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Uncertainty Evaluation and Validation of a Comparison Methodology to Perform In-house Calibration of Platinum Resistance Thermometers using a Monte Carlo Method

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Abstract The uncertainty required by laboratories and industry for temperature measurements based on the practical use of platinum resistance thermometers (PRTs) can commonly be achieved by calibration using temperature reference conditions and comparison methodologies (TCM) instead of the more accurate primary fixed-point (ITS-90) method. TCM is suitable for establishing internal traceability chains, such as connecting reference standards to transfer and working standards. The data resulting from the calibration method can be treated in a similar way to that prescribed for the ITS-90 interpolation procedure, to determine the calibration coefficients. When applying this approach, two major tasks are performed: (i) the evaluation of the uncertainty associated with the estimate of temperature (a requirement shared by the ITS-90 method), based on knowledge of the uncertainties associated with the temperature fixed points and the measured electrical resistances, and (ii) the validation of this practical comparison considering that the reference data are obtained using the ITS-90 method. The conventional approach, using the GUM uncertainty framework,

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requires approximations with unavoidable loss of accuracy and might not provide adequate uncertainty evaluation for the methods mentioned, because the conditions for its valid use, such as the near-linearity of the mathematical model relating temperature to electrical resistance, and the near-normality of the measurand (temperature), might not apply. Moreover, there can be some difficulty in applying the GUM uncertainty framework relating to the formation of sensitivity coefficients through partial derivatives for a model that, as here, is somewhat complicated and not readily expressible in an explicit form. Alternatively, uncertainty evaluation can be carried out by a Monte Carlo method (MCM), a numerical implementation of the propagation of distributions that is free from such conditions and straightforward to apply. In this paper, (a) the use of MCM to evaluate uncertainties relating to the ITS-90 interpolation procedure, and (b) a validation procedure to perform in-house calibration of PRTs by comparison are discussed. An example illustrating (a) and (b) is presented.

Keywords Monte Carlo method · Platinum resistance thermometer calibration · Uncertainty evaluation

1 Introduction, Objectives, and Main Contributions

Platinum resistance thermometers (PRTs) are among the most common measuring instruments used in thermometry, and are applied in primary laboratories, calibration and testing laboratories, and industrial laboratories, for each of which different measurement uncertainties generally apply.

The International Temperature Scale of 1990 (ITS-90) [1] describes a procedure for the calibration of PRTs based on measurements at defining fixed points. The use of this procedure provides very small temperature uncertainties, but requires expensive metrological infrastructures that are generally inappropriate for testing and industrial laboratories. Instead, it is common practice to calibrate reference standards in primary laboratories according to the ITS-90 definition, and to perform in-house calibrations of transfer and working standards using temperature comparison methodologies.

There are two major issues associated with this practice: (i) the need to evaluate measurement uncertainties in a context where the GUM (Guide to the Expression of Uncertainty in Measurement) uncertainty framework [2] might not always be appropriate or might be difficult to apply, and (ii) the validation of the TCM approach.

The aims of this study were (a) to validate an instance of the TCM approach in comparison with the fixed-point methodology, (b) to use the Monte Carlo Method (MCM) to obtain measurement uncertainties reliably and straightforwardly, and (c) to apply the whole process to an actual calibration to check the fulfillment of metrological requirements.

The case study reported here concerns the calibration of PRTs in the range from 0°C to the freezing point of tin (231.928°C).

2 Brief Description of the Two Calibration Methods

The ITS-90 specifies procedures to calibrate PRTs in several temperature intervals and, in particular, in the interval for this study, 0–231.928°C. In these procedures, calibration is carried out (a) at specified sets of defining fixed points in terms of the ratio of the resistance $R(T_{90})$ at temperature T_{90} and the resistance $R(273.16\ \text{K})$ at the triple point of water, namely (using T rather than T_{90}),

$$W(T) = \frac{R(T)}{R(273.16\ \text{K})}, \tag{1}$$

and (b) using specified reference and deviation functions for interpolation at intermediate temperatures. For the temperature interval of this study, according to ITS-90 [1] the thermometer is calibrated at the triple point of water ($t_0 = 0.01°\text{C}$), and at the freezing points of indium ($t_1 = 156.5985°\text{C}$) and tin ($t_2 = 231.928°\text{C}$), using the deviation function given by

$$W(T) - W_{\text{r}}(T) = a[W(T) - 1] + b[W(T) - 1]^2, \tag{2}$$

with the values of a and b obtained by measurement at the defining fixed points.[1] In Eq. 2, $W_{\text{r}}(T)$ represents the reference function given by

$$W_{\text{r}}\ (t) = C_0 + \sum_{i=1}^{9} C_i \left[\frac{(t - 481)}{481}\right]^i, \tag{3}$$

with the C_0 and C_i constants given in the text of ITS-90 [1].

