FITTING CURVES TO DESCRIBE ERRORS OF INDICATIONS IN CALIBRATION OF MEASURING INSTRUMENTS

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1. INTRODUCTION

Measuring instruments usually are calibrated at discrete values; however, it is very useful for the user to have formulae to describe the errors[a] of indications (and their uncertainties) as a function of the readings of the instrument.

The Guidelines on the Calibration of Non-Automatic Weighing Instruments [1, 2] offers advice on how to derive formulae to describe errors related with the indications in use (R) by continuous functions. For this reason, it is interesting to make a comparative study of results arising from such approaches.

In this paper, though, we analyzed only the different approaches stated in [1, 2] for weighing instruments calibration, these methods may apply for different kind of measuring instruments.

2. FUNCTIONAL RELATIONS

2.1. Linear interpolation

This method assumes a linear relation between two consecutives errors $E(I)^b$ and their uncertainties evaluated in calibration at the given indication (I_k, I_{k+1}) [1, 2],

$$E(R) = E_k + (R - I_k)(E_{k+1} - E_k)/(I_{k+1} - I_k) \quad (1)$$

$$u(R) = u_k + (R - I_k)(u_{k+1} - u_k)/(I_{k+1} - I_k) \quad (2)$$

2.2. Approximation by polynomials

This method is based on the "minimum χ^2" approach,

$$\chi^2 = \sum_{j=1}^{n} p_j v_j^2 = \sum_{j=1}^{n} p_j \left(f(I_j) - E_j\right)^2 = \text{minimum} \quad (3)$$

where,

- p_j weighing factor corresponding to indication j (proportional to $1/u_j^2$)
- v_j residual corresponding to indication j
- f approximation function containing n_{par} parameters

Approximation by polynomial yields the general function,

$$E(R) = f(R) = a_0 + a_1 R + a_2 R^2 + ... + a_n R^n \quad (4)$$

where a_i are the fitting coefficients and R is the reading of the measurement instrument.

The evaluation of the coefficients is solved by weighing least squares [1, 2],

$$\mathbf{a} = \left(\mathbf{X}^T \mathbf{P} \mathbf{X}\right)^{-1} \mathbf{X}^T \mathbf{P} \mathbf{e} \quad (5)$$

where,

- $\mathbf{X}$ matrix whose m rows are (1, I_j, I_j^2 ,..., I_j^n)
- $\mathbf{a}$ column vector whose components are the coefficients a_0, a_1, , a_n of the approximation polynomial
- $\mathbf{e}$ column vector whose m components are the E_j
- $\mathbf{P}$ weighing matrix ($\mathbf{P} = \mathrm{cov}(\mathbf{e})^{-1}$), whose main diagonal is formed by the inverse of the variance of the errors.

Variance and covariance of the fitting coefficients are given by the following matrix [1, 2]:

[a] The meaning of "error" (of indication) considered in this work corresponds to "measurement error" (with regard to the indication) according to the new VIM [8].
[b] The notation I is used for the indication (reading) of the instrument at calibration, and the notation R is used for the indication (reading) in use after calibration.

$$\mathrm{cov}(\mathbf{a}) = \left(\mathbf{X}^{\mathrm{T}}\mathbf{P}\mathbf{X}\right)^{-1} \tag{6}$$

To calculate the error of the indication for any reading (different to the indications evaluated in calibration), it can be evaluated with (4) with coefficients a_i obtained from (5). The uncertainty associated to this indication error is calculated with the combination of the uncertainty of the fitting coefficients, their covariance and the uncertainty of the indication R.

2.3. Approximation by straight line

This method is the particular case of 2.2 with $n = 1$,

$$E(R) = f(R) = a_0 + a_1 R \tag{7}$$

Other possibility is to consider that the error in zero (indication) is null. In [1, 2] is proposed an approximation to a straight line that crosses through zero ($a_0 = 0$) in non-matrix notation,

$$E(R) = f(R) = a_1 R \tag{8}$$

$$a_1 = \sum pIE \Big/ \sum pI^2 \tag{9}$$

$$u^2(a_1) = 1 \Big/ \sum pI^2 \tag{10}$$

The evaluation of the error of the indication and its associated uncertainty are evaluated in the same way that in 2.2.

