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CALCULATIONS OF UNCERTAINTY IN MEASUREMENTS

K. Chrzanowski*, R. Matyszkiel** and M. Szulim***
* Military Univ. of Technology, Inst. of Optoelectronics, 00-908 Warsaw, Poland
** Military Institute of Communication, 05-130 Zegrze Pld., Poland
*** Military Univ. of Technology, Faculty of Electronics, 00-908 Warsaw, Poland

Abstract: Rules of evaluation of uncertainty as a measure of measurement accuracy are *presented in the well-known "Guide to the expression of uncertainty in measurement". There are a few examples of uncertainty calculations in literature. However, all these examples refer to the case when the output quantity is determined on the basis of known input quantities by an analytical formula. In this paper a case when the output quantity is determined on basis of known input quantities by solving numerically a set of equations is discussed. It was shown that the rules recommended in the Guide cannot be used directly to calculate the standard uncertainty of the output quantity in this case but the calculations can be done using Monte Carlo simulations. Next, a software package that enables quick determination of the combined standard uncertainty or the extended uncertainty not only in case of analytical models of measurement process but also when the measurement result is calculated by numerical methods or algorithms is presented.*

Keywords: metrology, uncertainty, software.

1 INTRODUCTION

The well known "Guide to the expression of uncertainty in measurement", commonly abbreviated as Guide, published in 1993 in the name of the seven main international metrological organizations recommends uncertainty as a measure of measurement accuracy and presents methods of its calculations [1]. Publications [2,3] from the National Institute of Standards and Technology in USA and from the European Cooperation for Accreditation precise recommendations of the Guide.

There are a few examples of calculation of uncertainty of different measurement results in the Guide. More examples are presented in EA publications [4-11]. Nevertheless, all these examples generally refer to a situation when the measurement model can be presented in the form of a relatively simple analytical formula in situations when in practice measurement results are often determined by complicated analytical formulas, algorithms, or by solving numerically a set of equations etc. Additionally, calculations of the measurement uncertainty according to procedures recommended in the Guide or publications [2-3] are very time consuming even in the case of simple measurement processes. Therefore it seems that there are still many problems in practical application of the uncertainty theory in laboratories and industry.

2 SUMMARY OF PROCEDURES FOR CALCULATION OF UNCERTAINTY

According to the Guide the procedures to be followed for evaluation of the uncertainty of the result of a measurement can be summarised as follows:

1. Express mathematically the relationship between the measurand Y and the input quantities X_i on which Y depends.
2. Determine x_i, the estimated value of input quantity X_i, either on the basis of the statistical analysis or by other means.
3. Evaluate the *standard uncertainty* $u(x_i)$ of each input estimate x_i.
4. If the values of any two input quantities are correlated, evaluate their covariances.
5. Calculate the estimate y of the measurand Y from the functional relationship f using for the input quantities X_i the estimates x_i obtained in step 2.
6. Determine the combined standard uncertainty $u_c(y)$ of the measurement result y from the standard uncertainties and covariances of the input estimates.
7. If it is required to give an expanded uncertainty U then multiply the combined standard uncertainty $u_c(y)$ by a coverage factor k, typically in the range 2 to 3, to obtain $U=k\,u_c(y)$.

A bit different algorithms are recommended by European Cooperation for Accreditation or by National Institute of Standards and Technology in USA. However, the latter algorithms can be treated as modified versions of the original algorithm presented above.

3 EXAMPLES

In this section we will analyse two models of a measurement processes. First, the output quantity is determined on the basis of known input quantities by using a simple analytical formula. In the second one, the output quantity is determined on the basis of known input quantities by solving numerically a system of non-linear equations. In both cases we will try to calculate the combined standard uncertainty of the output quantity using the algorithm presented above.

Example 1. Calculate combined standard uncertainty of a measurement result of the transmission coefficient t_l of a optical plate measured using a spectroradiometer. The transmission coefficient t_l is calculated by using the formula $t_l = I / I_w$, where: I – indication of the spectroradiometer when the radiation passes through the tested plate, I_w - indication of the spectroradiometer when there is no an optical plate. Observations of the I i I_w were repeated 10 times. There are following measurement observations: I={50.7, 49.8, 51.6,47.9, 50.4, 51.6,47.9, 49.2, 48.9,52.2};I_w= {154.5, 146.5, 151.2,147.9, 149.5, 154.,147.6,146.9, 154.,147.7}.

