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PRESENT METROLOGICAL STANDARDS IN MATHEMATICAL MODELING PROCEDURES**

1. INTRODUCTION

In the years 1993–1994 metrology with associated branches of science and fundamental techniques experienced changes related to the introduction of basic and general term of uncertainty in measurement. Their beginning is connected with international recommendations *Guide to the Expression of Uncertainty in Measurement* edited by *International Organization for Standardization (*ISO) in 1993, a result of cooperation of a number of institutions on uncertainty in measurements. In 1994 the standard ISO 5725:1986 *Precision of test methods – Determination of repeatability and reproducibility for a standard test method by interlaboratory tests* was substituted by a standard edited in six parts under the heading of *Accuracy (trueness and precision) of measurement methods and results*.

The Polish counterpart documents are:

– publication *Expressing uncertainty in measurement. Guide*, edited by the Central Office of Measure (Główny Urząd Miar – GUM) in 1999;
– standard PN-ISO 5725 *Accuracy (trueness and precision) of measurement methods and results*, edited in six parts by the Polski Komitet Normalizacyjny (PKN) in 2002.

It should be stated that the notion of 'uncertainty of measurement' appeared in the Polish literature already in the 1970's. The commonly used term 'measuring error' was substituted with 'uncertainty of measurement' by prof. Henryk Szydłowski from A. Mickiewicz University of Poznań, incorporating both 'maximum error', and also all statistical

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parameters describing the precision of performed measurements [15]. The commonly applied term 'error' is very misleading, as in reality instead of error only uncertainty of measurement result occurs.

The standard PN-ISO 5725-1 contains Polish counterparts of English terms given in ISO 5725-1, and which are a collection of terms that are partly different from basic and general metrology terms presented in the *International Vocabulary of Basic and General Terms in Metrology*, ISO 1993, ed. GUM 1996. The differences refer to the scope of the terms and some notions, e.g. accuracy and trueness.

The scope of the standard ISO 5725 justifies the use of a specific set of notions that are sometimes modified. In 2000–2002 the following publications were also edited:

- extensive, 13-sheet long, standard PN-ISO 31: *Physical quantities and units of measure*, in that, e.g. sheet 0: *General principles* introducing to, e.g. units of measure 'singularity' referring to a quantity equal to one (dimensionless until then) and sheet 11: *Mathematical signs and symbols for physical sciences and techniques*;
- standards PN-ISO 3534: *Statistics. Terminology and symbols*, covering 4 sections, in that, e.g. section 3: *General terms referring to observation of measurement results*.

2. MOST IMPORTANT CHANGES IN METROLOGICAL TERMS

Accounting for the above mentioned standards when determining quantitative indices characterizing the quality of measuring methods and used for working out the results, the following notions and terms should be taken care of:

Assumed reference value – value used as a reference for the comparison, substituting the true (real) unknown; it is established on the scientific bases, research works or as an expected value, i.e. average value for a given population (series) of measurement results.

Trueness – a degree of congruence of the mean value obtained from a large population of results and the assumed reference value, expressed as loading; previous trueness was presented as 'accuracy of mean value'.

Accuracy – degree of congruence between the result of measurement and the assumed reference value; if this refers to a set of results, it covers random components and common systematic error or loading component (previously the notion 'accuracy' covered only the component which is now called trueness).

Loading – a difference between expected value and the assumed reference value, i.e. total systematic error (unlike random error).

Precision – degree of congruence between independent results obtained in definite conditions, only dependent on the distribution of random errors.

Repeatability – accuracy in repeatability conditions met, i.e. when independent results of the same units are obtained with the same method, in the same laboratory, by the same operator with the same equipment and in short spans of time.

Reproducibility – precision when reproducibility conditions are met, i.e. when the results of analyses of the same research units are obtained with the same method in various laboratories by various operators with the use of different equipment.

Uncertainty of measurement – evaluation related with the result of measurement characterizing intervals, inside of which an unknown true value can be expected (with no systematic error, the random uncertainty component can be interpreted as a statistical confidence interval); two types of uncertainty can be distinguished: *type A* – uncertainty which can be defined with mathematical statistics methods, and *type B* – uncertainty which can be determined using various methods, e.g. on the basis of literature data, material certificates and proofs, technical data of measuring device, own experience and available knowledge, etc.

The changes in measurements at the stage of result elaboration resulted in:

- obtaining correct results, which signifies identification of systematic errors or their elimination;
- quantitative evaluation of quality of final results by evaluation of their uncertainty (instead of a classical count of errors).