Even when it is assumed that the line crosses trough zero ($a_0 = 0$), this assumption has an associated uncertainty, $a_0 \pm u(a_0)$. This uncertainty is not considered in [1, 2], hence the uncertainty due to the fitting is underestimated.

2.4. Numerical simulation by Monte Carlo's method

In order to evaluate the performance of the different methods to generate the continuous function $E = f(R)$, the results from such methods are compared against results arising from numerical simulation of Monte Carlo's method [3].

The Monte Carlo's method considered in [3], applies to a model of several input quantities and just one output quantity,

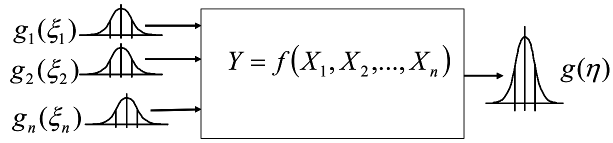

Figure 1. *Propagation of distributions for a measurement model with several input quantities and only one output quantity.*

However, a generalization [5, 7] to the model with several input quantities and several output quantities will be done in this paper,

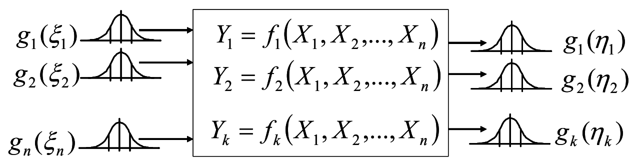

Figure 2. *Propagation of distributions for a measurement model with several input quantities and several output quantities.*

In general, the evaluation of the errors of the indications in use is solved in two steps: first, the fitting coefficients of the polynomial are calculated and second, the error for the reading in use R is calculated by means of such polynomial.

In the numerical simulation developed for this work, the errors of the indications in use were calculated in one step, taking as the mathematical model for the simulation the combination of (4) and (5). The input quantities considered for simulations were I_j, E_j and R_k, where I_j, and E_j were the indications and the errors found in calibration, and R_k, were the indication in use (readings).The output quantities were the errors for the instrument $E(R_k)$.

The mean values and the standard uncertainties of the input quantities were considered as the means and the standard deviations for the input pdfs (probability density functions) $g_i(\xi_i)$, and the means and standard deviations of the output pdfs $g_k(\eta_k)$ were taken as the mean values and the standard uncertainties of the output quantities.

3. NUMERICAL EXAMPLES

3.1. Errors characterized by a straight line

For the numerical example, the results of the example G1 of [1, 2] were taken. The example shows the calibration of a weighing instrument of

200 g of maximum capacity, and resolution of d = 0.1 mg. Calibration results are shown in table 1.

The errors for different nominal values were evaluated.

The standard uncertainty associated to a single indication, I_j, and to R_k was 0.14 mg (k=1), according to the example G1 of [1, 2]. The uncertainty associated to a single indication is the combination of the contributions of both resolution and repeatability of the measuring instrument.

Table. 1. *Discrete errors of indications evaluated in calibration and their standard uncertainties.*

Indication g	Error mg	unc. k = 1 mg
0	0.00	0.14
30	0.10	0.19
60	0.30	0.19
100	0.40	0.19
150	0.60	0.23
200	0.90	0.24

The fitting coefficients for a straight line and the variance-covariance matrix calculated with the above values are,

$\mathbf{a} =$

$a_0 =$ **$-5.143\ 1 \times 10^{-6}$ g**
$a_1 =$ **$4.317\ 8 \times 10^{-6}$**

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 1.193 \times 10^{-8}\ \mathrm{g}^2 & -9.150 \times 10\text{-}^{11}\ \mathrm{g} \\ -9.150 \times 10^{-11}\ \mathrm{g} & 1.342 \times 10^{-12} \end{vmatrix}$$

The fitting coefficients a_i for the approximation to the straight line that crosses through zero and their uncertainties are,

$a_0 =$ **0.00 g ± 0.14 mg** (k=1) [c]
$a_1 =$ **$4.27 \times 10^{-6} \pm 7.6 \times 10^{-7}$** (k=1)

Figure 3 shows the graph of errors of indications calculated by different methods. In Figure 3 are presented only the bars of the uncertainties evaluated in calibration combined with the contribution of the indication in use of the instrument.