Values for a and b are determined by solving the pair of linear algebraic equations given by Eq. 2 using the measured values of $W(T)$ for $T = T_1$ and $T = T_2$, forming the corresponding values of $W_{\text{r}}(T)$ using Eq. 3.

Following the calibration of a PRT as above, the temperature corresponding to a resistance ratio $W_{\text{r}}(T)$ subsequently measured using the PRT is determined by the inverse use of Eq. 3. This use is facilitated by the provision of the explicit approximation,

$$t = D_0 + \sum_{i=1}^{9} D_i \left[\frac{W_{\text{r}}(t) - 2.64}{1.64}\right]^i, \tag{4}$$

equivalent to Eq. 3 within 0.13 mK, where again the D_i's are provided constants [1].

TCM uses the same formulation as the ITS-90 procedure, being different only in (a) the definition of the temperature reference condition, thermometric baths being used, and (b) the use of reference PRTs to obtain the reference-temperature values rather than the fixed-point reference temperatures. The measurement uncertainties so obtained are, naturally, greater than for the ITS-90 procedure.

In summary, the steps in the evaluation are as follows:

Calibration mode

1. Measure electrical resistance R_0, R_1, R_2 at reference temperatures T_0, T_1, T_2, respectively;

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[1] The notation used is that each temperature expressed in lower case (say t_0) is in °C and has a corresponding temperature expressed in the corresponding upper case (that is, T_0) in K.

2. Form the resistance ratios $W_1 = R_1/R_0$, $W_2 = R_2/R_0$;
3. Use Eq. 3 to evaluate $W_r(T_1)$ and $W_r(T_2)$;
4. Solve the pair of equations $W_i - W_r(T_i) = a(W_i - 1) + b(W_i - -1)^2$, $i = 1, 2$ for a and b.

Calibrated measurement mode

5. Measure electrical resistance R at the unknown temperature T;
6. Form the resistance ratio $W = R/R_0$ (possibly using a new measured value for R_0);
7. Form the reference resistance ratio $W_r = W - a(W - 1) - b(W - 1)^2$;
8. Use the inverse function, Eq. 4, to obtain the required temperature T.

This evaluation procedure can straightforwardly be applied using the nominal values for T_0, T_1, T_2 in step 1, and the measured values for the electrical resistances R_0, R_1, R_2, delivering the required estimate $\hat{T}$, say, of the unknown temperature T in step 8. The procedure can also be followed in terms of applying the GUM uncertainty framework: given standard uncertainties associated with the nominal values for T_0, T_1, T_2 and the measured values of R_0, R_1, R_2 (and, if appropriate, covariances associated with pairs of these values), (i) the standard uncertainty associated with $\hat{T}$ can be evaluated and (ii) an expanded uncertainty U related to $\hat{T}$ can be formed. In (i), the law of propagation of uncertainty would be applied, and in (ii), T would be characterized by a Gaussian distribution to deduce U.

The hardest part of the uncertainty evaluation relates to step 4, in which a and b are obtained by solving a pair of equations. White and Saunders [3] provide an elegant approach. Meyer and Ripple [4] derive equations for the uncertainty evaluation based on the application of the GUM uncertainty framework. In doing so, they take account of further influencing factors. Also, see Lira et al. [5].

3 Discussion of the Use of the GUM Uncertainty Framework and a Monte Carlo Method

Although the GUM uncertainty framework is commonly applied to evaluate measurement uncertainty, other approaches are increasingly used, especially a Monte Carlo method that implements the propagation of distributions [6]. In this section, we discuss the relative merits of using that framework and MCM for the problem investigated in this work. Both approaches use a functional model relating the input quantities (fixed-point temperatures T_0, T_1, T_2 and electrical resistances R_0, R_1, R_2, R) to a single (scalar) output quantity T. Moreover, both approaches consider that the input quantities are characterized by probability density functions (PDFs) obtained from knowledge of these quantities. The GUM uncertainty framework utilizes only summary parameters of those PDFs (expectations and standard deviations), whereas MCM uses the PDFs themselves. Furthermore, the GUM uncertainty framework characterizes the output quantity by a Gaussian PDF (or a scaled and shifted t-distribution), whereas MCM derives the PDF for the output quantity, whatever its form.

