New model function for SPRT calibration at the defining fixed points of ITS-90

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Abstract. *The paper presents a new method for evaluating the combined standard uncertainty in the case of SPRT calibration at the defining fixed points of ITS-90. The main feature of the proposed method is the form of the model function, in which the input quantities are elementary and do not depend upon common variables, thus reducing drastically the incidence of correlations among them. The analytical expressions of the sensitivity coefficients are determined using a dedicated computer programme, developed in a software environment with symbolic processing facilities. The capabilities of the model are illustrated on a sample set of input data, assembled from research projects in NIM Bucharest and from the reference literature.*

1. Introduction

The calibration of Standard Platinum Resistance Thermometers (SPRTs) at the defining fixed points of the International Temperature Scale of 1990 (ITS-90) [1] is the basis for the definition of the T_{90} temperatures in the range from 13.803 3 K to 961.78 ºC.

Temperatures are determined in terms of the ratio:

$$W(T_{90}) = R(T_{90}) / R(273.16K) \tag{1}$$

by means of a reference function $W_r(T_{90})$ and of a deviation function $\Delta W(T_{90})$:

$$W(T_{90}) = W_r(T_{90}) + \Delta W(T_{90}). \tag{2}$$

$W_r(T_{90})$ is a power series with coefficients provided in ITS-90. $\Delta W(T_{90})$ is a function with a general form, but the values of its coefficients are specific to the SPRT under calibration and are determined from measurements at the defining fixed points.

The uncertainties associated with the SPRT resistance measured at the temperatures of the fixed points are propagated at any intermediate temperature within the calibration range of the SPRT by using the interpolation relations (2).

The measurement uncertainty is usually evaluated using a mathematical model of the measurement and the law of propagation of uncertainty. The only measurements involved in determining the characteristic $W=f(T_{90})$ of an SPRT are the measurements of its resistance at the fixed points. Hence, the model functions for these measurements are of critical importance. The identification of the input quantities that the measurand depends upon, their characterization, and their representation in the model function are done based on the physical phenomena involved in the measurement process.

Important efforts of researchers in thermometry were focused lately on evaluating the uncertainties of realization of the Scale [2], [3], [4], [5], [6], [7], [8], [9], but only few available documents deal explicitly with the issue of the model function [2], [3], [4].

2. Model functions

The model function of an SPRT calibration at a defining fixed point expresses in a mathematical form the functional relationship between the measurand (i.e. the resistance of an SPRT, measured at that fixed point) and the input quantities that the measurand depends upon. The set of input quantities includes, in addition to the repeated observations, various influence quantities that are inexactly known. In the present approach, the measurand is eventually expressed as a function of the genuine input quantities, that are:

- quantities directly measured, and
- quantities directly characterized using scientific judgement.

The resulting form of the model function enables a systematic and consistent approach on the correlations issue. It also has the advantage of enabling the outline of the contributory variances of the genuine input quantities. This way, it substantiates the identification of those input quantities that have a heavy weight in the combined variance, as well of those that tolerate large margins of variation (in terms of associated uncertainties) without a significant impact on the uncertainty of measurement.

Let R_{TPW} be the SPRT resistance at the triple point of water (TPW) and R_{FP} the SPRT resistance at any other fixed point (FP). By using the notations:

$R_{s/TPW}$ – resistance of the standard resistor;

r_{TPW} – reading of the bridge at fixed point temperature,

the proposed model function is:

$$R_{TPW} = (R_{s/TPW} + C_{5/TPW} + C_{6/TPW})(r_{TPW} + C_{7/TPW} + C_{8/TPW}) + (C_{1/TPW} + C_{2/TPW} + C_{3/TPW}) / K \, R_{TPW} \left.\frac{dW_r}{dT_{90}}\right|_{T_{90}=273.16\,K} \tag{3}$$

where the approximation $\left.\frac{dW}{dT_{90}}\right|_{T_{90}} \cong \left.\frac{dW_r}{dT_{90}}\right|_{T_{90}}$ was used, with $\left.\frac{dW_r}{dT_{90}}\right|_{T_{90}}$ evaluated by means of equations (9a) or (10a) in [1]. The model function includes the corrections C_i that have to be applied to compensate for the systematic effects involved in the realization of the fixed point and in the resistance measurement:

C_1 – the correction for the influences of the chemical impurities or for the variation of the isotopic composition of water, respectively;

C_2 – the correction for parasite heat fluxes (departure from the thermal equilibrium);

C_3 – the correction for the effect of the hydrostatic pressure;

C_5 – the drift of the resistance of the standard resistor since its latest calibration;

C_6 – the correction for the variation with the temperature of the standard resistance;

C_7 – the correction for the self heating effect;

C_8 – the correction for the systematic effects that arise in the measurement bridge (due to the non-linearity, to the limited resolution, and so on).

