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EXAMPLES OF APPLYING MONTE CARLO SIMULATIONS IN THE FIELD OF MEASUREMENT UNCERTAINTIES OF THE STANDARD OF LENGTH

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Abstract -Recently, the Monte Carlo simulations (MCS) have been increasingly applied in the field of estimating the measurement uncertainties. The MCS method is based on random number generation from the probability density functions for each input value and forming of experimental probability density function of the output value. The paper presents calculation examples of the measurement uncertainty in calibration of the standard of length by using the MCS method. The MCS method is implemented for validation of the realised measurement uncertainties by GUM method in calibrating the standard of length.

Keywords: standards of length, measurement uncertainty, Monte Carlo simulation, calibration

1. INTRODUCTION

Compared to the standardised procedures (GUM method) of calculating the measurement uncertainty, this method has a whole range of advantages, but it also has some disadvantages. However, according to the experience acquired at the Laboratory for Precise Measurement of Length (LFSB) the advantages of this method are greater, and especially at levels where it is necessary to calculate the measurement uncertainty, and the knowledge (statistics, differential calculus) and experience are lacking. In other words, the greatest advantage of simulation is that the obtained result is experienced visually and the uncertainty calculus often turns into "fun".

It is precisely the impossibility of visual presentation of the measurement uncertainty which is probably the worst drawback of the GUM method.

Further, an example of comparison application of the MSC method with GUM method is presented, in the calibration procedure of PGM length of 0,5 and 100 mm, by comparison method.

2. CALCULATION OF THE MEASUREMENT UNCERTAINTY BY APPLYING GUM AND MCS METHOD

The length of gauge blocks of nominal lengths 0,5 and 100 mm is determined by their comparison with the known standards of the same nominal lengths.

The mathematical model of measurement has been given by expression (1):

$$L_e = L_{ref} + \delta L_D + \delta L + \delta L_C - L_{ref}\left(\theta_e \delta\alpha + \alpha_{ref}\delta\theta\right) - \delta L_V \quad (1)$$

which yield the following:

$$\delta\theta = \theta_e - \theta_{ref}$$
$$\delta\alpha = \alpha_e - \alpha_{ref}$$

where:

- δL measured difference in the length between calibrated and reference standard,
- L_e length of the calibrated standard at a temperature of 20 °C,
- L_{ref} length of the reference standard at a temperature of 20 °C,
- α_e linear coefficient of temperature expansion of the calibrated standard,
- α_{ref} linear coefficient of temperature expansion of the reference standard,
- θ_e temperature deviation of the calibrated standard of 20°C
- θ_{ref} temperature deviation of the reference standard of 20 °C
- δL_D influence of time ageing of the material of the standard,
- δL_V influence of the central point on the measurement surface of the standard,
- δL_C influence of the non-linearity comparator.

From the equation (1) it may be seen that the length of the calibrated standard L_e, i.e. the uncertainty of the obtained result of functions of the following variables:

$$L_e = f\left(L_{ref}, \delta L_D, \delta L, \delta L_C, \alpha_{ref}, \theta_e, \delta\alpha, \delta\theta, \delta L_V\right) \quad (2)$$

The thus composed standard uncertainty $u_c(L_e)$ can be calculated from the expression (3).

$$
\begin{aligned}
u_c^2(L_e) = {} & c_{L_{ref}}^2 u^2(L_{ref}) + c_{\delta L_D}^2 u^2(\delta L_D) + c_{\delta L}^2 u^2(\delta L) + \\
& + c_{\delta L_C}^2 u^2(\delta L_C) + c_{\alpha_{ref}}^2 u^2(\alpha_{ref}) + c_{\theta_e}^2 u^2(\theta_e) + \\
& + c_{\delta\alpha}^2 u^2(\delta\alpha) + c_{\delta\theta}^2 u^2(\delta\theta) + c_{\delta L_V}^2 u^2(\delta L_V) + \\
& + c_{\delta\alpha,\theta_e}^2 u^2(\delta\alpha) u^2(\theta_e) + c_{\alpha_{ref}\delta\theta}^2 u^2(\alpha_{ref}) u^2(\delta\theta)
\end{aligned} \tag{3}
$$

The yields of components of the standard measurement uncertainty for the standards of 0,5 mm and 100 mm which include also the members of the higher order of the function development into the Taylor order are presented in Table I.