The series shown in Figure 3 correspond to the following approaches,
1. Calibration,
2. Linear interpolation,
3. Approx. by first order polynomial,
4. Approx. by straight line that cross through zero, and
5. Numerical simulation.

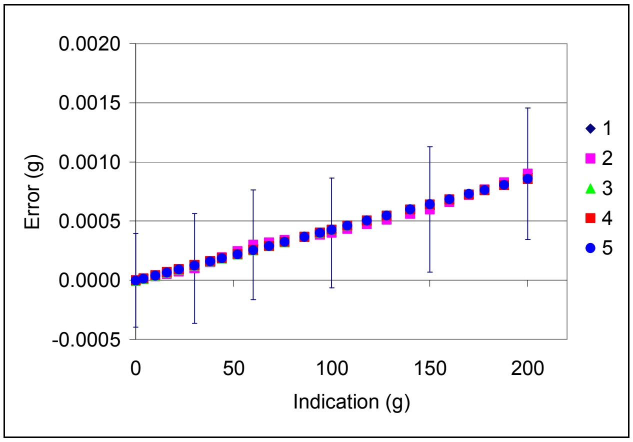

Figure 3. *Errors of indications in use of the instrument calculated by different approximation methods.*

In Figure 4 the uncertainties calculated by the different approximation methods are shown.

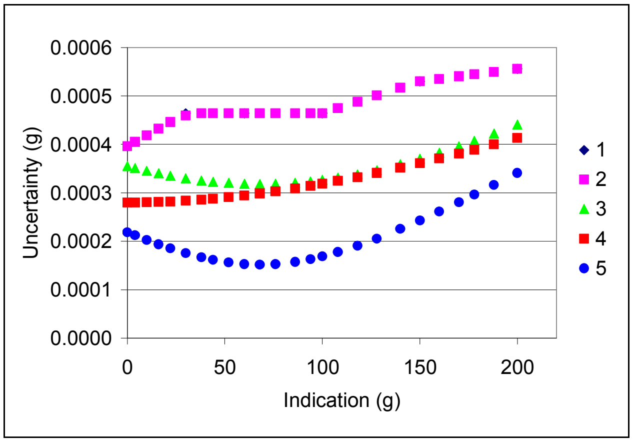

Figure 4. *Expanded uncertainties associated to the errors of the indications evaluated by different approximation methods.*

From Figure 3, it can be noted that the errors evaluated by the different methods have almost the same values, but the uncertainties evaluated by

[c] The value of a_0 is assumed as zero, but it should be assigned an uncertainty value equal to a single reading of the instrument in use. For the calculation of the uncertainty of the error $E(R)$ for this method, the correlation between a_0 and a_1 is not considered.

those methods show differences indeed (see Figure 4).

3.2. Approximation by second order curve

With the purpose to evaluate the performance of the approximation method by a second order polynomial, values of table 1 were intentionally modified to characterize a second order function. The modified errors and their corresponding uncertainties (without modification) are listed in table 2.

Table 2. *Discrete errors of indications (intentionally modified) and their standard uncertainties.*

Indication g	Error mg	unc. k=1 mg
0	0.00	0.14
30	0.10	0.19
60	0.40	0.19
100	1.20	0.19
150	3.00	0.23
200	6.50	0.24

The values of the fitting coefficients for the second order function and the covariance matrix, evaluated by (5) and (6), are listed next,

$\mathbf{a} =$

$a_0 =$ 6.881 9 x 10^{-5} g
$a_1 =$ -8.437 2 x 10^{-6}
$a_2 =$ 1.989 1 x 10^{-7} g^{-1}

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 1.655 \times 10^{-8}\ g^2 & -3.320 \times 10^{-10}\ g & 1.324 \times 10^{-12} \\ -3.320 \times 10^{-10}\ g & 1.384 \times 10^{-11} & -6.884 \times 10^{-14}\ g^{-1} \\ 1.324 \times 10^{-12} & -6.884 \times 10^{-14}\ g^{-1} & 3.791 \times 10^{-16}\ g^{-2} \end{vmatrix}$$

With the above values, errors for selected indications as in normal use of the instrument were evaluated.