The results of measurement of physical values are presented as intervals (not points!), which is justified practically and theoretically. This stems from the metrological postulate that the so-called sensitivity thresholds of measurement methods are bigger than zero, e.g. [14].

This is explained by:

1) technical-biological causes: limited (imperfect) accuracy of tools and systems used in the measuring process, and also our senses;
2) physical nature of investigated objects and phenomena: matter has a grain texture, whereas a number of physical effects have a quantum character; constant measurable quantities in a given interval can assume infinitely numerous values, differing by infinite elemental increases, where the smallest possible one is an elemental quantum (grain) of the measured value;
3) theoretical premises resulting from the probability calculus and mathematical statistics: probability of the fact that continuous random variable X, which is used for the quantitative analysis of measurement results, assumes an arbitrary point value a and is equal to zero:

$$P(X = a) = \lim_{b \to a} P(a \le X \le b) = \lim_{b \to a} \int_a^b f(x)dx = \int_b^a f(x)dx = 0 \tag{2.1}$$

where $f(x)$ is a density function of probability random variable X or briefly: density of probability [16]; probability P bigger than zero refers to situations when variable X assumes values from an arbitrary finite interval (a, b): $a \le X \le b$, where the difference $(b - a)$ is bigger than zero, which means interval evaluation.

Above remarks justify the unquestionable metrological axiom saying that the result of measurement has a form of an interval on a dimensional axis. Above presented rules, according to which the physical measurables are presented, should also find its representation in practical procedures of mathematical modeling.

3. PRINCIPLES OF MATHEMATICAL MODELING

3.1. Basic notions in modeling

Modeling aims at presenting a real object or technological process as a model, which should enable one to investigate and analyze it and get the most efficient description of the object or actual process. The purpose for which the model has been elaborated is most important as it determines the way in which the model is made at the assumed simplification level.

The basic notion in modeling is the model. The actually existing objects or processes are original, whereas the model is a simplified (abstract or physical) representation, neglecting all the properties which are not subject of the study. By doing this, the model becomes more convenient to handle and analyze than the original, which is frequently too complex.

The model is a quantitative and qualitative representation of the original, thanks to which the dependence between analyzed factors can be accounted for. This is always a compromise between tending to obtain a true and detailed representation of reality and the tendency to simplify have only an approximation, which should be satisfactory from the practical point of view. If the simplifications go too far, the model stops describe the reality properly; on the other hand, a true model is usually unattainable (too complex) and devoid of economic justification. Models should be verified practically, i.e. experimentally.

The notion of a model is very broad, hence the detailed classification of models is very difficult and sometimes ambiguous [1, 4, 10]. Generally, all the models can be divided into cognitive (conceptual, notional) and material (physical, real) ones. According to the modern theory and philosophy of science strongly attached to the modeling reality [6]: *„Models blur the boundaries between the thought and an object. There exist conceptual models of physical processes and physical models of rational processes”*. When creating material models employing criteria of similarity with the study object, other models, similar to the prototype, can be distinguished: geometrical, physical and mathematic ones [10].

The scientific-technical publications representing various disciplines of science differ in the classifications of models and modelings.

For instance, the most frequent models encountered in hydrogeology [8] are the following: a) physical (hydraulic), natural or artificial, depending on the material used; b) analogy, making use of analogies of mathematical description of physically varying effects; c) mathematical, most frequently deterministic type, based on strict analytical solutions or approximated numerical solutions.

In a work on environmental engineering [7], two groups (categories) of models are distinguished: a) physical, being laboratory paradigms of the studied systems; b) mathematical, sometimes commonly called ‘computer’ ones, represented by deterministic simulation models or stochastic empirical models.

In modeling of dynamic systems after [11], the models are divided into notional and real ones, where the latter can be represented by physical and/or mathematical models.

The above information and rich literature devoted to modeling clearly reveal that in practice a two-category division dominates: physical and mathematical models. This classification is fully justified as in many disciplines (e.g. mechanics) the analysis of the object or effect has to be preceded by its physical model, and only then realized based on the mathematical modeling (e.g. [1, 23]).

3.2. Characteristic of mathematical models

Gutenbaum [1] defines mathematical model as a set of symbols and mathematical relations and operation principles, when these symbols and relations refer to definite elements of modeled reality area.