Table I. Yields of components of standard uncertainty, and sources of uncertainty

Components of standard uncertainty	Source of uncertainty	Amount of standard uncertainty	$c_i = \frac{\partial f}{\partial x_i}$	Yield to measurement uncertainty, nm	
				L=5 mm	L=100 mm
$u(L_{ref})$	Calibration of length of the reference standard	10+0,150 L nm	1	10,1	25,0
$u(\delta L_D)$	Temporal ageing of the material	8+0,102 L nm	1	8,1	18
$u(\delta L)$	Measurement of length differences	2,5 nm	1	2,5	18,2
$u(\delta L_C)$	Comparator non-linearity	18,5 nm	1	18,5	18,5
$u_c(\theta_e)$	Deviation of the temperature of standard	0,234 °C	$\delta\alpha L \approx 0$	0	0
$u(\delta\theta)$	Difference in the temperature of standard	0,058 °C	$-L\cdot 11{,}5\cdot 10^{-6}$	0,33	66,7
$u(\alpha_{ref})$	Coefficient of linear extension of reference standard	$0{,}577\cdot 10^{-6}$ K^{-1}	$L\theta_e$ θ_e =0,1 °C	0	5,8
$u(\delta\alpha)$	Difference of linear extension coefficients	$0{,}816\cdot 10^{-6}$ K^{-1}	$-L\theta_e$ θ_e =0,1 °C	0,1	8,2
$u(\delta L_V)$	Measuring length near the central point	3,2+0,0067 L nm	-1	3,2	3,9
			$c_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$		
$u(\delta\alpha)u(\theta_e)$	Members of the 2nd order	$0{,}191\cdot 10^{-6}$	$-L$	0	19,1
$u(\alpha_{ref})u(\delta\theta)$	Members of the 2nd order	$0{,}033\cdot 10^{-6}$	$-L$	0	3,3
Combined variance $u_c^2(L_e)$:			**$u_c^2(L_e) = (23^2 + 0{,}53^2 L^2)$ nm^2, L u mm**		
Linearised expanded measurement uncertainty U, k=2, P=95%:			**$U = (0{,}05 + 1{,}1L)$ µm, L u m**		

For the standards of 0,5 mm and 100 mm a calculation of the measurement uncertainty (validation) has also been performed, by means of MCS method. Apart from the output value L_e certain components were simulated as well, such as $\delta\alpha$, $\delta\alpha\cdot\theta$ i ($\theta_e\cdot(\alpha_{ref} - \alpha_e) + \alpha_{ref}\cdot\delta\theta$). The mentioned examples show clearly the advantages of the MCS method in relation to the GUM method. From the obtained experimental pdf there follows an estimate of the output value y, the estimated standard deviation, and the estimate of the interval $(y_{((\frac{1-P}{2})\cdot M)},\ y_{((\frac{1+P}{2})\cdot M)})$ for the given probability P. All the probability density functions of the output values have been obtained by M=100000 simulations.

The probability density function g($\delta\alpha$) has been simulated by the MCS method based on the expression (4).

$$\delta\alpha = \alpha_{ref} - \alpha_e \tag{4}$$

The input values x_i are defined by probability density functions g(x_i) as presented in Table II.