The uncertainty values of the indication errors in use were evaluated taking into account the uncertainty contributions due to the fitting coefficients, their covariance and the uncertainty contribution due to the indication in use, (0.14 mg k=1).

Subsequently, a numerical simulation by Monte Carlo's method was performed and their results were compared against matrix method results.

In Figure 5, the indication errors evaluated by both methods, and also the errors of indications found in calibration (table 2) are shown. The uncertainty values include the uncertainty contributions due to the calibration and due to the indication in use of the instrument. In Figure 5 only the expanded uncertainty bars for the discrete calibration values are shown.

The data series correspond to,
1.- Calibration,
2.- Approx. by second order polynomial,
3.- Numerical simulation.

From Figure 5, as in the case of the straight line approximation, it can be noted that the errors evaluated by an approximation by second order polynomial and numerical simulation methods have almost the same values, but, the uncertainty values evaluated by these methods show differences with the calibration values and among them too, see Figure 6.

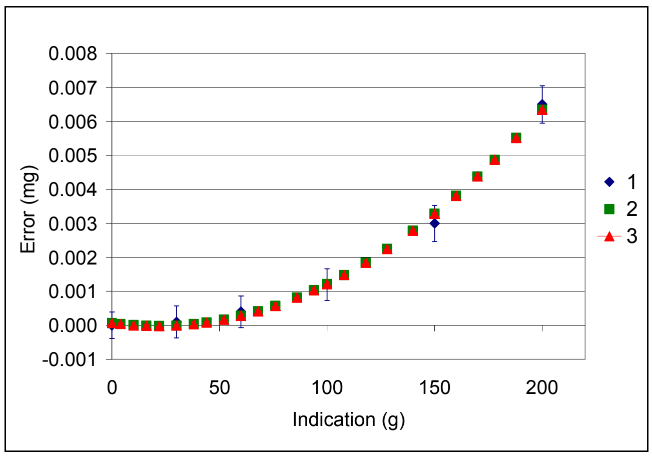

Figure 5. *Errors of indications calculated by different approximation methods*

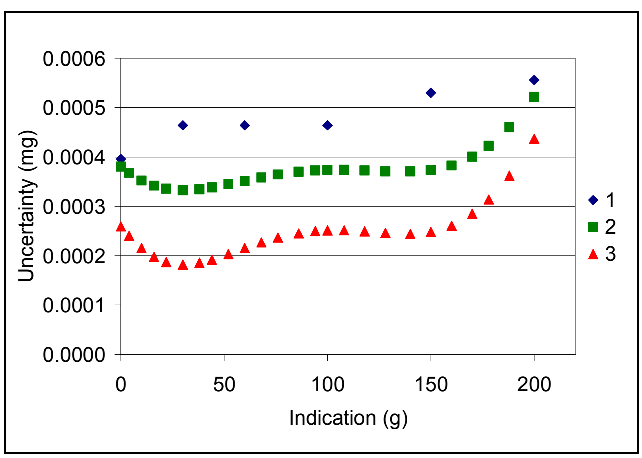

***Figure 6.** Expanded uncertainties associated to the errors of the indications calculated by different approximation methods*

4 INTERPOLATION AND EXTRAPOLATION

Usually, procedures for calibration of instruments should include the testing of limiting values of the range of the instrument (Min and Max), and as many as possible of nominal values to be tested between the limiting values; however, this is not possible to do for some calibrations, that is why it is important to analyse both interpolation and extrapolation calculations.

4.1. Interpolation

In order to evaluating the performance of the approximation by polynomials, the data of examples 3.1 and 3.2 were evaluated with the following modification: values of 60 g and 150 g were eliminated as if they never were tested, in order to have lower number of tested nominal values.