The interpretation of symbols and mathematical relations leads to the construction of a model. Mathematical modeling is interdisciplinary and universal in nature, i.e. allows for analyses and can be used in various disciplines. Hence, it has been commonly used, especially over the last decades, also in disciplines that have been considered to be non-mathematizable, e.g. humanities. As already mentioned, to investigate an object or effect one should build its physical model first. This is a concept how to describe an object or effect and establish parameters that have influence on it. This particularly refers to mechanics, where the measured quantity is sometimes defined as a ‘measurand’ and presented as a mathematical model (e.g. [23]). In other disciplines of science mathematical modeling is preceded by the phase of conceptual modeling (cognitive, conceptual, notional).

Making of the mathematical model should be understood as a mathematical notation of physical laws valid for the studied processes and objects. These can be various algebraic equations, normal differential equations or partial ones, differential-integral equations, difference equations, etc. with possible boundary and initial conditions. The mathematical model of a definite object or physical effect can have many equivalent mathematical forms, differing in the applied notation, i.e. mathematical form [1, 4, 11].

Depending on the assumed criteria, mathematical models can be classified in a number of ways, tracing back to mathematics, physics and related sciences, e.g. static-dynamic, stationary-non-stationary, linear-non-linear ones. In practice, however, the most important division as far as technical sciences are concerned, is the general classification of models, resulting from the cause-and-effect postulate for the causative (deterministic, determined) and random (random, probabilistic, stochastic, statistical) models [4]. In causative (deterministic) models only the cause-and-effect function relations take place for all the physical quantities. If at least one relation that is not of cause-and-effect type occurs, the model is called a random model. In literature devoted to this subject one can find a number of various opinions and proposals, which are sometimes ambiguous, or even exclusive. In his comprehensive work [1] J. Awrejcewicz gives the following mathematical models, as referred to mechanics:

a) deterministic – all parameters are determined;
b) probabilistic – at least one of the parameters is a random with unknown distribution of probability;
c) statistical – at least one of the parameters is a random variable with unknown distribution of probability;
d) strategic – at least one of the parameters can assume one of defined values.

In the work devoted to environmental protection [7] P. Holnicki-Szulc distinguishes computer model, including mathematical models:

a) simulation (deterministic) analytical models (with accurate solutions) and numerical models (with approximated solutions);
b) empirical (stochastic) models – based on semi-empirical statistical data, illustrating relations between measured values and available data.

Similarly, in an extensive monograph [3] on reservoir engineering the authors discuss computer models, which in practice is reduced to the realization of various equivalent models: mathematical, numerical, network, difference, and reservoir models in particular.

In work on hydrogeology [9] the following mathematical models are distinguished:

a) deterministic, covering analytical and numerical models;
b) stochastic (statistical);
c) combined models, linking elements of above-mentioned models.

M. Sobczyk in his highly recommended handbook on statistics [6] distinguishes two types of relations between variables:

a) functions – a given value of a variable (independent, explanatory X) has one and only one corresponding other variable (dependent Y);
b) stochastic (probabilistic) – with a change of value of one variable, the distribution of probability of the other variable changes too; a specific case of this relation is a (statistical) correlation, when the determined values of one variable have strictly corresponding mean values of the other variable.

In the light of the review of various mathematical model classifications, the simplest and best justified division of models, as far as the character of measurable physical values in technical sciences goes, is a division into three classes of mathematical models, partly congruent with the one proposed in [17, 19, 20, 21]:

a) deterministic (functions);
b) random (stochastic), including statistical ones;
c) deterministic-statistical.

The following quantities can be distinguished in the structure of the mathematical model [4, 23]:

- input $X = \{x_i : i = 1, n_x\}$;
- output $Y = \{y_i : i = 1, n_y\}$;
- characterizing the model, i.e. regarded to play an important role of its attributes, also called quantities influencing the result, $H = \{h_i : i = 1, n_h\}$;
- remaining quantities, especially various types of unexpected disturbances $Z = \{z_i : i = 1, n_z\}$.

In the metrological categories the output quantities Y should be treated as the results of measurements of analyzed values, whereas input quantities X – as auxiliary quantities, appearing in formulae defining values of type

$$Y = f(X_i; i = 1, n_x) \tag{3.1}$$

in transient measurements. Relations between values characterizing the model make up its characteristic.

The basic types of analyses of mathematical models are [4]:

- analysis, i.e. simple task,
- control, i.e. reverse task,
- sensibility analysis,
- identification.

Analysis of the model is a simple task lying in determining output quantities knowing the characteristic of the model and input data. The results of analysis of the model are frequently used for model verification: analysis of its congruence with the object of study and accuracy of model.

Control is a reverse task, which means such a selection of input quantities that the required output data are obtained for a known characteristic of the model.