Table II. Input values and pdf in simulating of value $\delta\alpha$

Input value		Probability density function g(x_i)
Title	Symbol x_i	
Linear coefficient of temperature expansion of the reference standard	α_{ref}	Rectangular distribution ($10{,}5\cdot 10^{-6}$ K^{-1}, $12{,}5\cdot 10^{-6}$ K^{-1})
Linear coefficient of temperature expansion of the calibrated standard	α_e	Rectangular distribution ($10{,}5\cdot 10^{-6}$ K^{-1}, $12{,}5\cdot 10^{-6}$ K^{-1})

The estimated standard deviations of the output value amounts to $0{,}817\cdot 10^{-6}$ K^{-1} which confirms the uncertainty determined by the GUM method. The probability density functions of the output values are presented in Fig. 1

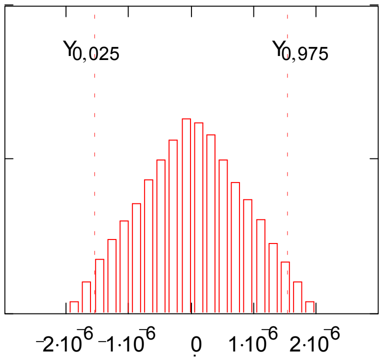

Fig. 1. Probability density function g($\delta\alpha$)

The output value $\delta\alpha$ is within the interval:

($Y_{0,025} = -1{,}556\cdot10^{-6}$ K^{-1}; $Y_{0,975} = 1{,}557\cdot10^{-6}$ K^{-1}) P= 95%

The analysis of the relations of the probability density functions assigned to input values obviously shows that the convolution of two rectangular distributions of the same parameters will yield symmetric triangular distribution (Fig. 1).

The probability density function g($(\alpha_{ref} - \alpha_e)\cdot\theta$) has been simulated by the MCS method based on the expression (5).

$$(\alpha_{ref} - \alpha_e)\cdot\theta \qquad (5)$$

The input values x_i are defined by the probability density functions g(x_i) as shown in Table III.

Table III. Input values and pdf in simulating of value $\delta\alpha\cdot\theta$

Input value		Probability density function g(x_i)
Title	Symbol x_i	
Linear coefficient of temperature expansion of the reference standard	α_{ref}	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}; $12{,}5\cdot10^{-6}$ K^{-1})
Linear coefficient of temperature expansion of the calibrated standard	α_e	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}, $12{,}5\cdot10^{-6}$ K^{-1})
Temperature of the standard	θ	Rectangular distribution (-0,5 °C; 0,3 °C)

The convolution of the distribution of the input values defined in Table III. yields the experimental pdf shown in Fig. 2.

The estimated standard deviations of the output value amount to $2{,}057\cdot10^{-7}$.

The output value $\delta\alpha\cdot\theta$ is within the interval:

($Y_{0,025} = -4{,}56\cdot10^{-7}$; $Y_{0,975} = 4{,}53\cdot10^{-7}$) with P= 95%

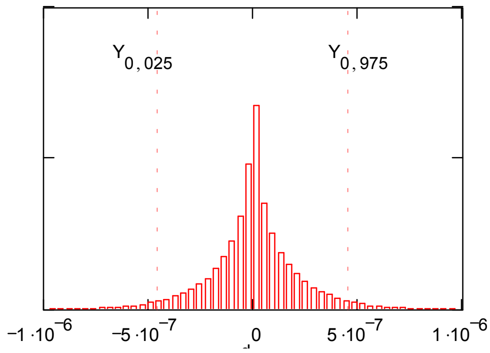

Fig. 2. Probability density function g($\delta\alpha\cdot\theta$)

The yield to the combined uncertainty of value L_e due to the temperature influence has been simulated by the MCS method according to the expression (6).

$$\theta_e\cdot(\alpha_{ref} - \alpha_e) + \alpha_{ref}\cdot\delta\theta \qquad (6)$$

The input values x_i are defined by the probability density functions g(x_i) as shown in Table IV.