According to data from the manufacturer, the intrinsic limit error of the spectroradiometer equals ±1% of the readings.

Mathematical model of this measurement process can be presented in the following form

$$t = \frac{I + \Delta I}{I_w + \Delta I_w} \tag{1}$$

where I, I_w - measurement result of the quantities I, I_w ; ΔI, ΔI_w - unknown systematic errors of the measuring system during measurement of the quantities I, I_w..

It is easy to carry out all steps of the algorithm presented above using only a simple calculator or even without it. Results of such calculations presented in form recommended by the EA are shown Tab. 1. Nevertheless, calculation of the combined standard uncertainty of the output quantity connected associated with a few input quantities using even this simple analytical formula are quite time consuming as it is necessary to carry out the following steps:

1. calculation of the estimates of the quantities I, I_w ; ΔI, ΔI_w using statistical analysis of the observations presented above and on the basis of the information provided by the manufacturer;
2. calculation of the standard uncertainties of estimates of the input quantities I, I_w ; ΔI, ΔI_w
3. calculation of the correlation coefficient between the input quantities I, I_w ; ΔI, ΔI_w,
4. calculation of the estimate of the output quantity t,
5. calculation of the sensitivity coefficient c_i (it is necessary to carry out a few operations of differentiation),
6. calculation of the partial uncertainties and the combined standard uncertainty of the quantity t.

Tab. 1. Results of calculations presented in the form recommended by the EA

qunatity X_i	*estimate* x_i	standard uncertainty $u(x_i)$	probability distribution	sensitivity coefficient c_i	partial uncertainty $u_i(y)$
I	50,02 mW	0.49 mW	normal	0.00667	0.03268
DI	0 mW	0.288 mW	rectangular	0.00667	0.00192
I_w	149,98 mW	1.01 mW	normal	0.00222	0.002242
DI_w	0 mW	0.866 mW	rectangular	0.00222	0.001922
t	0.335				0.005

It can be estimated that many people working in industrial laboratories will need a few hours to solve this really simple case and to calculate results shown in Tab. 1. It is often necessary to estimate uncertainty of thousands or more results of measurements. Therefore, we can conclude that users of measuring instruments should spend a lot of time calculating uncertainty of measurements in order to fulfil recommendations of the metrological organisations mentioned above, especially if they are working in industrial plants or laboratories that implemented the quality systems.

The uncertainty calculations for the analysed case are time consuming but at least it is well known how to carry out the required calculations, as there are a few examples of uncertainty calculations that refer to this case [3-11]. Therefore, although a specialised software that could shorten time of calculation would be helpful, the calculations can be done without it, too. There is, however, a case of measurement process where the output quantity depends on many input quantities by complex numerically solved formulas and the uncertainty calculations can be done only by a specialised software, especially that there no solutions how to solve such a case available in literature offered by the metrological organisationsearlier mentioned.

Example 2. Let us analyse here a case when the final measurement result is determined by solving numerically a system of non-linear equations. It occurs, for example, in multiband pyrometry when the output temperature T_{out} can be calculated by solving numerically a following set of non-linear equations [12]

$$\begin{cases} S_1 = k_1 (a_0 + a_1 l_1 + a_2 l_1^{\,2}) \dfrac{s(l_1)\Delta l_1}{l_1^5 \left[\exp\left(\dfrac{c_2}{l T_{out}} \right) - 1 \right]} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots, \\ S_4 = k_4 (a_0 + a_1 l_4 + a_2 l_4^{\,2}) \dfrac{s(l_4)\Delta l_4}{l_4^5 \left[\exp\left(\dfrac{c_2}{l T_{out}} \right) - 1 \right]} \end{cases} \tag{2}$$

where S_1,..., S_4 are the electrical signals measured at the four different spectral bands of the pyrometer, a_o,.a_1,a_2 are unknown coefficients of the polynomial interpolating emissivity function of the tested object, l_n is the effective wavelength of center of system the n spectral band, Dl_n is the n-th band width, t_{Fn} is the transmittance of the optical filter used in n spectral band, $s(l)$ is the relative spectral sensitivity of the detector, and k_n is the design constant of the n spectral band, c_2 is the Planck constant.