Moreover, the proposed solutions found in related research studies apply the conventional GUM uncertainty framework using Gaussian approximations [4,7,8], implementing differential calculus and procedures to handle correlation (e.g., resulting from the ratios in calibration and in measurement using the same reference value of R_0) [9].

There are several intermediate quantities in the above evaluation procedure, the coefficients a and b being particularly important: they describe the calibration of the PRT.

There are some topics meriting discussion in the approach to this problem, especially when using the GUM uncertainty framework:

1. Whether to work with a single model of evaluation, namely, T in terms of T_0, T_1, T_2, R_0, R_1, R_2, and R, or a pair of such models: (i) a and b in terms of T_0, T_1, T_2, R_0, R_1, and R_2, and (ii) T in terms of a, b, R_0, and R. It is arguably more reasonable to consider a pair of models, since they correspond to the two distinct stages: PRT calibration and use of the calibrated PRT;
2. The influence of model non-linearity, regarding the provision of an estimate of T, and the evaluation of the corresponding standard and expanded uncertainties. The difficulty of determining the partial derivatives required is one relevant consideration.

In the problem considered, the electrical resistance is regarded as having a Gaussian PDF. However, resistance ratios are used, which would then have non-Gaussian PDFs, as would the quantities (coefficients and temperatures) subsequently obtained from them. In fact, six of the above steps involve non-linear operations, all contributing to possible departures from normality. The GUM mainly considers the use of models that are linear or mildly non-linear, for which first-order partial derivatives must be evaluated, but states (clause 5.1.2) that higher-order derivatives must be used when non-linearity is significant. MCM makes no assumption regarding the output PDF and, therefore, does not impose any particular limitation related to input or output PDFs (only the ability to make random draws from the input PDFs). It combines them according to the mathematical model used, no judgment being required concerning whether contributions are significant. (The partial derivatives of first order within the GUM uncertainty framework provide valuable sensitivity coefficients. It is possible to implement a numerical procedure to provide information constituting a non-linear counterpart of a sensitivity coefficient [10]).

For the second stage of the two-stage approach, the GUM uncertainty framework requires the covariance associated with the estimates of the two coefficients. MCM deals with this aspect straightforwardly, since such covariance effects are readily handled (Sect. 5).

A further point of comparison concerns the uncertainty related to the estimate of T. In the approach used in the GUM uncertainty framework, an approximate solution is unavoidable, as a consequence of the model non-linearity. The extent of that approximation is very difficult to assess, emphasizing the advantage of MCM.

4 Uncertainty Evaluation Method and Experimental Data

The uncertainty evaluation is applied to a sequence of models (*chain* of functions) presented in the following steps and illustrated diagrammatically in Figs. 1 and 2.