For the data of 3.1, table1 (except for 60 g and 150 g), the fitting coefficients and the variance-covariance matrix are,

$\mathbf{a} =$

$a_0 =$ -1.627 64 x 10^{-5} g

$a_1 =$ 4.442 31 x 10^{-6}

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 1.340 \times 10^{-8}\ \mathrm{g}^2 & -9.618 \times 10^{-11}\ \mathrm{g} \\ -9.618 \times 10^{-11}\ \mathrm{g} & 1.678 \times 10^{-12} \end{vmatrix}$$

For the data of 3.2, table 2 (except for 60 g and 150 g), the fitting coefficients and the variance-covariance matrix are,

$\mathbf{a} =$

$a_0 =$ 3.921 8 x 10^{-5} g

$a_1 =$ -7.812 6 x 10^{-6}

$a_2 =$ 2.000 7 x 10^{-7} g^{-1}

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 1.692 \times 10^{-8}\ \mathrm{g}^2 & -3.410 \times 10^{-10}\ \mathrm{g} & 1.317 \times 10^{-12} \\ -3.410 \times 10^{-10}\ \mathrm{g} & 1.872 \times 10^{-11} & -9.165 \times 10^{-14}\ \mathrm{g}^{-1} \\ 1.317 \times 10^{-12} & -9.165 \times 10^{-14}\ \mathrm{g}^{-1} & 4.929 \times 10^{-16}\ \mathrm{g}^{-2} \end{vmatrix}$$

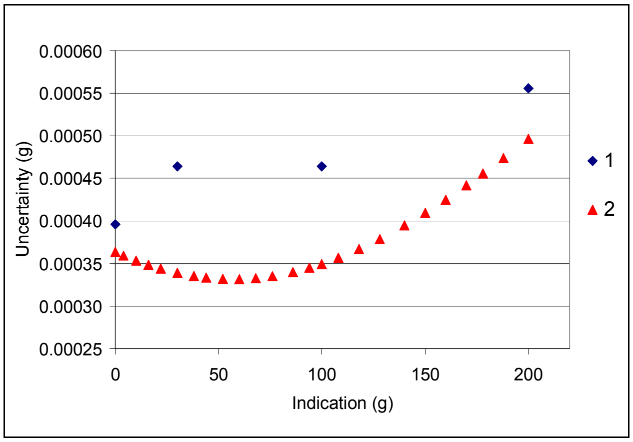

***Figure 7.** Expanded uncertainties associated to the errors of the indications calculated by calibration (series 1) and by the approximation by polynomial (series 2) for data of table 1 (except values of 60 g and 150 g).*

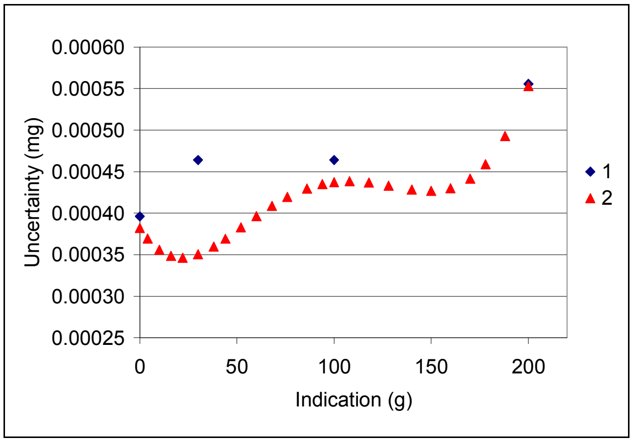

***Figure 8.** Expanded uncertainties associated to the errors of the indications calculated by calibration (series 1) and by the approximation by second order polynomial (series 2) for data of table 2 (except values of 60 g and 150 g).*

In both examples, the calculated errors from different approaches are quite similar to those values evaluated in 3.1 and 3.2, but regards to the uncertainty values there are some differences. The uncertainty values calculated by the polynomial function remain under the values of the uncertainties calculated in calibration, even when these results are slightly larger than if the tested values of 60 g and 150 g were included, see Figures 8 and 9.

4.2. Extrapolation

In order to evaluate the performance of the approximation by polynomials, the data of examples

3.1 and 3.2 were evaluated with the following modification: values of 0 g and 200 g were eliminated as if never were tested, in order to avoid the limits of the range of the instrument.