There are four unknowns T_{out}, and coefficients in the systems of equations (2) and four measured electrical signals S_1,..., S_4. It is possible to solve the system (2) using different mathematical methods and determine all unknowns mentioned above, however, the most important if the temperature T_{out}. Errors of measurement of the signals S_1,..., S_4 are usually the main source of errors of determination of the output quantity T_{out}. Therefore we can assume that only the signals S_1,..., S_4 are input quantities measured with limited accuracy; and that errors of determination of the other quantities like k_n, l_n, Dl_n, t_{Fn}, c_2 are negligible. On the basis of some knowledge about design of the pyrometer it is possible calculate the standard uncertainties of the signals S_1,..., S_4 as required in the presented earlier algorithm. However, the set of equations (2) cannot be solved analytically. Therefore, it is not possible to carry out directly the steps number 5 and 6 of this algorithm as we cannot derive analytical relationships between the combined standard uncertainty of the output quantity T_{out} and the standard uncertainties of the input quantities S_1,..., S_4.

Although we cannot use directly the algorithm presented above we can still determine the combined standard uncertainty of the output quantity T_{out} using another way based on Monte Carlo simulation.

The signals S_1,..., S_4 used during measurement process for the calculation of the output quantity T_{out} are constants. However, these input quantities can be treated as random variables whose random variations generate dispersion of values of the output quantity T_{out}. The combined standard uncertainty $u_c(T_{out})$ of the output quantity T_{out} can be calculated as the standard deviation of this dispersion. In order to calculate the uncertainty $u_c(T_{out})$ it is necessary to simulate random behaviour of the input quantitiesmentioned above, solve numerically the system of equations (2) many times, and finally determine $u_c(T_{out})$ as the standard deviations of dispersion of calculation results.

For the following data: S_1= 0.000511262, S_2= 0.000923934, S_3= 0.00136961, S_4= 0.0018296595, k_1=k_2=k_3=k_4=0.185294, l_1=3, l_1=3.5, l_1=4, l_1=4.7, $\Delta\lambda_1$=$\Delta\lambda_2$=$\Delta\lambda_3$=$\Delta\lambda_4$=0.1, s_1=0.53, s_2=0.661, s_3=0.81, s_4=0.99, $u(S_1)$= $u(S_2)$= $u(S_3)$= $u(S_4)$= 0.00000016667, and T_{out}=600K assuming normal distribution of the random variables S_1,..., S_4 we can calculate the combined standard uncertainty $u_c(T_{out})$ as equal to 3.765K.

On the basis of the examples presented above we can conclude that a specialised software package that could handle both analytical and numerical models of measurement processes would help significantly users of measuring instruments to estimate uncertainty of measurement results.

4 SOFTWARE PACKAGE

A software package called Assistant was developed. It can handle time consuming uncertainty calculations of both analytical and numerical models and free its users to concentrate on the real metrological challenges. The software can handle the examples analysed earlier within a few seconds after the user has entered all the necessary input data.

The developed software package Assistant requires from its user to make six following steps.

1. Determine and insert the number of input quantities X_1,..., X_n that influence the output quantity Y.
2. Determine and insert of the relationship between the input quantities X_1,..., X_n with the output quantity Y.
   Any analytical formula, numerical algorithm, system of equations etc. that connect the quantities X_1,..., X_n with the quantity Y should be given.
3. Insert parameters enabling identification of probability distributions of the input quantities X_1,.., $X_{n.}$
   The are two options of inserting the necessary information about probability distributions of the any input quantity X_i. When the quantity X_i was repeatedly observed then the user can choose the first option and insert the results of repeated observations of this quantity. In case of single observation of the quantity X_i when only a single value is known for this quantity the user must choose second option and insert type of the assumed probability distribution of this quantity and other parameters necessary to precise the assumed probability distribution. These parameters can be the standard deviation of this probability distribution, interval for a certain confidence level, limits within which all values of the quantity X_i. The second option can be chosen by the user in case of repeatedly observed quantity X_i, too.
4. Determine correlation coefficient between the input quantities.
   The software package Assistant independently calculates correlation coefficient between quantities identified by the user by inserting results of their repeated observations. However, it needs from the user some information about correlation between other quantities. When the user does not have any information about correlation between the input quantities the Assistant assumes that they are independent.
5. Insert information whether the extended uncertainty should be calculated. In case of a positive answer choose option of determination of the coverage factor.
   The user can determine the coverage factor k by himself or the suitable values of the k can be calculated by the program using the Welsh-Satterthwaite formula.
6. Determine the form of presentation of results calculations of uncertainty of the output quantity y.
   The user of the Assistant can choose between two options. First is a shortened form of presentation when only output estimate and its combined standard uncertainty or expanded uncertainty are generated according to the rules from the Guide. The second is an extended form when both input quantities, input estimates, sensitivity coefficients, output estimate and their combined standard uncertainty or expanded uncertainty are presented in a formalised table recommended by European Cooperation for Accreditation like in Tab. 1.

