

APPLICATION OF MONTE CARLO METHOD FOR EVALUATION OF UNCERTAINTIES OF TEMPERATURE MEASUREMENT BY SPRT

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Abstract - Procedure for evaluation of uncertainties of the ITS-90 based on the propagation of distributions using the Monte Carlo method is presented. It is based on generation of pseudo-random numbers for input variables of the multivariate Gaussian distribution. This allows to take into account the correlations between the resistances at the defining fixed points. Assumption of Gaussian probability density function is acceptable with respect to the several sources of uncertainties of resistances.

Keywords: Correlation, International Temperature Scale 1990 (ITS-90), Monte Carlo method, Standard Platinum Resistance Thermometer (SPRT), Uncertainty

1. INTRODUCTION

Evaluation of the uncertainties of the temperature scale ITS-90 realization is an important task in metrological practice. Approaches are based on the GUM [1] and Supplements 1 and 2 [2, 3]. Widespread practices are based on the law of uncertainty propagation. There are also approaches based on orthogonal polynomials. The overview is presented in [4-9]. Propagation of distributions using Monte Carlo Methods (MCM) based on Supplement 1 to the GUM [2] occurs in a few isolated cases [10].

This paper presents a method based on the propagation of distributions by Monte Carlo method. The procedure is based on the generation of pseudo-random numbers of input variables (SPRT resistances at defining fixed points (DFPs), SPRT resistances in temperature measurements) of multi-dimensional distribution. Multi-dimensional distribution is used because it allows to take into account correlation between the SPRT resistances from calibration and in temperature measurement. In the case of uncorrelated resistances it is sufficient to generate data from the one-dimensional distribution of input variables.

For the actual implementation of MCM for propagation of distributions is necessary to know the probability distributions of input quantities and in the case of correlated input quantities multivariate distribution function. We assumed normal distribution for all input SPRT resistances and for correlated resistances multivariate normal distribution. This assumption is eligible regarding to several sources of uncertainties of SPRT resistances at the DFPs. E.g. chemical impurities of the substance in the DFPs,

hydrostatic-head effect (corresponding to location of SPRT sensing element in DFP), self-heating effect of the SPRT, immersion effect of the SPRT, effect of gas pressure in the DFPs, choice of fixed point value from plateau isotopic variations (for triple point of water (TPW) only), residual gas pressure in TPW cell, changes of resistances of standard resistor caused by changing of its temperature, non-linearity of the resistance bridge, uncertainty of calibration of resistance standard etc.

The aim of this study is

- a) presentation of the procedure for MCM method for uncertainty evaluation of the temperature scale by using SPRT calibrated at DFPs;
- b) validation of the process by using the law of uncertainty propagation according to the GUM for specific conditions.

The procedure should allow to take into account the correlation between the SPRT resistances calibrated at the DFPs and in temperature measurements.

Influences such as temperature gradients, fluctuations, drifts and further, there are not analysed. Also, the uncertainties due to non-uniqueness and consistency subranges are not covered. These questions are presented e.g. in [4].

The case study concerns the determination of uncertainties of temperature scale realization using SPRT calibrated in the range from 0 °C to the freezing point of aluminium (660.323 °C).

2. INTERNATIONAL TEMPERATURE SCALE ITS-90 – THEORETICAL BASES

Temperature according to the ITS-90 can be determined from the inverse function

$$T = f(W_r) \quad (1)$$

For the corresponding subranges of the ITS-90 from 0 °C the functions (1) are stated in [11]. Function W_r is given by

$$W_r - W = \sum_{i=1}^N a_i f_i(W) \quad (2)$$

where

$$W = \frac{R}{R_{TPW}} \quad (3)$$

while

R is the SPRT resistance at temperature T and R_{TPW} is the SPRT resistance at TPW,
 $f_i(W)$ are functions of the individual subranges in [11],
 a_i are the coefficients of deviation function from SPRT calibration at DFPs and

$a_i = g_1(R_{TPW1}, \dots, R_{TPWN}, R_{DFP1}, \dots, R_{DFPN})$ or

$a_i = g_2(W_{DFP1}, W_{DFP2}, \dots, W_{DFPN})$.