For data of 3.1 (except for 0 g and 200 g), the fitting coefficients and variance-covariance matrix are:

$\mathbf{a} =$

$a_0 =$ 1.293 03 x 10^{-5} g
$a_1 =$ 3.974 15 x 10^{-6}

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 4.184 \times 10^{-8}\ \mathrm{g}^2 & -4.104 \times 10^{-10}\ \mathrm{g} \\ -4.104 \times 10^{-10}\ \mathrm{g} & 5.177 \times 10^{-12} \end{vmatrix}$$

For data of 3.2 (except for 0 g and 200 g), the fitting coefficients and the variance-covariance matrices are,

$\mathbf{a} =$

$a_0 =$ 0.000 129 31 g
$a_1 =$ -5.692 x 10^{-6}
$a_2 =$ 1.6531 x 10^{-7} g^{-1}

$$\mathrm{cov}(\mathbf{a}) = \begin{vmatrix} 1.758 \times 10^{-7}\ \mathrm{g}^2 & -4.398 \times 10^{-9}\ \mathrm{g} & 2.254 \times 10^{-11} \\ -4.398 \times 10^{-9}\ \mathrm{g} & 1.239 \times 10^{-10} & -6.713 \times 10^{-13}\ \mathrm{g} \\ 2.254 \times 10^{-11} & -6.713 \times 10^{-13}\ \mathrm{g} & 3.795 \times 10^{-15}\ \mathrm{g}^{-2} \end{vmatrix}$$

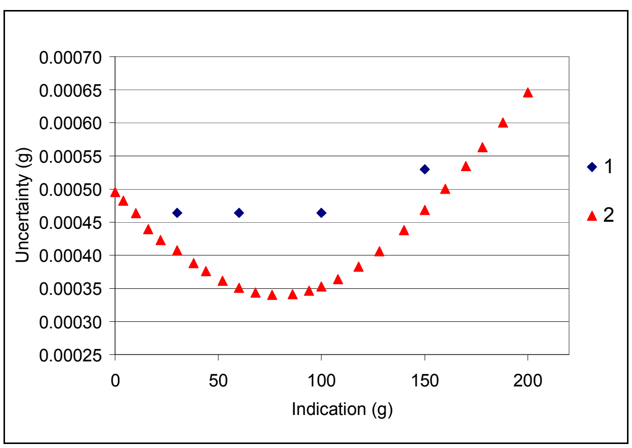

Figure 9. *Expanded uncertainties associated to the errors of the indications calculated in calibration (series 1) and by the approximation by polynomial of first order (series 2), for data of table 1 (except 0 g and 200 g).*

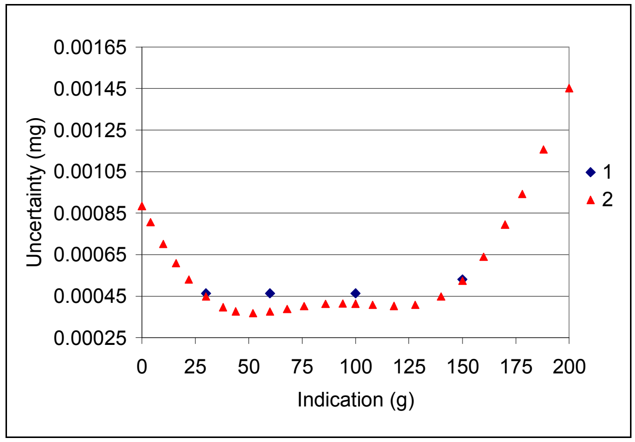

Figure 10. *Expanded uncertainties associated to the errors of the indications calculated in calibration (series 1) and by approximation of polynomial of second order (series 2), for data of table 2 (except 0 g and 200 g).*

In both examples, similar than in section 4.1, the main differences of results are in the uncertainties associated to the error of indications. The extrapolation of the indication errors throws larger values of uncertainty for nominal values out of the calibration range, especially for the second order polynomial function, see Figures 10 and 11.

5. PROPOSAL FOR THE CALCULATION OF A POLYNOMIAL FUNCTION FOR THE EVALUATION OF THE INDICATION ERRORS AND A POLYNOMIAL FUNCTION FOR THE ASSOCIATED UNCERTAINTIES

