ,  $t_{bath2/i}$ ,  $t_{bath1/H_2O}$  and  $t_{bath2/H_2O}$  are uncorrelated,
- s)  $u(t_{bath1/i}) = u(t_{bath2/i}) = u(t_{bath1/H_2O}) = u(t_{bath2/H_2O}) = u(t_{bath})$ .

It should be noted that some of the approximations are on the verge of nonsense, such as  $X_{1/i} = X_{2/i} = X_{1/H_2O} = X_{2/H_2O} = X$ . It refers to the term

$$\frac{1}{X_{H_2O}^2} \frac{(I_2^4 + I_1^4)}{(I_2^2 - I_1^2)^2} \beta^2 u^2(t_{bath})(1 + W^2) X^2 \quad (3)$$

in (8.21), where "X" is not identifiable for the reader; it can equally stand for  $X_i$  or for  $X_{H_2O}$ . The correct expression of the term  $(1 + W^2) X^2$  in (3) above is  $(X_i^2 + W^2 X_{H_2O}^2)$ . The use of  $X_i$ , i.e.

$(1 + W^2) X_i^2$  - case a)

or, alternatively, of  $X_{H_2O}$ :

$(1 + W^2) X_{H_2O}^2$  - case b)

induces significant increase or decrease of the uncertainty related to the stability of the resistor temperature, depending on the value of  $W$ :

$$\text{case a)} \quad \left( \frac{(1 + W^2) X_i^2}{X_i^2 + W^2 X_{H_2O}^2} \right)^{1/2} \cong \left( \frac{1 + W^2}{2} \right)^{1/2}$$

or

$$\text{case b)} \quad \left( \frac{(1 + W^2) X_{H_2O}^2}{X_i^2 + W^2 X_{H_2O}^2} \right)^{1/2} \cong \left( \frac{1 + W^2}{2W^2} \right)^{1/2}$$

More specifically:

- an increase of up to 3 times (case a)) or a decrease of up to 1.4 times (case b)), for  $t > 0$  °C, and
- a decrease of up to 1.4 times (case a)) or an increase of up to 84 times (case b)), for  $t < 0$  °C.

With the above revealed simplifications, approximations and errors included<sup>7</sup>, the equations (8.20) and (8.21) are used in all examples of "total uncertainty" calculation that are dealt with in Section 9.

The approximation reaches its peak in these examples, as **the variances in the measurement of the resistance  $u^2(R_{\text{meas}})$  at the triple point of water and at all other fixed points in a calibration subrange are considered equal among themselves.** Whereas the simple presence in one of the terms of  $u(R_{\text{meas}})$  of  $X$  (actually,  $X_i$ ) – that obviously has different values at the different fixed points – would suffice to exclude this equality.-

In this context, we also have to point at the strange, inconsistent combination between (9.13)

$$u_{\text{total}}^2(W_r) = \frac{1}{R_{\text{H}_2\text{O}}^2} \left[ u^2(R) + W^2 u^2(R_{\text{meas}}) + (1-Z)^2 W^2 u^2(R_{\text{H}_2\text{O,ox}}) \right. \\ \left. + \sum_{i=1}^N u^2(R_i) f_i^2(W) + u^2(R_{\text{meas}}) \sum_{i=2}^N (1+W_i^2) f_i^2(W) + \sum_{i=2}^N (1-Z_i)^2 W_i^2 f_i^2(W) u^2(R_{\text{H}_2\text{O,ox}}) \right]$$

and (9.15) (which is derived from equation (8.20) by using **an additional set of simplifying assumptions!** See Section 9.9):

$$u^2(R_{\text{meas}}) = R_S^2 \frac{(I_2^4 + I_1^4)}{(I_2^2 - I_1^2)^2} \left( u^2(X_{\text{DNL}}) + X_i^2 \beta^2 u^2(t_{\text{bath}}) + u^2(X_{\text{noise}}) \right).$$

In this case, although  $u^2(R_{\text{meas}})$  is not expressed as a function of  $X$ , but of  $X_i$ , the different values that would result from (9.15) can not be substituted in (9.13) because there  $u^2(R_{\text{meas}})$  is defined by a unique value for all fixed points! That is through a unique  $X$  (which is not identified and is not quantified). The same happens in (9.16) and (9.18).

The priority of the authors seems to be fewer lines in the expressions of uncertainties, at the expense of accuracy, rigor and generality. That is an inappropriate, obsolete, and damaging objective. We live for some time already in the microchip era, symbolic computation is nowadays a standard software tool, and therefore easing pen on paper calculation should be less than a minor concern.

Approximations and simplifications used in the methods for calculating uncertainty in Document CCT generate errors in the calculated value of the uncertainty associated with the result of the measurement. The thus generated errors, be they less significant, or considerable, should all be estimated and presented explicitly in the Document; that way, the user would be enabled for an informed decision to either ignore errors as negligible, or eliminate errors by discarding those assumptions which led to them.

**5)** The method for the evaluation of the measurement uncertainty presented in the Document CCT/08-19/rev erroneously treats the problem of correlation. The models in [2, 8, 9] whereby the evaluation of the correlations can be avoided are applied only partially, in association with the method for the propagation of uncertainty in [10, 11, 12].