For the calculation of the coefficients of deviation function can be used matrix notation. If the relationship (2) is applied to N fixed points, than

$$\begin{pmatrix} \Delta W_{DFP1} \\ \vdots \\ \Delta W_{DFPN} \end{pmatrix} = \begin{pmatrix} f_1(W_{DFP1}) & \cdots & f_N(W_{DFP1}) \\ \vdots & \ddots & \vdots \\ f_1(W_{DFPN}) & \cdots & f_N(W_{DFPN}) \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} \quad (4)$$

where $\Delta W_{DFPi} = W_{r,DFPi} - W_{DFPi}$, W_{DFPi} are resistance ratios for corresponding DFPi and $W_{r,DFPi}$ are from the document ITS-90 [11].

Equation (4) is written in the form

$$\Delta \mathbf{W}_{DFP} = \mathbf{M}_{DFP} \mathbf{a} \quad (5)$$

Coefficients of deviation function are then (because there exists $\mathbf{M}_{DFP}^{-1}$)

$$\mathbf{a} = \mathbf{M}_{DFP}^{-1} \Delta \mathbf{W}_{DFP} \quad (6)$$

Then the equation (2) can be rewritten

$$W_r = W + \mathbf{a}^T \mathbf{f}(\mathbf{W}) \quad (7)$$

3. APPLICATION OF MONTE CARLO METHOD FOR EVALUATIONM UNCERTAINTY OF THE TEMPERATURE SCALE

3.1 The input data

Input data for MCM are the SPRT resistances at DFPs from calibration and SPRT resistances from temperature measurement, so input quantities vector of dimension $2N + 2$

$$\mathbf{R} = (R, R_{TPW}, R_{TPW1}, \dots, R_{TPWN}, R_{DFP1}, \dots, R_{DFPN})^T \quad (8)$$

and covariance matrix and vector of input quantities of type $(2 + 2N) \times (2 + 2N)$.

The SPRT resistances are determined on the basis of SPRT calibration at DFPs, i.e. vector

$$\mathbf{R}_{cal} = (R_{TPW1}, \dots, R_{TPWN}, R_{DFP1}, \dots, R_{DFPN})^T$$

and their uncertainties and covariances. It means covariance matrix of type $2N \times 2N$.

SPRT resistances R corresponding to measured temperatures T , SPRT resistance at TPW R_{TPW} and their uncertainties and covariances are determined in phase of temperature measurement. It means the vector $\mathbf{R}_{mess} = (R, R_{TPW})^T$ and its covariance matrix.

Furthermore, it is necessary to consider the covariances between SPRT resistances from calibration and from temperature measurement.

Then we can write the covariance matrix of the vector (8) in the form

$$\mathbf{V}_R = \begin{pmatrix} \mathbf{V}_{R_{mess}} & \mathbf{V}_{R_{mess}, R_{cal}} \\ \mathbf{V}_{R_{mess}, R_{cal}} & \mathbf{V}_{R_{cal}} \end{pmatrix} \quad (9)$$

In equation (9) covariance matrix $\mathbf{V}_{R_{mess}}$ expresses the uncertainties of SPRT resistances and covariances between them for temperature measurements. Covariance matrix $\mathbf{V}_{R_{cal}}$ expresses uncertainties of SPRT resistances and covariances between them for calibration of SPRT at DFPs. Matrix $\mathbf{V}_{R_{mess}, R_{cal}}$ expresses the covariances between the SPRT resistances from measurement and resistances from calibration. Matrix $\mathbf{V}_{R_{mess}, R_{cal}}$ has a nonzero values in-house temperature realization. I.e. the case when SPRT resistance at TPW is used from calibration. If we assume that the measurements of SPRT resistances for temperature measurement are under the same conditions as it was in calibration process then there could exist also covariances between SPRT resistances for temperature measurement and SPRT resistances from calibration.

Normally in practice the covariances between resistances are not considered, except for SPRT resistances at TPW. Two cases are considered here, 1) the use of SPRT in the laboratory (in-house), 2) the use of SPRT outside the laboratory. Covariance matrix $\mathbf{V}_{R_{mess}}$ has in both cases zero elements. The covariance matrix $\mathbf{V}_{R_{mess}, R_{cal}}$ for the use of SPRT in-house has in the second line the first N elements different values from zero and other elements are zero. For the use of the SPRT outside the calibration laboratory covariance matrix $\mathbf{V}_{R_{mess}, R_{cal}}$ is zero. The total covariance matrix of vector of input resistances is for these cases given below.