Considering that the Monte Carlo's method is one of the best methods to evaluate the uncertainty associated to the indication errors evaluated by a polynomial function, but as this method is not simple to apply by the final users, the authors recommend to the metrologist the following procedure for the evaluation of the fitting curve to describe errors of indications on calibration of measuring instruments (as a polynomial function) which include the information of Monte Carlo's method for the uncertainty evaluation but expressed as a polynomial function too:

a) To calibrate the instrument and to calculate the errors of indications and their associated uncertainties for discrete values (regular calibration),

b) If it is possible, the nominal values tested at calibration should include the minimum and the maximum capacity or the measuring range for the “normal” use of the instrument. The metrologist should keep in mind that more nominal values tested represent a lower uncertainty but higher cost of calibration,

c) To find the fitting curve by the use of the weighing least squares method, (5). This fitting curve could be a first or second order polynomial, (4),

d) To apply the chi-squared test χ^2 in order to check if the polynomial selected fits properly,

e) To estimate along the all measurement range of the instrument, include enough indication errors (at least ten) in the simulation by Monte Carlo’s method using the mathematical model of weighted least squares (5) for a polynomial function (4). The errors of indications found in calibration a), and their associated uncertainties should be taken as the means and as the standard uncertainties of the pdfs of the input quantities. If the nominal values tested could be considered as input quantities with variability (as it is assumed in the total least squares approach [6]), this situation should be modeled on the simulation,

f) From the pdfs of the indication errors resulting from the simulation, a polynomial function should be calculated in order to have a function of the uncertainty of the indication errors in relation with the nominal values of the indications of the instrument. This function could be calculated by ordinary least squares.

$$\mathbf{a}' = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{S} \tag{11}$$

where $\mathbf{a}'$ is a column vector of the fitting coefficients for the function of uncertainty (related to the indication error) and $\mathbf{S}$ is the column vector of the standard deviations of the pdfs of the output quantities of the simulation.

For the numerical examples of sections 3.1 and 3.2, the formulae to describe the indication errors and their standard uncertainties are:

for the straight line function,

$$E(R) = -5.143\times10^{-6} + 4.318\times10^{-6}R$$
$$u(E_R) = 1.068\times10^{-4} - 7.954\times10^{-7}R + 5.752\times10^{-9}R^2$$

and for the second order polynomial function,

$$E(R) = 6.882\times10^{-5} - 8.437\times10^{-6}R + 1.989\times10^{-7}R^2$$
$$u(E_R) = 1.079\times10^{-4} + 5.377\times10^{-8}R - 2.226\times10^{-9}R^2 + 2.102\times10^{-11}R^3$$

With these formulae, the user can evaluate the indication error and the standard uncertainty related to any reading of the instrument in normal use. The standard uncertainty calculated by these functions should be combined with the rest of contributions that are involved in the specific mathematical model where is used the calibrated instrument.

6. CONCLUSIONS

In this work the methods of approximation to describe errors in relation to indications mentioned in [1, 2] were analyzed, results from those methods were compared against values calculated by Monte Carlo’s simulation method.

The uncertainty of the fitting coefficients of the polynomial will depend on the number of nominal values tested and on the selected approximation for the fitting of the indication errors. For the matrix model dealt in this paper to calculate approximation function to describe errors related to the indications, the fitting could be tested with χ^2 test [1, 2].

Indeed it is not recommended to calculate errors of indications by an approximation function out of range of the nominal values tested; because of that, calibration should include the limits of the measurement range (*Min* and *Max*) of the instrument and as many as possible of nominal values to be tested.

Results (indication errors) of numerical simulation by Monte Carlo’s method are practically the same than results calculated by the approximation by polynomials (2.1).

The evaluation of the uncertainty for the straight line that crosses through zero approximation specified in [1, 2] does not consider the contribution of the uncertainty due to the assumption that a_0 is zero, but this supposition has an associated uncertainty, which in this work was considered identical to the uncertainty of a single indication.

The evaluation of the uncertainty for the error of the reading in use by linear interpolation method recommended in [1, 2], formula (2), considers that the uncertainty of the readings in use will be described by a linear interpolation too, in similar way as the calculation of the errors, however if the uncertainty of the errors is calculated using the law of propagation of uncertainty [3] applied to the mathematical model (1), the arising uncertainty is lower than that estimated by (2).

The closer approximation to the uncertainty evaluated by Monte Carlo's method is that evaluated by the polynomial method, even when this calculation throws uncertainties values higher than those evaluated by numerical simulation method.

A proposal for the calculation of the indication errors and their uncertainties by polynomials functions is presented in this paper, see chapter 5.

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