A similar expression is obtained for R_{FP}, with the only difference that the model function could include (if is not a triple point) the correction for the deviation of the gas pressure in the fixed point cell from the reference pressure [1], C_4:

$$R_{FP} = (R_{s/FP} + C_{5/FP} + C_{6/FP})(r_{FP} + C_{7/FP} + C_{8/FP}) + (C_{1/FP} + C_{2/FP} + C_{3/FP} + C_{4/FP})/K\, R_{TPW} \left.\frac{dW_r}{dT_{90}}\right|_{T_{90}=T_{FP}} \quad (4)$$

It is worth noting that, by converting $C_{1/FP}$, $C_{2/FP}$, $C_{3/FP}$ and $C_{4/FP}$ in ohms in relation (4), R_{TPW} turns into an input quantity for R_{FP}, with two important consequences: the calibration uncertainty at TPW propagates into the calibration uncertainty at FP, and correlations among input quantities of both R_{TPW} and R_{FP} have to be considered when uncertainty is evaluated for R_{FP}.

Some of the input quantities (R_s, C_5 and C_6 ; r_{FP} or r_{TPW}, C_7 and C_8) are correlated, as they depend upon one or more common variables. Those input quantities will be expressed in this model as functions of the independent variables they all depend upon, thus reducing drastically the incidence of correlations among them.

On the other side, input quantities C_3 and C_4 are themselves measurands and they depend upon other quantities. Therefore, C_3 and C_4 will be also expressed as functions of the input quantities they depend on.

With the notations:

- b_{TPW}, b_{FP} – the coefficient of the drift of the resistance of the standard resistor since its latest calibration;
- t_{TPW}, t_{FP} – the time of the calibration of SPRT at TPW and FP, respectively;
- t_0 – the time of the calibration of the standard resistor ($\{t_0\}_{\mathrm{d}} = 0$);
- α_{TPW}, α_{FP} – the temperature coefficient of the standard resistor;
- $T_{b1/TPW}$, $T_{b1/FP}$, $T_{b2/TPW}$, $T_{b2/FP}$ – the temperatures of the oil bath for the maintenance of the standard resistor during the measurements, using the currents I_1 and I_2, respectively;
- T_r – the calibration temperature of the standard resistor ($\{T_r\}_{\mathrm{K}} = 293.15$);
- $r_{1/TPW}$, $r_{1/FP}$, $r_{2/TPW}$, $r_{2/FP}$ – the ratios of the resistance measured using the currents I_1 and I_2, respectively;
- $r_{c1/TPW}$, $r_{c1/FP}$; $r_{c2/TPW}$, $r_{c2/FP}$ – the correction factors for the readings of the bridge r_1 and r_2, respectively [10], [9];
- $I_{1/TPW}$, $I_{1/FP}$, $I_{2/TPW}$, $I_{2/FP}$ – the measurement currents of the bridge;
- A_{FP}, A_{TPW} – the coefficient of variation of the temperature with the immersion depth;
- h_{FP}, h_{TPW} - the immersion depth;
- B_{FP} – the coefficient of variation of the FP temperature with the deviation of the gas pressure in the cell from the reference pressure;
- δp_{FP} – the deviation of the gas pressure in the cell from the reference pressure,

the expressions of R_{TPW} and R_{FP} become:

$$R_{TPW} = \frac{R_{s/TPW}\,[1 + b_{TPW}\,(t_{TPW} - t_0)]}{(I^2_{2/TPW} - I^2_{1/TPW})\left[1 - (C_{1/TPW} + C_{2/TPW} - A_{TPW}\,h_{TPW})/K \left.\frac{dW_r}{dT_{90}}\right|_{T_{90}=273.16\,K}\right]} \times$$

$$\times \{[1 + \alpha_{TPW}(T_{b1/TPW} - T_r)]\, r_{1/TPW}\, r_{c1/TPW} I^2_{2/TPW} - [1 + a_{TPW}(T_{b2/TPW} - T_r)]\, r_{2/TPW}\, r_{c2/TPW} I^2_{1/TPW}\,]\} \quad (5)$$

$$R_{FP} = R_{s/FP}\,[1 + b_{FP}(t_{FP} - t_0)]\,\{[1 + \alpha_{FP}(T_{b1/FP} - T_r)]\,r_{1/FP}\,r_{c1/FP}\,I_{2/FP}^2 - \\ -[1 + \alpha_{FP}(T_{b2/FP} - T_r)]\,r_{2/FP}\,r_{c2/FP}\,I_{1/FP}^2]\}/(I_{2/FP}^2 - I_{1/FP}^2) + \\ +(C_{1/FP} + C_{2/FP} - A_{FP}\,h_{FP} - B_{FP}\,\delta p_{FP})/K\,R_{TPW}\left.\frac{dW_r}{dT_{90}}\right|_{T_{90}=T_{FP}} \tag{6}$$

With the exception of [2], other models reported in the reference literature, by using a summative function similar with (3) and (4), do not express the model function as an analytical expression of the genuine input quantities and they stop short from taking into account the correlations among input quantities.