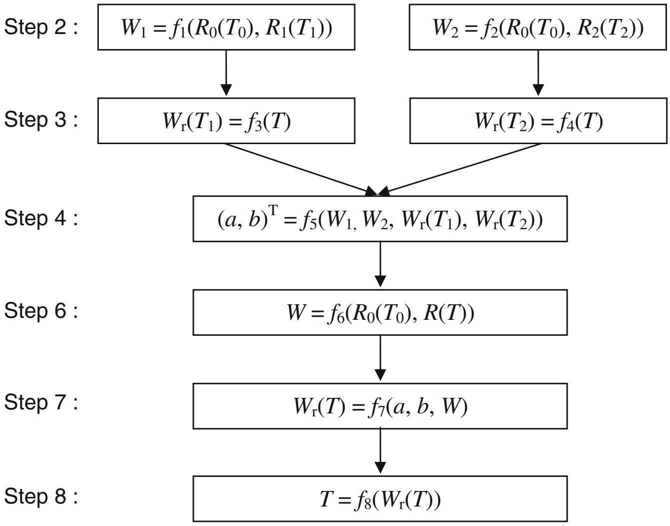

Fig. 1 Chain of functions related with calibration and evaluation of temperature

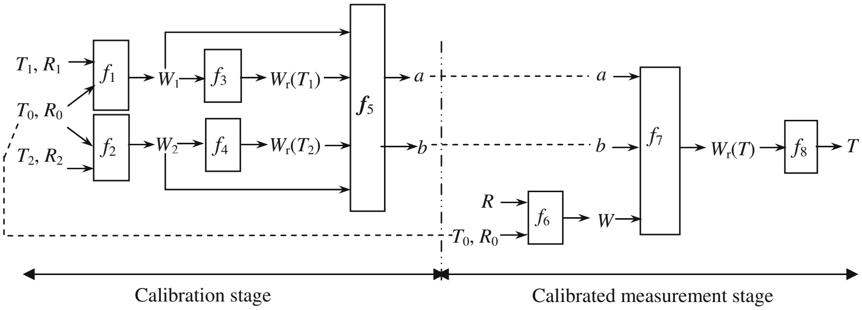

Fig. 2 Chain of functions. Single-stage process: taking the input quantities T_0, T_1, T_2, R_0, R_1, R_2, R to the output quantity T. Two-stage process: taking the input quantities T_0, T_1, T_2, R_0, R_1, R_2 to the intermediate quantities a and b, and thence a and b, with T_0, R and R_0, to the output quantity T

The conventional approach considers a two-stage model. The input quantities in the first stage are T_0, T_1, T_2, R_0, R_1, and R_2, and the output quantities a and b. The input quantities in the second stage are a, b, T_0, R_0, and R, and the output quantity T. The alternative is a single model, with input quantities T_0, T_1, T_2, R_0, R_1, R_2, and R, and output quantity T. A function with form inferred from the above is denoted by f_j.

With step numbers related to the sequence introduced in Sect. 2, the functions in the chain are as follows:

By applying the chain rule of differential calculus to the sequence of functions constituting the single model, the partial derivatives of T with respect to T_0, T_1, T_2, R_0, R_1, R_2, and R can be determined, and the standard uncertainty associated with the estimate $\hat{T}$ of T evaluated given the standard uncertainties (and covariances where appropriate) associated with the fixed points T_0, T_1, T_2 and the measured values of R_0, R_1, R_2, and R.

For the two-stage model, at the end of the first stage there will be an uncertainty matrix (covariance matrix) **cov**, say, associated with the estimates $\hat{a}$ and $\hat{b}$ of the elements of the vector $(a, b)^T$, containing as diagonal elements the squares of the standard uncertainties associated with $\hat{a}$ and $\hat{b}$ and in the off-diagonal positions the covariance associated with $\hat{a}$ and $\hat{b}$. The standard uncertainties associated with the estimates of R and R_0, together with **cov**, are used in the second stage to provide the standard uncertainty associated with $\hat{T}$.

It is emphasized that **cov** is not needed when the single model is used, since (implicitly, or explicitly, but clumsily) T can be expressed functionally in terms of T_0, T_1, T_2, R_0, R_1, R_2, and R.

A difficulty is the evaluation of the standard uncertainties associated with the estimates of the coefficients a and b in Eq. 2. These uncertainties are required in the evaluation of the uncertainty associated with $\hat{T}$ provided by the calibrated PRT. The difficulty arises because of the complicated way in which T depends on a and b and, in turn, the way in which a and b depend on the fixed points and on the electrical resistances measured at the calibration stage. In this work, the two-stage model was considered since it corresponds better with practice, but the additional difficulty created by the need to know the covariance associated with estimates of a and b should be taken into account in deciding which approach to adopt. An appraisal of both approaches will be attempted in future studies.

It is emphasized that U is not needed when the single-stage model is used, since (implicitly, and explicitly, but clumsily) T can be expressed functionally in terms of R_0, R_1, R_2, and R.

Now we will describe how MCM can be used for the problem addressed. Like the GUM uncertainty framework, MCM operates with a mathematical model relating an output quantity to a set of input quantities [11]. The input quantities are fixed points and electrical resistances, and the output quantity the required temperature T. MCM propagates a large number of random draws from distributions characterizing the input quantities through the mathematical model to provide random draws from the distribution for T. This procedure avoids the mentioned limitations of the GUM uncertainty framework. A best estimate of T, the associated standard uncertainty, and a coverage interval for a prescribed coverage probability can then readily be obtained from the distribution for T constructed from the large number of draws characterizing the distribution.