Table IV. Input values and pdf in simulating of value $\delta\alpha\cdot\theta$

Input value		Probability density function g(x_i)
Title	Symbol x_i	
Linear coefficient of temperature expansion of the reference standard	α_{ref}	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}, $12{,}5\cdot10^{-6}$ K^{-1})
Linear coefficient of temperature expansion of the calibrated standard	α_e	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}, $12{,}5\cdot10^{-6}$ K^{-1})
Temperature deviation of the standard of 20 °C	θ_e	Rectangular distribution (-0,5 °C; 0,3 °C)
Temperature difference between the reference and calibrated standard	$\delta\theta$	Rectangular distribution (-0,1 °C; 0,1 °C)

The estimated standard deviations of the output value amount to $6{,}96\cdot10^{-7}$ which confirms the uncertainty determined by the GUM method. The probability density function of the output value is presented in Figure 3. The output value $\theta_e\cdot(\alpha_{ref} - \alpha_e) + \alpha_{ref}\cdot\delta\theta$ is within the interval:

($Y_{0,025} = -1{,}18\cdot10^{-6}$; $Y_{0,975} = 1{,}19\cdot10^{-6}$) with P= 95%

By convolution of the four rectangular distributions according to expression (6) normal distribution has not been realised, but the output value can be rather described by trapezoid distribution (Figure 3.).

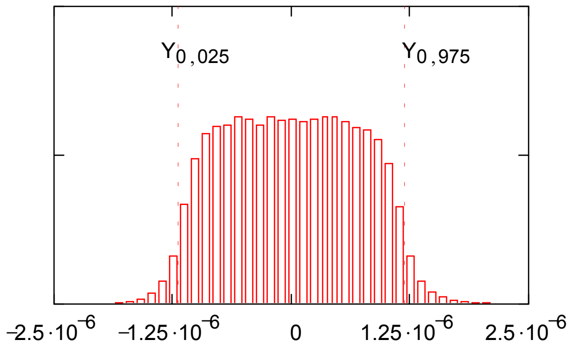

Fig. 3. Probability density function g($\theta_e\cdot(\alpha_{ref}$ - $\alpha_e)$ + $\alpha_{ref}\cdot\delta\theta$)

The input values and the probability density function for the standards of nominal lengths of 0,5 mm and 100 mm, are presented in Tables V. and VI. Experimental probability density functions of the output value L_e, for the mentioned standards, obtained by MCS method and normal distribution curve assumed by the GUM method, are presented in Figures 4. and 5.

Table V. Input values and pdf in simulating of value L_e for gauge block nominal length of L=0,5 mm.

Input value		Probability density function g(x_i)
Title	Symbol x_i	
Length of the reference standard	L_{ref}	Normal distribution (0,5 mm; 10,1 nm)
Influence of temporal ageing of the material	δL_D	Normal distribution (0 mm; 8,1 nm)
Measured difference in length of the calibrated and reference standard	δL	Normal distribution (0 mm; 2,5 nm)
Influence of comparator non-linearity	δL_c	Rectangular distribution (-32nm; 32 nm)
Temperature deviation of the standard of 20 °C	θ_e	Rectangular distribution (-0,5 °C; 0,3 °C)
Coefficient of temperature expansion of the calibrated standard	α_e	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}; $12{,}5\cdot10^{-6}$ K^{-1})
Coefficient of temperature expansion of reference standard	α_{ref}	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}; $12{,}5\cdot10^{-6}$ K^{-1})
Temperature difference in the reference and calibrated standard	$\delta\theta$	Rectangular distr. (-0,1 °C; 0,1 °C)
Influence of the standard central point	δL_V	Rectangular distribution (-5,5 nm; 5,5 nm)

Table VI. Input values and pdf in simulating of value L_e for gauge block nominal length of L=100 mm.