3. The evaluation of calibration uncertainty at the triple point of water

According to ITS-90, T_{90} temperatures are determined as functions of the ratio $W(T_{90})$ between the resistance measured at each specified fixed point other than TPW and the resistance measured at the TPW. Therefore, the calibration uncertainty at a fixed point is not of interest. Nevertheless, the calibration uncertainty at TPW is useful for monitoring the stability of the SPRT.

An essential feature of the model function proposed here for the calibration of SPRTs at the TPW (equation (5)) is that the input quantities $X_1, X_2, \ldots, X_{14}$ are independent, thus eliminating the necessity of evaluating the correlations among them. There are, still, two input quantities correlated on technical grounds, I_1 and I_2, but their correlation coefficient can be approximated reasonably well by 1.

For economy of notation, the same symbol is used below for a quantity and for its estimate.

The combined standard uncertainty associated with R_{TPW} is determined using the law of propagation of uncertainty for correlated input quantities [11], that becomes:

$$u_c^2(R_{TPW}) = \sum_{i=1}^{14}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + \left(\frac{\partial f}{\partial I_{1/TPW}}u(I_{1/TPW}) + \frac{\partial f}{\partial I_{2/TPW}}u(I_{2/TPW})\right)^2 \tag{7}$$

where $x_1, x_2, \ldots, x_{14}, I_{1/TPW}, I_{2/TPW}$ are the input estimates and f is the model function:

$$R_{TPW} = f(x_1, x_2, \ldots, x_{14}, I_{1/TPW}, I_{2/TPW}) \tag{8}$$

with its analytical form given by equation (5).

The model was implemented by means of a dedicated computer programme, using a software environment with symbolic processing facilities. The resulting analytical expressions of the sensitivity coefficients are much too large to be interpreted, presented or handled other way but by electronic means.

A sample use of the model is presented below for a set of input data, shown in Table 1, set assembled from research projects in NIM Bucharest and from the reference literature.

Table 1. Input data for R_{TPW}

Quantity	Estimate	Standard uncertainty
$R_{s/TPW}$	9.999 947 Ω	3×10^{-6} Ω
b_{TPW}	-5.48×10^{-10} d^{-1}	1.92×10^{-10} d^{-1}
t_{TPW}	100 d	1 d
α_{TPW}	16.36×10^{-6} K^{-1}	6×10^{-8} K^{-1}
$T_{b1/TPW}$, $T_{b2/TPW}$	293.171 K	0.007 K
$r_{1/TPW}$	2.552 565 4	3×10^{-7}
$r_{2/TPW}$	2.552 595 9	3×10^{-7}
$r_{c1/TPW}$, $r_{c2/TPW}$	1.000 000 0	1×10^{-7}
$I_{1/TPW}$	1.000×10^{-3} A	1.6×10^{-5} A
$I_{2/TPW}$	1.414×10^{-3} A	1.6×10^{-5} A
$C_{1/TPW}$	0.0000 K	1×10^{-4} K
$C_{2/TPW}$	0.00000 K	5×10^{-5} K
A_{TPW}	0.73×10^{-3} K m^{-1}	6×10^{-5} K m^{-1}
h_{TPW}	187×10^{-3} m	3×10^{-3} m

Table 2 summaries the values of the sensitivity coefficients and of the contribution to $u_c(R_{TPW})$, computed for each input quantity. For the set of values presented in Table 1, the value of the combined standard uncertainty associated with R_{TPW} is $u_c(R_{TPW})$=1.85 x 10^{-5} Ω, that is 0.18 mK.

The chart in Fig. 1 presents the greatest nine contributory variances of input quantities that result from the Table 2. On the same chart, the contribution of the group of correlated quantities I_1 and I_2 is also represented and labeled "I_1I_2".