3.2 Procedure of calculation

Procedure for calculating the temperature and its uncertainty by propagation of distributions by using Monte Carlo method can be expressed in the Fig. 1.

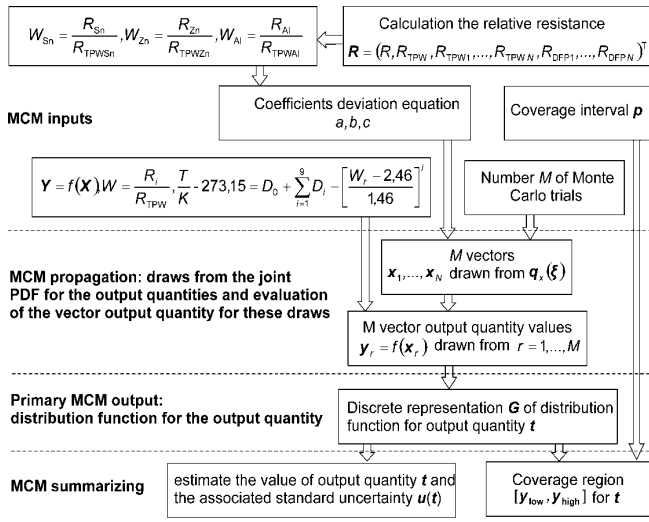


Fig.1. Computing phase of uncertainty evaluation by using Monte Carlo simulation for calculation the temperature and its standard uncertainty

3.3 Generating pseudo-random numbers from probability distributions

To calculate the uncertainties using MCM and the creation of applications with graphical interface support was used software Matlab (version 7.14, the 64-bit version), which uses a pseudo-random numbers generator Marsen Twister, which have undergone by a large number of tests for testing pseudo-random numbers. This program allows you to generate pseudo-random numbers with the required probability distributions of input quantities and rectangular, triangular and Gaussian distributions. In our case is assumed that all input quantities have a Gaussian distribution and in general they are correlated.

To construct a generator of pseudo-random numbers from a multi-dimensional normal distribution $N(\mu, V)$ is necessary to establish dimension n of multidimensional normal distribution, vector of mean values μ of dimension $n \times 1$, covariance matrix V of dimension $n \times n$ and the number of pseudo-random numbers that we want to generate.

Furthermore, it is necessary to generate a matrix X of dimension $n \times q$. From the covariance matrix V by using the Cholesky decomposition ($V = R^T R$) we obtain R^T . We will generate a matrix Z of dimension $n \times q$ from the normal distribution. We compute $X = \mu \mathbf{1}^T + R^T Z$, where $\mathbf{1}$ denotes the unit vector of dimension q (see [2]).

To calculate the estimate of temperature T and its standard uncertainty $u(T)$ by adaptive Monte Carlo method is necessary to determine the number M of Monte Carlo trials which are necessary to carry out for each sequence (h). For the output quantity T we consider the reference probability p and number of significant decimal digits n_{dig} from a standard uncertainty $u(T)$. Number M of Monte Carlo trials increases ($M \times h$) by each additional sequence of calculation (h) due to stabilization of the required statistical output quantities.

4. EVALUATION OF UNCERTAINTY AND EXPERIMENTAL DATA

We calculated the uncertainties of temperature for specific data from the Slovak Institute of Metrology (SMU) for the sub-range from triple point of water up to freezing point of aluminium.

4.1 Input data

The input data are given in Table 1. We measured temperature in the calibration laboratory (in-house) and also outside the calibration laboratory. We used one TPW cell for SPRT calibration. When we considered the SPRT resistances at TPW after tin, zinc and aluminium correlated (for simplicity we considered the correlation coefficient $r=1$), SPRT resistance of temperature measurement was considered uncorrelated with the other SPRT resistances. The SPRT resistances at DFPs are considered uncorrelated (cases a)-in house, b)-outside laboratory), or correlated (cases c)-in house, d)-outside laboratory). The correlations between resistances at TPW and at DFPs are considered uniformly $r=0,4$ and between the resistances at DFPs uniformly $r=0,3$. The results of MCM simulation are presented in table 2 and table3.