Sensitivity analysis is an analysis of influence of parameters of the model on output quantities. The results of sensitivity analysis and the results of analysis allow for an evaluation of influence of various quantities on the results of the studies model, especially evaluation of the influence of disturbances or remaining uncontrolled quantities of the model on these results.

Identification of the model lies in characterizing the model on the basis of known input and output quantities. The analysis of the model can be treated as identification of the model. Identification may focus of the structure of the model (structural identification) or parameters (parametric identification).

From the point of view of mathematical modeling of objects (systems), the following three models can be distinguished [1, 7]:

a) phenomenological (education) – describes and explains the mechanism of the system operation;

b) prognostic (simulation) – allows for predicting future behaviour of the model and analyzing actual object (system) by comparative simulation, i.e. analysis of mathematical model;
c) decision (management-aiding) – allows for proper selection of input reactions meeting required conditions (values of input quantities).

Over the last years we have observed an intense development of a new approach to the analysis of large data sets and mathematical models construed on this basis. This is the youngest (dating back to the 1980's) and quickly developing part of computer science known as data mining [12, 13]. It links the algorithms worked out over the last 30 years for data analysis and finding trends and regularities with classic statistical methods, probability calculus and database technologies. One of the main segments of data exploration is modeling, with its final objective of finding practical solutions of definite problems, especially as far as predicting, simulating and management aiding (decision taking) are concerned [12].

4. EVALUATION OF RESULTS OF MATHEMATICAL MODELING

4.1. Identification of possible systematic errors

The present theory of uncertainty assumes the random model of inaccuracy of measurements, whereas the ways of evaluating their uncertainty are referred to correct measurements, i.e. not burdened with systematic error.

Systematic error in its definition has a specified value and sign, therefore is determined, not random. If it is determined, the result of the measurement can be easily corrected by introducing the same value but with the opposite sign. If the value of the correction is unknown, which signifies that the result of the measurement was incorrect, it should be treated as additional random uncertainty. Hence a great practical significance of identification of possible systematic errors referring to the measurement of output values Y and input quantities X in the mathematical model (function of measurement) (3.1).

If a given quantity Y or X is measured in laboratory conditions (the so-called active experimental analyses), the identification of systematic error (loading of the laboratory, in terms of metrology) can be realized by additional measurements (for verification purposes) in a laboratory accredited by the Polish Centre for Accreditation and confirmed with a respective certificate. An example of this type of procedure is depicted in the publication [22].

If the output quantity of model Y undergoes measurements in industrial conditions (the so-called passive experimental analyses), then in favourable conditions model's congruence with the object (effect) can be checked out and verified. This gives an opportunity to find out the so-called loading of model, being its additive or multiplicative systematic error, the value of which can estimate (predict) differences between arithmetic means of actual measurements and the point results of mathematical modeling.

4.2. Evaluation of uncertainty of modeling results

Statistical models

The interval form of presentation of mathematical modeling results has been valid for random (stochastic) mathematical models for years. This especially refers to the most commonly applied statistical (correlation) models, which after verification are willingly applied as predictive regression models for predicting output values of *Y*. The statistical regression models frequently made as a version of polynomial multiple linear or pseudo curvilinear regression, can be presented in the following form [2, 16, 19]:

$$Y = f(X_i : i = 1, n_x) + \varepsilon \tag{4.1}$$

where:

- Y – dependent variable, the value of which we want to explain or predict;
- X_i – independent variable, also called explanatory variable or predicator;
- ε – random error, also called random disturbances (source of randomness in the model); has from definition a normal distribution, expected value equal to zero an no autocorrelation.

The statistical model (4.1) evidently differs from the function of measurement (3.1) only with random error (disturbance) ε. In this case the regression interval prediction is construed as a classic interval of confidence, known from mathematical statistics [2, 16].

The width of the confidence interval $\langle a, b \rangle$ depends on the assumed level of confidence *ă*, determining the probability *P* of the fact that interval $\langle a, b \rangle$ contains an unknown evaluated parameter *Y*, i.e. $P(a \le Y \le b) = \gamma = 1 - \alpha$, where α – level of significance of tested statistical hypotheses. In the natural and technical studies, the 95%-level of confidence is most frequent, i.e. $\gamma = 95\%$.