Table 2. Values of the sensitivity coefficients and of the contributions to $u_c(R_{TPW})$

X_i	$c_i = \partial f/\partial x_i$	$u_i(R_{TPW})$ /(10^{-6} Ω)
$R_{s/TPW}$	2.552 54	7.658
b_{TPW}	2 552.5 Ω d	0.490
t_{TPW}	-1.398 x 10^{-8} Ω d^{-1}	0.014
α_{TPW}	0.536 Ω K	0.032
$T_{b1/TPW}$	8.352 x 10^{-4} Ω K^{-1}	5.846
$T_{b2/TPW}$	- 4.176 x 10^{-4} Ω K^{-1}	2.923
$r_{1/TPW}$	20.000 Ω	6.000
$r_{2/TPW}$	-10.000 Ω	3.000
$r_{c1/TPW}$	51.051Ω	5.105
$r_{c2/TPW}$	-25.526 Ω	2.553
$I_{1/TPW}$	0.862 7 Ω A^{-1}	13.803
$I_{2/TPW}$	-1.220 0 Ω A^{-1}	19.520
$C_{1/TPW}$	0.101 808 Ω K^{-1}	10.181
$C_{2/TPW}$	0.101 808 Ω K^{-1}	5.090
A_{TPW}	-1.9043 x 10^{-2} Ω K^{-1} m	1.142
h_{TPW}	7.43 x 10^{-5} Ω m^{-1}	0.223

The variation of the isotopic composition of the water in the triple point cell provides the dominant contribution to $u_c(R_{TPW})$. If, for example, $u(C_1)$ was 3 times smaller, the calibration uncertainty at TPW would get 15 % smaller and the weight of the contributory variance of C_1 to $u_c^2(R_{TPW})$ would decrease from 30 % to 4 %.

One can notice that, although $\frac{\partial f}{\partial C_2} = \frac{\partial f}{\partial C_1}$, the weight of the contributory variance of C_2 in $u_c^2(R_{TPW})$ is of only 8 %, because $u(C_2) = u(C_1)/2$.

Another major contribution to $u_c(R_{TPW})$ comes from the uncertainty of the standard resistor calibration. To lower the calibration uncertainty at TPW with almost 10 %, the value of $u(R_s)$ should be 1x10^{-6} Ω, that is 3 times smaller than in the original set of data.

The impact of the sensitivity coefficients, so of the form of the model function, on the combined standard uncertainty can be easily shown up for the following pairs of input quantities, for which the associated uncertainties are equal: r_1 and r_2, T_{b1} and T_{b2}, r_{c1} and r_{c2}. Doubling the uncertainties of these quantities determines increases of $u_c(R_{TPW})$ substantially different between the members of each pair, due to their sensitivity coefficients that stay in a 2:1 ratio:

- 15 % increase if r_1 or T_{b1} doubles, and 4 % increase, in r_2 and T_{b2} cases;
- 11 % increase, if r_{c1} doubles, and 3 % increase, in r_{c2} case (smaller impact because their contributions to $u_c(R_{TPW})$ are smaller).

It is also worth pointing out that neglecting the correlation between the currents I_1 and I_2 determines a value of the calibration uncertainty at TPW of 0.30 mK, that is an overestimation with 60 %.

The other input quantities (A, b, h, α and t) have small or negligible contributions to the calibration uncertainty at TPW. That is emphasized by the fact that $u_c(R_{TPW})$ turn out augmented by less than 1 % when the uncertainty associated with the input quantity increases:

- 2.5 times, in the case of A;

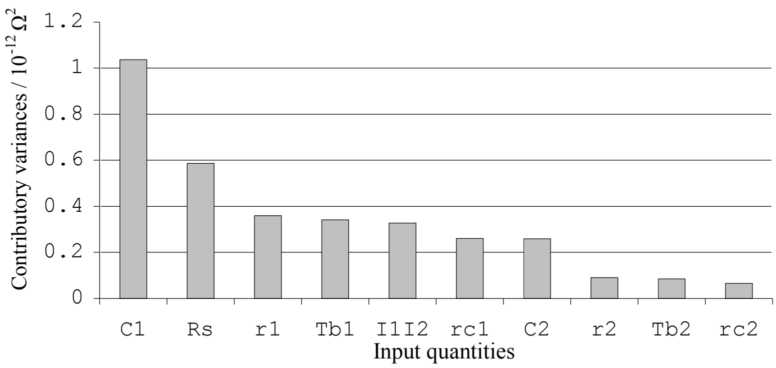

Figure 1. Contributory variances to the combined variance $u^2_c(R_{TPW})$

- 5 times in the case of *b*;
- 10 times in the case of h;
- 80 times in the case of α ;
- 150 times in the case of *t*.

4. Conclusions

The paper addressed the evaluation of the combined standard uncertainty in the case of SPRT calibration at the defining fixed points of ITS-90.

By using an elaborated form of the model function, based on input quantities at an elementary level, the impact of correlations was minimized and a direct, systematic, and coherent approach to evaluating the combined standard uncertainty was enabled. After overcoming the complexity of the analytical expressions, by taking advantage of the symbolic processing facilities offered by modern computer software, the model proved itself a powerful tool, that can provide the combined standard uncertainty associated with the result of the measurement, as well as the contributory variances of each input quantity. These features were illustrated in the case of the triple point of water. The model is flexible and easily expandable to include further input quantities discovered as relevant.

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