The use of MCM requires a validated pseudo-random uniform number generator, transformation algorithms to convert uniform random sequences into other sequences with given PDFs (for example, the Box–Muller transformation [12] converts uniform random sequences into sequences with Gaussian PDFs), and algorithms to order the sequence, and to assess the numerical precision of the results obtained [10]. This last aspect can be handled using an adaptive Monte Carlo procedure that automatically determines the number of draws that would be required to deliver a specified numerical precision.

Table 1 NMI calibration data (Serial Number 25286/3)

Id.	Fixed-point temperature (°C)	Standard uncertainty (°C)	Measured resistance (Ω)	Standard uncertainty (Ω)
T_{S1}	0.0100	0.0050	99.9976	0.00010
T_{S2}	29.7646	0.0050	111.5831	0.00011
T_{S3}	231.9250	0.0075	187.5670	0.00019

Table 2 In-house TCM calibration data

Id.	Reference temperature (°C)	Standard uncertainty (°C)	Measured resistance (Ω)	Standard uncertainty (Ω)
T_{M1}	0.010	0.007	99.997	0.00010
T_{M2}	29.771	0.007	111.584	0.00011
T_{M3}	231.532	0.008	187.422	0.00019

The basis for the comparison of the fixed-point and TCM approaches was the experimental data[2] for the calibration of PRTs in a National Metrology Institute (NMI) and specifically that related to the in-house calibration given in Tables 1 and 2.

In-house calibration standard uncertainties were obtained by considering all relevant contributions to the uncertainty budget, namely, the calibration uncertainty of the reference PRT, PRT stability and self-heating, bridge uncertainties (resolution, linearity, connectors, etc.), standard resistor uncertainties (calibration, temperature influence), oil bath and ethanol/water mixture, bath stability and uniformity.

5 Measurement Uncertainty Evaluation Using a Monte Carlo Method

As mentioned earlier, a major aspect of the uncertainty evaluation for the two-stage process, using MCM for the fixed-point method and the TCM, is the calculation of the calibration coefficients a and b (Eq. 2), and thus it was decided to focus this investigation on that aspect of the uncertainty evaluation. We outline how to carry out the evaluation to assess the uncertainty related to the estimated temperature T, which is relatively straightforward. In each case, a sequence of draws was made from Gaussian PDFs assigned to the input quantities T_0, T_1, T_2, R_0, R_1, and R_2; Gaussian PDFs rather than scaled and shifted t-distributions were used since the available experimental data are based on a large effective degrees of freedom due to extensive study and knowledge of the measurement system. For the fixed-point method, the expectations of these quantities were taken as the temperatures and measured resistances in Table 1 and the standard deviations as the associated standard uncertainties given there. For the TCM, the data in Table 2 were correspondingly used. For each method, a sequence of random draws from each of these PDFs was made, and for each set of values in the sequence

[2] Temperatures as requested by the customer. In comparison with the ITS-90 procedure, this imposes a non-standard sub-range calibration. However, the pseudo-ITS-90 and TCM approaches are based on similar substitutions for T1, so their comparison should not be invalidated by this fact.

the pair of values of a and b formed. The draws were based on the Mersenne Twister uniform random number generator and the Box-Muller transformation.

Figure 3 illustrates how MCM is applied in this particular evaluation process, namely, (1) the generation of random number sequences (PRNG), (2) their transformation to other sequences with Gaussian PDFs for the two types of input quantities (temperature values T_i and electrical resistance values R_i, $u\left(\hat{T}_i\right)$ and $u\left(\hat{R}_i\right)$ being the standard uncertainties associated with estimates $\hat{T}_i$ and $\hat{R}_i$), (3) the combination of the modified sequences according to the generic mathematical model $[\mathbf{Y}] = f[\mathbf{X}]$, and (4) the treatment of the model values (output sequences), yielding PDFs for the coefficients a and b, and hence estimates $\hat{a}$ and $\hat{b}$ of a and b, and their associated standard uncertainties $u(\hat{a})$ and $u(\hat{b})$.