Input value		Probability density function g(x_i)
Title	Symbol x_i	
Length of the reference standard	L_{ref}	Normal distribution (100 mm; 25 nm)
Influence of temporal ageing of material	δL_D	Normal distribution (0 mm; 18,2 nm)
Measured difference in the length of calibrated and reference standard	δL	Normal distribution (0 mm; 2,5 nm)
Influence of comparator non-linearity	δL_c	Rectangular distribution (-32nm; 32 nm)
Temperature deviation of standard of 20 °C	θ_e	Rectangular distribution (-0,5 °C; 0,3 °C)
Coefficient of temperature expansion of the calibrated standard	α_e	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}; $12{,}5\cdot10^{-6}$ K^{-1})
Coefficient of temperature expansion of reference standard	α_{ref}	Rectangular distribution ($10{,}5\cdot10^{-6}$ K^{-1}; $12{,}5\cdot10^{-6}$ K^{-1})
Temperature difference between reference and calibrated standard	$\delta\theta$	Rectangular distribution (-0,1 °C; 0,1 °C)
Influence of central point of standard	δL_V	Rectangular distribution (-6,7 nm; 6,7 nm)

The probability density function (pdf) of the output value L_e has been simulated by the MCS method on the basis of expression (1). Figures 4 and 5 show the probability density functions of the output value L_e thus confirming the normal distribution of the output value.

The curve in Figures 4 and 5 marks the distribution obtained by the GUM method whereas columns represent the distribution density function by the MCS method.

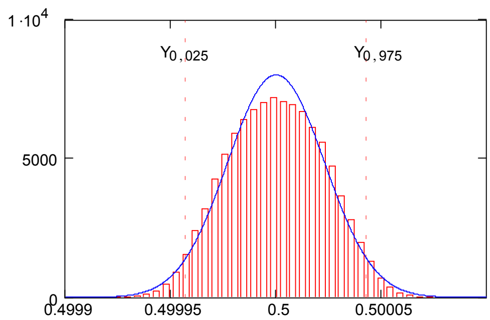

Fig. 4. Probability density function g(L_e) for the nominal length of standard of 0,5 mm

The estimated standard deviation of the output value L_e for the standard of nominal length of 0,5 mm amounts to 23 nm. The output value L_e is within the interval range:

($Y_{0,025}$ = 0,4999571 mm; $Y_{0,975}$ = 0,5000431 mm) P=95%

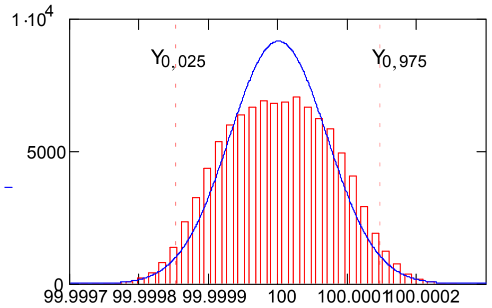

Fig. 5. Probability density function g(L_e) for the nominal length of standard of 100 mm

The estimated standard deviation of the output value L_e for the standard of nominal length of 100 mm amounts to 79 nm. The output value L_e is within the interval range:

($Y_{0,025}$ = 99,999853 nm; $Y_{0,975}$ = 100, 000145 nm)P=95%

While the GUM method assumes normal distribution of the output value, the MCS method yielded experimental distribution of the output value that may more or less match the assumed normal distribution. The form of the experimental curve will depend primarily on the probability density function of the most significant input value. In this case, due to the dominant influence of temperature on the measurement uncertainty, the normal distribution assumes, through length increase, the characteristics of a trapezoid distribution (see Fig. 3).

3. CONCLUSION

The presented example confirms the advantages of the MCS method in relation to the calculation of the measurement uncertainty when the GUM method is applied. Therefore, the following may be stated for the MCS method:

1. A combination of different probability density functions is possible, which define the input values,
2. The obtained experimental pdf provide an estimate of the output value y, estimated standard deviation, and the interval estimate $(y_{((\frac{1-P}{2})\cdot M}, y_{((\frac{1+P}{2})\cdot M)})$ for the given probability P.
3. The calculation includes higher orders of the function development into Tayler's order.
4. Unknown systemic errors are simulated,
5. If present, the correlation between input values is simulated.

In the presented examples the Monte Carlo simulations have been primarily used for the validation of the values obtained by means of the GUM method. All the examples have fully confirmed the GUM values of influencing the measurement uncertainty. The graphical presentation of the output probability density functions has expanded the knowledge about the mentioned influences.

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