Table 1. Measured values of SPRT resistances at DFPs

Defining fixed point	Resistance (Ω)	Standard uncertainty of resistance (Ω)
TPW _{Sn}	24,8002001	$1,27 \cdot 10^{-5}$
TPW _{Zn}	24,8001927	$1,27 \cdot 10^{-5}$
TPW _{Al}	24,8001872	$1,27 \cdot 10^{-5}$
Sn	46,9397533	$3,85 \cdot 10^{-5}$
Zn	63,7056752	$4,98 \cdot 10^{-5}$
Al	83,7191875	$6,32 \cdot 10^{-5}$

To exclude the impact of uncertainty of resistance measurements for measurement of temperature T , we did not consider the uncertainty of the SPRT resistance at T , i.e. we consider the value of R for a given temperature as a constant. Then for the vector of input quantities $R = (R_{TPW}, R_{TPWSn}, R_{TPWSzn}, R_{TPWSAl}, R_{Sn}, R_{Zn}, R_{Al})^T$ we generated pseudo-random numbers from 7 dimensional Gaussian distribution and the resistance value R for the temperature was considered to be constant. In case we wanted to include in the calculation the measurement uncertainty of R for temperature measurement, we generated value of R from 8 dimensional Gaussian distribution.

We consider $M = 10^5$ Monte Carlo trials. For the output quantity T we consider the reference probability $p = 0.95$ or 95% - confidence interval and the number of significant decimal digits $n_{\text{dig}} = 2$, from standard uncertainty $u(T)$.

Histogram, for example for the resistance R_{Sn} from $N(\mu, V)$ distribution. is shown in Fig. 2

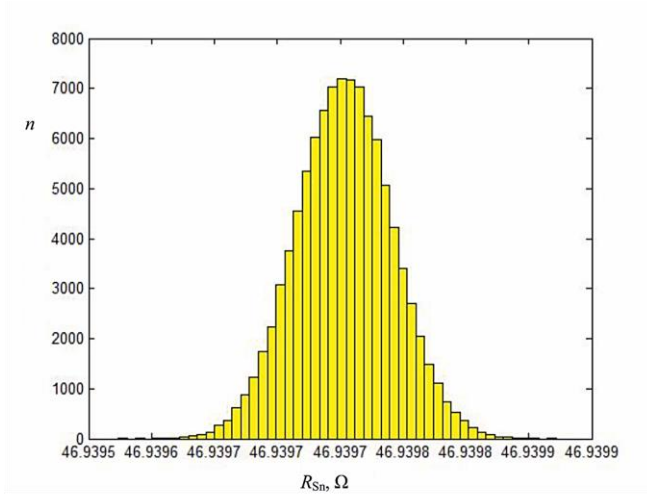


Fig. 2 Histogram for input resistances R_{Sn}

The coefficients a, b, c of deviation function can be determined from equation (6) for pseudo-random generated values for the input quantities and we get a_1 to a_{10^5} . The procedure for calculation of coefficients of deviation function is shown in Fig.3. Histogram of coefficient a is presented in Fig. 4. Coefficients b and c have similar histograms.

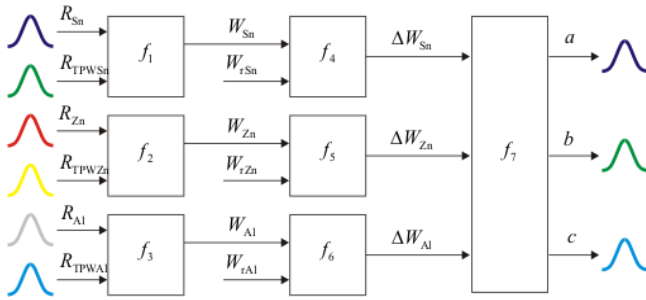


Fig. 3 Model of calculation of temperature and its standard uncertainty, part - calculation of the coefficients

The coefficients of deviation function a, b, c (in vector form) were calculated by Monte Carlo method in the previous chapter in order to calculate of estimation of the unknown temperature, associated standard uncertainty and confidence interval.

The measured resistance R at temperature T , mentioned above, is considered to be uncorrelated with other resistances and it can be generated from the one-dimensional probability distribution. It is supposed in our analysis as a constant (the uncertainty is equal to zero), so the problem can be analysed without influencing the measurement uncertainty of the resistance for temperature measurements. For specific measurement uncertainty we use a specific type of distribution.