The output PDFs for a and b for the fixed-point method are shown in Figs. 4 and 5. Although they are close to Gaussian in form, no distributional assumption is made in the use of MCM. In a similar way, the PDFs for the coefficients for the

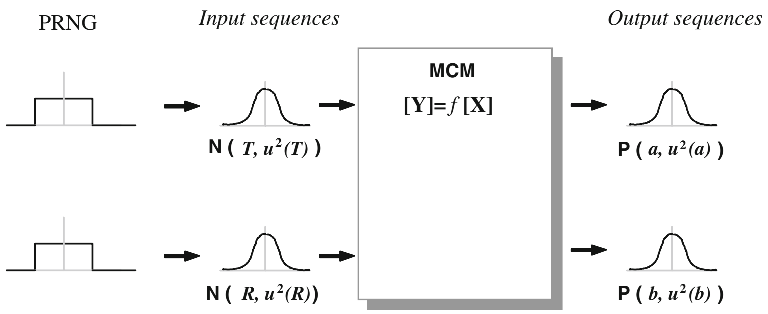

Fig. 3 Propagation of distributions using MCM

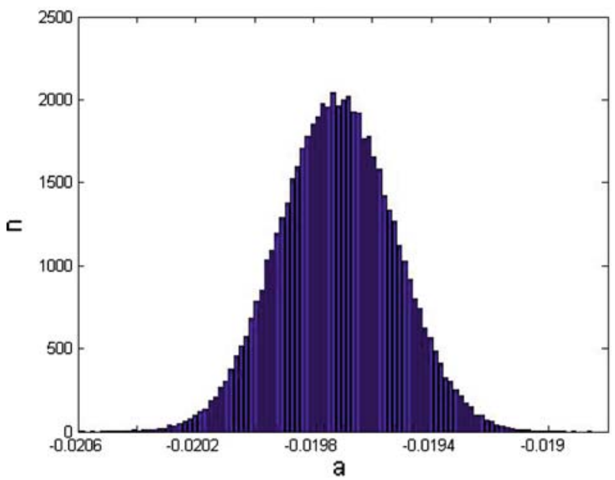

Fig. 4 PDF for coefficient a for the fixed-point method

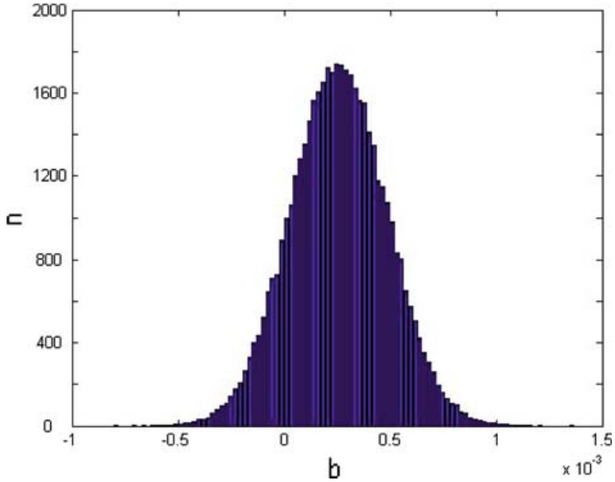

Fig. 5 PDF for coefficient b for the fixed-point method

TCM data are obtained. They are very similar in appearance to the PDFs for a and b for the fixed-point method.

The complete set of drawn pairs of coefficients (a, b) is shown in Fig. 6 for the fixed-point method results. The coefficients are clearly strongly correlated (correlation coefficients were -0.987 for the fixed-point method and -0.993 for TCM), which indicates the importance of accounting for that effect in the second stage, namely, the use of the calibrated PRT for subsequent measurement. To apply MCM to the second stage requires the re-use of the sequence of drawn pairs of coefficients (a, b). For each such pair, and the corresponding draws for T_0, R_0, and R, the corresponding value of the required temperature T is determined.[3]

6 Comparison of Results and Validation of TCM Procedure

The comparison of the results obtained is based on the evaluation of the temperature deviation function (the difference between the fixed-point-based function and the TCM function), presented in Fig. 7, where the electrical resistance is the input quantity, allowing the ratio $W(T) = R(T)/R(273.16\,\mathrm{K})$ to be evaluated, and, subsequently, the reference ratio $W_r(T)$ from Eq. 2, which is applied in the calculation of the temperature using Eq. 4 in both cases (fixed point and TCM).

Based on this result, an acceptance criterion of 0.01°C can be adopted, and a contribution to the uncertainty budget considered based on this estimate.

[3] It would be invalid to use the sequence of drawn pairs of coefficients (a, b) to form an uncertainty matrix associated with the estimates of these coefficients, and to sample from the multivariate Gaussian distribution having expectation equal to the vector defined by these two estimates and covariance equal to this uncertainty matrix. Doing so would be counter to the concept of the propagation of distributions in which no assumption is made about the form of "output" PDFs.