When using prediction regression models, in practice their quality is frequently characterized with the use of absolute values of $S_{y/x}$ or/and relative $S_{y/x} / \bar{y}$ standard residual errors of the model, where $S_{y/x}$ is a square root of residual variance (average square of residual variable), whereas $\bar{y}$ – mean (average) value of predicted parameter. The residual variance $S_{y/x}^2$ is an estimator of variance, and $S_{y/x}$ – estimator of standard deviation of random model, which can be used for assessing boundaries of confidence intervals of evaluations $\hat{y}$ of predicted parameter *y* provided that the obtained regression model is correct.

The way of verifying the trueness (adequacy) of the regression model and detecting possible systematic error of loading of residual regression variables can be found in mathematical statistics handbooks or some publications, e.g. [19].

Deterministic models

The evaluation of uncertainty of results of deterministic (functional) modeling is based on the present theory of uncertainty which, as already observed, is based on the random model of uncertainty and correct results of measurements. For evaluating the uncertainty in a general case with respect to the deterministic model one should use the measuring function (3.1) on the assumption that both values of output Y and input variables X can be determined with the direct and/or indirect measurements method, and the input quantities can be correlated.

The principles of estimating measurements are discussed in detail in a number of handbooks and guides on measurements, e.g. [5, 12, 18, 23]. In this work the authors give only the most important notions and strategies of assessing uncertainty.

The uncertainty of measurement u is a parameter thanks to which the boundaries of interval, which with the assumed probability encloses an unknown real value of the measured quantity, can be determined. It is assumed that the total uncertainty is always random and that standard deviation S of measurement series or multiplication kS is its figure measure. The uncertainty of measurement may include many components, both of A and B type.

It can be assumed that owing to the source of origin the A-type uncertainty corresponds to errors caused by random effects, whereas B-type uncertainty corresponds to errors generated by systematic factors. In the analysis of measurement uncertainty of A and B type it is assumed that all known corrections were accounted for during the measurement.

The most frequent source of uncertainty caused by systematic effects is imperfect measuring apparatuses. In this case the boundary value of a classic error Δg allows for evaluation of variance or standard deviation for the assumed distribution of uniform or triangular probability.

The theory of uncertainty introduced the following important notions:

Standard uncertainty $u(x)$ – expressed by standard deviation S of results of a number of measurements performed in constant reference conditions.

$$u(x) = S \tag{4.2}$$

Cumulative (total) uncertainty – standard uncertainty of the result of transient measurement obtained from the measurement of a few input quantities, equal to a geometric sum of components being variances and covariances (in the case of correlated quantities) of these quantities multiplied by the respective coefficients of sensitivity dependent on the function of type measurement (3.1).

$$u_\tau = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f}{\partial X_i} \right)^2 u_i^2} \tag{4.3}$$

Covered uncertainty – determines the interval of values around the result of measurement equal to the product of total uncertainty and coverage factor k.

$$U = k \cdot u_{\tau} \tag{4.4}$$

The coverage factor k is a standardized variable, determined for the assumed level of confidence from normal distribution or t-Student and depending on the assumed confidence level and number of degrees of freedom.

In some cases of the values of coefficient $k = 2$ or $k = 3$ can be arbitrarily assumed, with the corresponding probability (level of confidence) $p = 0.95$ and $p = 0.99$, respectively. However, it should be remembered that this is a simplification which may decrease the correctness of evaluation of boundaries of the assessed interval [5, 23].

5. CONCLUSIONS

The paper presents the most important meritoric issues related to the theory and practice of mathematical modeling, which loomed after 1993, and which stemmed from the fundamental changes in metrology introduced by international and home standardization and metrological institutions and organizations. They especially refer to the evaluation of the quality of measurements of physical quantities and are related with the introduced notion of uncertainty in measurement. The principles of mathematical modeling and classes (types) of mathematical models were given in more detail. Special attention was paid to the evaluation of the results of mathematical modeling, in that identification of possible systematic errors and before all, evaluation of uncertainty of the results of statistical and deterministic modeling. The mathematical modeling method, and consequently simulations in mining and geology develop very dynamically, making use of, among others, the newest calculation methods and analyses of large databases, e.g. artificial neural networks, the so-called data mining. The efficient practical use of mathematical modeling requires proper knowledge and experience and, on the other hand, sufficient amount of information about the modeled object (process), frequently obtained during field studies. The properly construed model is calibrated and verified, then can be used in practice for predicting. The quantitative evaluation of the prediction results can be acquired through the analysis of sensitivity of prediction to the changing parameters of the model. In practice the model should be preferably construed simultaneously with the field studies and successively improved. The correct feedback from modeling to field studies and the other way round creates conditions for obtaining correct results.

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