The calculation procedure is shown in Fig. 5, where:

$$f_8 = \frac{R}{R_{TPW}}$$

from equation (2) is $f_9 = a(W-1) + b(W-1)^2 + c(W-1)^3$,

from equation (7) is $f_{10} = W - a(W-1) + b(W-1)^2 + c(W-1)^3$.

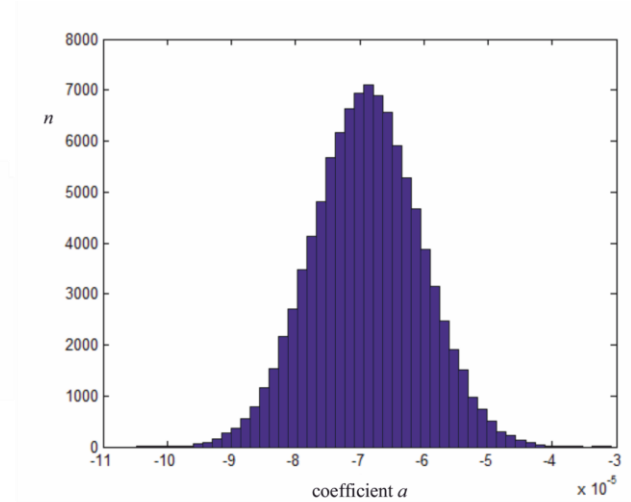


Fig. 4 Histogram for the coefficient a

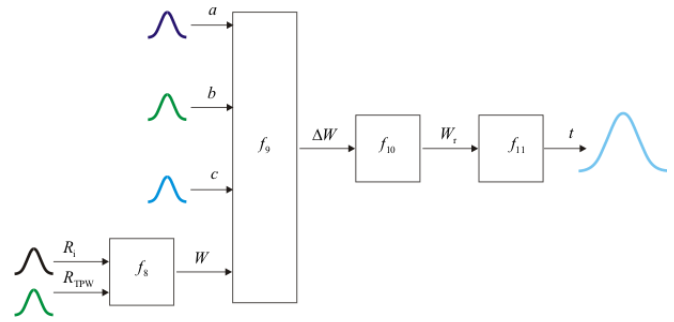


Fig. 5 Model of calculation of temperature and its standard uncertainty, part - calculation of temperature

Histogram of temperature is presented in Fig. 6.

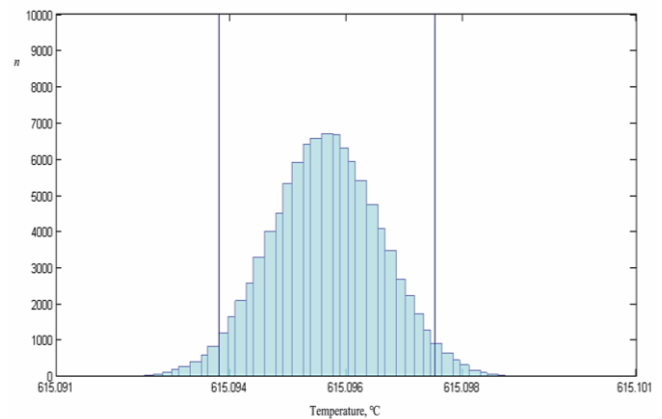


Fig.6 Histogram of temperature

4.2 Validation of uncertainty propagation law

It can be found out by calculation if the reference interval obtained by uncertainty propagation law and by Monte Carlo method is identical in certain numerical tolerance. This numerical tolerance is assessed from point of view of limit values of the reference interval and it gives expression of standard uncertainty $u(y)$ to the existing number of decimal places. Numerical expression of tolerance δ with an associated standard uncertainty $u(y)$ as described in [2] is as follows

$$\delta = \frac{1}{2} \times 10^r, u(y) = 68 \times 10^{-5} \text{ } ^\circ\text{C}, a = 68, r = -5,$$

$$\delta = \frac{1}{2} \times 10^{-5} = 0,000005 \text{ } ^\circ\text{C}$$

Absolute differences (of limit values) of both confidence intervals are determined from the relations

$$d_{\text{low}} = |y - U_{0.95} - y_{\text{low}}| \quad (9)$$

$$d_{\text{high}} = |y + U_{0.95} - y_{\text{high}}| \quad (10)$$

They are shown for different situations in Table 2 and Table 3. Table 2 shows that for the Adaptive MCM shortest coverage interval, GUF interval is slightly bigger. Table 3 shows the coverage interval MCM and GUF for various situations in measurement and calibration.