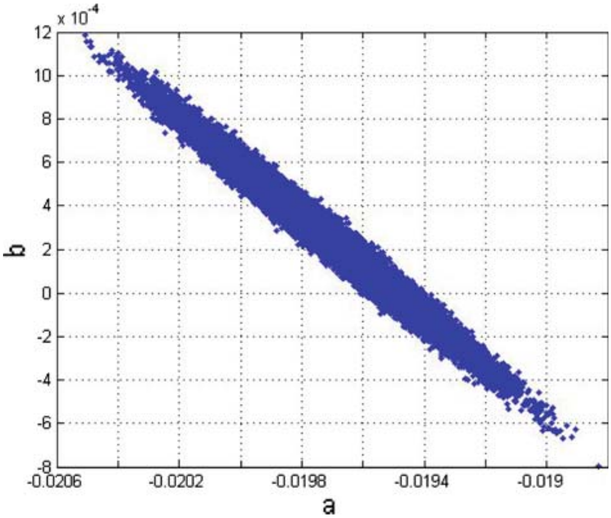

Fig. 6 Monte Carlo “draws” of the values of *a* and *b* for the fixed-point method

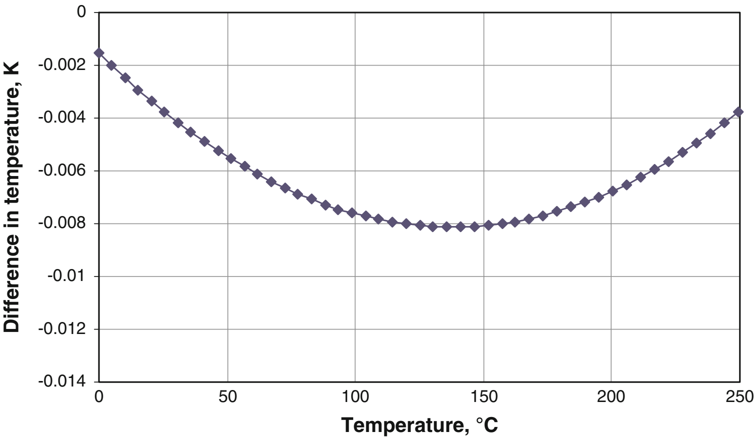

Fig. 7 Deviation in temperature between fixed-point-based and TCM curves

7 Conclusions

The first of the objectives given in the introduction was the validation of the temperature comparison methodology to perform in-house calibration. According to the results obtained, expressed for the case treated, the observed deviation in the temperatures provided by the two methodologies is less than 0.01°C. This degree of agreement is acceptable for many of the practical needs of industry and calibration and testing laboratories.

Regarding the objective of considering the use of MCM as a tool to perform this type of uncertainty evaluation, the main advantage is the avoidance of the need to apply the chain rule of differential calculus to evaluate the somewhat complicated partial derivatives of the models involved [3,4]. A further advantage would arise if the non-linearity of the model(s) considered is such that the conditions for valid application of the GUM uncertainty framework do not reasonably apply. That aspect requires further study.

This work shows that it is possible to obtain, straightforwardly using MCM, the joint PDF for the coefficients associated with the ITS-90 deviation functions for the temperature interval considered and the comparison methodology used. This joint PDF is represented by the sequence of "draws" of the values of these coefficients. It also shows how information is used in the evaluation of uncertainty in the following stage concerning the use of a calibrated PRT.

Further studies will be carried out to establish a comparison between the GUM uncertainty framework and MCM in the implementation of single and two-stage approaches so that a better knowledge of the difficulties and advantages related to both methods can be acquired. Taking into account the correlation existing among input variables is also intended in a further investigation. Even though, for the reasons stated, not all the conditions for the valid application of the GUM uncertainty framework apply, it is possible that, for the particular problem of concern, the results of the two uncertainty evaluations agree sufficiently for practical purposes. Although it would be difficult to draw general conclusions in this regard, it is expected that by examining a number of particular cases, some statements could be made that would apply to those cases and to cases sufficiently similar to them. Conversely, the result of such a study might indicate that MCM should perhaps be used for such problems to obtain uncertainty evaluations of greater reliability.

With this work, greater dissemination of metrology knowledge might be achieved, since the type of problems handled relate to a large user community of thermometry applications.

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