The structure of the application „Assistant" is based on the algorithm of calculation of uncertaintyearlier described. It consists of the following modules: the main module handling creating, editing, saving and visualisation of projects; the module analysing the mathematical expressions; the module introducing input quantities as results of series of measurements; the module introducing input quantities based on knowledge about them (the type of distribution and e.g. the range, or expected value and standard deviation); the module calculating uncertainties and expected values of the input quantities; the module determining the coefficients of correlation between input quantities; the module calculating the expected value of the output quantity; the module estimating the uncertainty of the output quantity, and the module estimating the extended uncertainty of the output quantity.

Most important features of the Assistant are presented below.

- It works in the following systems: Windows NT, Windows 98, Windows 95.
- It can handle both analytical and numerical models of measurement processes.
- A user can create a new project, save all input data and results of calculations in a file, as well as open such a file of an earlier project and analyse it.
- It enables calculations of the combined standard uncertainty and the expanded uncertainty.
- It supports following probability distributions: normal, t-, U, rectangular, triangular, trapezoidal.

- Automatic calculations of correlation between observations of different quantities.
- Two version of reports produced by Assistant: the simplified version (the estimate of the output quantity and its standard uncertainty of its extended uncertainty) or the full version (the table recommended by EA).
- Report may be printed, transferred via clipboard or to data files. Three different formats are supported (Text only format or HTML). The latter format is particularly important as it enables possibility to create sophisticated reports in a well known format and to run such applications like Internet Explorer, Netscape Navigator to interpret it and to print from this applications.
- The Assistant enables to use the following mathematical functions: sin, cos, tan, exp, sqrt, log, ln; and following mathematical operations: addition, subtraction, multiplication, division, power, numerical derivation; numerical integration. We can also attribute specific units to quantities.
- All examples from the Supplement to EAL-R2 and many others referring to real measurement processes are included in the help file.

5 CONCLUSIONS

It is possible to calculate using the recommended in the Guide and presented above algorithm the standard uncertainty of the extended uncertainty of any measurement result. However, calculation of the uncertainty of a measurement result can be very time consuming even in case of simple measurement models. Next, the examples from the Guide and from publications the EA show well how the uncertainty of a measurement result should be evaluated when the output quantity is determined on basis of known input quantities using an analytical formula. There are not known examples that would give precise guidelines how the uncertainty of a measurement result should be evaluated when the output quantity is determined on basis of known input quantities using numerical methods.

There are two main advantages of the developed software package Assistant. First, it significantly reduce the time necessary to determine uncertainty of results of measurements. Second, it can determine, uncertainty of the measurement results not only for typical case of simple analytical measurements models but also for case when the output quantity is determined using sophisticated analytical formulas, numerical algorithms, or by solving numerically systems of non-linear equations.

Because of these significant advantages the software package Assistant can help to implement the recommendations of the Guide in many industrials plants and laboratories that so far do not estimate accuracy of measurement results due to problems connected with uncertainty calculations.

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AUTHOR(S): K. Chrzanowski Ph.D, D.Sc., Eng., Military University of Technology, Inst. of Optoelectronics, 2 Kaliski Str., 00-908 Warsaw, Poland, phone 48-22-6857689, fax 48-22-6668950, E-mail: kchrza@wat.waw.pl;
R. Matyszkiel M.Sc. Eng., Military Institute of Communication, 05-130 Zegrze Pld., Poland, tel. 48-22-6885547, fax 48-22-7743865 E-mail matyszki@wil.waw.pl
M. Szulim M.Sc. Eng., Military University of Technology, Faculty of Electronics, 00-908 Warsaw, Poland, tel. 48-22-6857106