From the calculation of absolute differences (of limit values) d_{low} and d_{high} results that they are not larger than δ and verification of uncertainty propagation law is successful for cases of uncorrelated SPRT resistances at DFPs and unsuccessful for case of correlated resistances at DFPs. Of course, it is not to be applied for other conditions.

The resulting (total) time of calculation is given in Table 4.

5. CONCLUSIONS

This paper presents a procedure for the determination of uncertainties of temperature measurement by MCM. The procedure is based on generating of pseudo-random numbers for the input SPRT resistances at DFPs and at TPW.

In order to take into account the correlations between DFPs the approach of generating of pseudo-random numbers from multivariate distributions was used. We assumed a 7-dimensional Gaussian probability distribution. The assumption of Gaussian distribution is quite acceptable, given several sources of uncertainty of SPRT resistances at DFPs. If the correlations between the SPRT resistances at DFPs are negligible, it is possible to adapt the model so that the input resistances are uncorrelated and we can use one-dimensional distributions for each input resistance.

Table 2 Comparison and verification of uncertainty propagation law by the method of probability distribution by simulation MCM for one value t for the case a)

Method	M	t ($^\circ\text{C}$)	$u(t)$ ($^\circ\text{C}$)	95 % coverage interval	$d_{\text{low}}; d_{\text{high}}$	GUF validated ($\delta = 0.000005$)
GUF		615,095667	0,000635	[615,094424; 615,096911]		
MCM symmetric cov. int.	1×10^5	615,095668	0,000634	[615,094424; 615,096914]	0,000000 0,000003	Yes
Adaptive MCM symmetric cov.int.	$1,75 \times 10^7$	615,095666	0,000634	[615,094421; 615,096909]	0,000003 0,000002	Yes
Adaptive MCM shortest cov. int.	$1,75 \times 10^7$	615,095666	0,000634	[615,094429; 615,096904]	0,000005 0,000007	No

GUM uncertainty framework (GUF) [2]

Table 3 Comparison and verification of uncertainty propagation by method of probability distribution by simulation MCM for one value t for different cases ($M = 1 \times 10^5$)

Case	Method	t ($^\circ\text{C}$)	$u(t)$ ($^\circ\text{C}$)	95 % coverage interval	$d_{\text{low}}; d_{\text{high}}$	GUF validated ($\delta = 0.000005$)
a)	GUF	615,095667	0,000635	[615,094424; 615,096911]		
	MCM symmetric cov. int.	615,095669	0,000634	[615,094424; 615,096914]	0,000000 0,000003	Yes
b)	GUF	615,095667	0,000954	[615,093798; 615,0975437]		
	MCM symmetric cov. int.	615,095667	0,000954	[615,093800; 615,097533]	0,000002 0,000004	Yes
c)	GUF	615,095667	0,000721	[615,094255; 615,097080]		
	MCM symmetric cov. int.	615,095667	0,000671	[615,094349; 615,096987]	0,000094 0,000092	No
d)	GUF	615,095667	0,001013	[615,093687; 615,097653]		
	MCM symmetric cov. int.	615,095668	0,0008013	[615,094105; 615,097253]	0,000423 0,000400	No

GUM uncertainty framework (GUF) [2]

Table 4 The computational time for the main steps in the Monte Carlo simulation relating to model with one or more output quantities for $M = 2 \times 10^5$ Monte Carlo experiments

Operation	Time (s)
Generation $M=105$ of random numbers from multivariate Gaussian distributions	0,52
Calculation of coefficients of deviation function	5,5
Calculation of temperature t and standard uncertainty $u(t)$	0,7
Creation of $M = 2 \times 10^5$ values of model	2,3
Sorting $M = 2 \times 10^5$ values of model	8,5
Total	17,52

We also paid attention to validation of the use of uncertainty propagation law according to the GUM for particular conditions. For the case of uncorrelated input SPRT resistances at DFPs the validation is successful, the results obtained by using the uncertainty propagation law and by using MCM were consistent. In the case of correlated input resistances at DFPs this compliance was not achieved.

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