Let us now consider the simplest case - the calculation of the uncertainty associated with the resistance ratio at a fixed point  $i$ ,  $W_i = R_i/R_{\text{H}_2\text{O}}$  (Section 9.4). The two input quantities for  $W_i$  ( $R_i$

<sup>7</sup> The errors highlighted above were propagated in the EURAMET TC-T workshop held between 27–28 October 2011, at SMD, Bruxelles, where the presentation *Uncertainties related to resistance measurement* reproduced the entire contents of Section 8 of the Document CCT, with no amendment (not even a correction of the terms that are dimensionally incorrect in equations 8.15 and 8.19).

and  $R_{i,H_2O}$ ) are correlated, since they share several common input quantities. Nevertheless, in the Document, the uncertainty of the resistance ratio at the fixed point  $i$ ,  $u(W_i)$ , is given by (see (9.5))

$$u^2(W_i) = \frac{1}{R_{H_2O}^2} \left[ u^2(R_i) + W_i^2 u^2(R_{i,H_2O}) \right],$$

without taking into account the correlation between  $R_i$  and  $R_{H_2O,i}$ . The authors of the Document consider that "these types of correlation problems are best simplified by expanding the equations in terms of the measured quantities" (p. 65) and they express the  $R_i$  and  $R_{H_2O,i}$  in terms of a set of independent variables  $Z_{i,k}$  on which  $R_i$  and  $R_{H_2O}$  depend (equation (9.3)), as in [2, 9]<sup>8</sup>. But this solution is not sufficient. The evaluation of the correlation  $u(R_i, R_{H_2O})$  can be avoided [8, 9] provided that  $W_i$  is also expressed in terms of the uncorrelated variables  $Z_{i,k}$  (see (3) in [8]):  $W_i = G_i(Z_{i,1}, Z_{i,2}, \dots, Z_{i,m})$ . As a result,  $u(W_i)$  will be calculated directly by combining the variances of the independent variables  $Z_{i,k}$ .

In the Document CCT, the output quantity  $W_i$  is expressed in terms of  $R_i$  and  $R_{H_2O,i}$ , which are correlated quantities. As a consequence, the equation of the variance of  $W_i$  should include not only the variances of  $R_i$  and  $R_{H_2O}$ , as in (9.5), but also **their covariance**<sup>9</sup>,  $u(R_i, R_{H_2O})$ , like this:

$$u^2(W_i) = \frac{1}{R_{H_2O}^2} \left[ u^2(R_i) + W_i^2 u^2(R_{i,H_2O}) - 2W_i u(R_i, R_{i,H_2O}) \right] \quad (4)$$

where

$$u(R_i, R_{i,H_2O}) = \sum_{k=1}^m \frac{\partial R_i}{\partial x_{i,k}} \frac{\partial R_{H_2O}}{\partial x_{i,k}} u^2(x_{i,k}). \quad (5)$$

Obviously, in the case of the calculation of  $u^2(W_r)$ , the impact of correlations is much greater, because:

- more fixed points are involved, therefore more  $u(R_i, R_{i,H_2O})$  covariances come along with variances  $u^2(W_i)$  (see equation (4)), and
- $u^2(W_r)$  has to include, along with  $u^2(W_i)$ , the covariances among the resistance ratios  $u(W_i, W_j)$ :

$$u^2(W_r) \cong \sum_{i=2}^N f_i^2 u^2(W_i) + 2 \sum_{i=2}^{N-1} \sum_{j=3}^N f_i f_j u(W_i, W_j) + u^2(W).$$

But covariances  $u(W_i, W_j)$  are very difficult to evaluate. Worse even, including these new terms in the equations for  $u^2(W_r)$  in the Document is losing the main announced benefit of the method proposed by the authors, that is a simplified form for "total uncertainty".

To avoid the need to introduce these covariances in  $u^2(W_r)$  it is necessary [8, 9] that  $W_r(T_{90})$  be expressed in terms of the set of uncorrelated variables  $Z_{i,k}$  on which  $R_i$  and  $R_{i,H_2O}$  depend (see (5) in

<sup>8</sup> Equation (9.3) is almost identical to the equation (3) in [2]. The resemblance is not noticeable at a first look due to the different symbols used (for instance, the temperature coefficient is marked as  $\beta$  instead of the usual  $\alpha$ , the symbol consecrated for decades; the derivative  $\left. \frac{dW_r}{dT_{90}} \right|_{T_{90}=273.16 \text{ K}}$  is replaced by  $\frac{dW_1}{dt}$ ,  $C_1 \rightarrow \Delta t_{\text{iso}}$ ,  $C_7 \rightarrow \Delta X_{\text{sh}}$ , etc.). But, as

soon as we replace the notations used in the expression of one of the equations by the symbols used in the other for the same input quantities, the two equations are almost identical.

<sup>9</sup> Also, in [10], I. Lira expressed the temperature  $T$  (equivalent of  $W_r$ ) in terms of the coefficients of the deviation function,  $\phi_i$ , and not as a function of the uncorrelated variables on which they depend:  $\phi_i = f_i(x_1, x_2, \dots)$ . As a result, he had to include the covariance between  $\phi_i$  and  $\phi_j$  in the calculation of the uncertainty  $u(T)$ .

[8]). Thus,  $u^2(W_i)$  will be calculated directly by combining the variances of the independent variables  $Z_{i,k}$ .

Unfortunately, the authors use in an incomplete and ineffective manner the available means to avoid correlations among input quantities for  $W_i$  and  $W_r$ . Although correlations are still present, the significant contributions of the covariances  $u(R_i, R_{i,H_2O})$  and  $u(W_i, W_j)$  to  $u^2(W_i)$  and, respectively, to  $u^2(W_r)$  are omitted in the Document, with considerable impact on the calculated uncertainty.

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