What to know about risks of false decisions due to measurement uncertainties[1]

Q&A with Ilya Kuselman

Q: What is "conformity assessment"? Is this not a bureaucratic procedure?

International standard ISO/IEC 17000:2004 "Conformity assessment. Vocabulary and General Principles" defines conformity assessment as the demonstration that the specified requirements for a product or system have been met. For example, we want to drink, eat and drive while staying alive, being healthy and even having fun. This means that water, wine, food and transportation meet the established requirements. Testing (chemical analytical) laboratories provide a customer with the information necessary to conduct conformity assessment and should carry it out if the consumer is interested.

To this end, the measurement results obtained in such laboratories are compared with the requirements for substances and materials established as the limits of the specification intervals of contents or concentrations of the main components and impurities. These laboratories also undergo conformity assessment according to the international standard ISO/IEC 17025:2017 "General requirements for the competence of testing and calibration laboratories." One of the basic requirements of ISO/IEC 17025:2017 is calibration of the chemical analytical equipment and internal quality control of the measurement process using the relevant reference materials of composition and properties of substances and materials as the measurement standards. In turn, producers of reference materials should comply with the international standard ISO 17034:2016 "General requirements for the competence of reference material producers." At the top of the pyramid of this conformity assessment, there are requirements of the ISO Guide 35:2017 "Reference materials—Guidance for characterization and assessment of homogeneity and stability." ISO Guide 35:2017 recommends setting the limits of the specification intervals of the contents of components, impurities and/or other properties to be characterized in the reference material, already at the stage of the project for the development of this reference material.

Q: What are the risks? What can be wrong with a material if the actual content of any component or impurity is slightly more or slightly less than its specification limit?

As the French say: "one who risks nothing, gets nothing; one who risks everything, loses everything." We take risks in the bathroom at home: according to statistics, the most severe home injuries await us there. On roads in Israel, where citizens are generally law-abiding, an order of magnitude more people die in car accidents than in terrorist attacks. Of course, we risk choosing our friends, and even more so wives or husbands. However, the Russian writer Ivan Bunin may be right, arguing that the one who does not take risks, risks the most. In our case, we discuss the risks as probabilities of false decisions in conformity assessment of a substance or material, based on a comparison of measured values of contents of the main components and impurities with their specification limits. This is also applicable to a reference material. There is a producer's risk when a good product (a batch of a substance or material) is mistakenly recognized as nonconforming with the specifications and rejected. Simultaneously, the consumer's risk is the probability of the false decision for a product that does not meet the same specifications but is mistakenly recognized as conforming and released to the market. Both risks may be particular when related to conformity assessment of the content of one particular component or impurity in a substance or material. They are called "specific" for a specific batch, lot or environmental compartment, and "global", when an infinite statistical population of the batches, lots or compartments is discussed. There are also total risks in conformity assessment of a multicomponent object or system as a whole, divided into the producer's and consumer's, specific and global risks.

Q: How do measurement uncertainties affect risks, and what does the mass balance have to do with it?

If people know the actual (true) value of the measurand, the answer to the question "What is good

1. This is the main part of the interview given to the organizers of the Vth International Scientific Conference, "Reference Materials in Measurement and Technology," Ekaterinburg, Russia, 13-16 September 2022. The full version of the interview in Russian is available on the webpage https://uniim.ru/news/.

and what is bad?" would be much simpler in conformity assessment. However, the problem is that although improving the measuring technique can decrease the measurement uncertainty, some uncertainty always remains: "God only knows the truth, while the devil is in the details." Therefore, the measurement result consists of the measured value and its associated uncertainty, expressed as the standard deviation or confidence interval, which contains the true value with the specified probability. The measurement uncertainty causes the "gray zone" of risks of false decisions around a specification limit. The larger the measurement uncertainty is, the wider the "gray zone." Practitioners take that into account empirically using "intrafactory tolerances," which are de facto the acceptance intervals for measured values, more stringent for a producer than the specification intervals set in a standard or another regulatory document. Everything would be fine, but the measured values of different components of the same substance or material can be correlated for a variety of reasons. There are 1) metrologically related correlations, *e.g.,* in spectral analysis; 2) native correlations, *e.g.,* because of the stoichiometry of a substance, in which the contents of components/elements are constant under normal conditions; and 3) technological correlations caused by requirements to the ratio of quantities of the raw materials. Moreover, when the contents of all the main components are controlled for conformity assessment and their sum must be equal to 100 % (or 1 if the contents are expressed in mass or mole fractions), this limitation, called "mass balance," causes another kind of correlation. It was first described by the English mathematician Karl Pearson in the 19th century as the "spurious" correlation. Note that previously, in the 18th century, the works of the French naturalist Antoine Lavoisier and Russian scientist Mikhail Lomonosov were already known. Their names are always mentioned in connection with the history of the comprehensive conservation law, in particular, the law of conservation of mass. According to this law, the composition of a substance or material, object or system, close to the transfer of matter and energy, remains unchanged. Thus, the mass balance and the limitation of the sum of the contents of the components by 100 % (or 1) is one of the expressions of the law of conservation of mass. Similar to other types of correlation, "spurious" correlation affects the results of the conformity assessment and should be taken into account in the evaluation of risks—the probabilities of false decisions on conformity.

Q: Where can one find detailed guidelines on evaluation of the risks?

The Joint Committee for Guides in Metrology at BIPM issued the guide JCGM 106:2012 "The role of measurement uncertainty in conformity assessment," https://www.bipm.org/en/committees/jc/jcgm/publications. This guide explains conformity assessment methodology by comparing measurement or test results with their specification limits using the approach of Thomas Bayes, the English mathematician of the 18th century. The approach is based on the statement that knowledge about the measured value can be supplemented by information accumulated before the measurement as a random variable and expressed in terms of a probability density function. JCGM 106 concerns one (particular) measurand and is applicable in analytical chemistry "component by component." The Bayesian approach has been extended by us to multicomponent systems (multidimensional spaces of contents or concentrations of components) in the IUPAC/CITAC Guide: 2021 "Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty (IUPAC Technical Report)", published in *Pure and Applied Chemistry,* https://doi.org/10.1515/pac-2019-0906, and on the CITAC website, https://www.citac.cc/guides/. The next IUPAC/CITAC Guide "Evaluation of risks of false decisions in conformity assessment of a substance or material with a mass balance constraint (IUPAC Technical Report)" is being prepared for publication by the working group of the IUPAC Project, https://iupac.org/project/2019-012-1-500, expected in early 2023. In the last document, the Bayesian approach is applied in a non-Euclidean space (simplex) formed by contents of the components under the mass balance constraint, where the usual three-dimensional figures become flat, like shadows, and fit into a triangle; the contents of four components form a pyramid; *etc.* Solutions are found using the Monte Carlo method and R-programming. All the mentioned documents are available and will be available for open access.

Anyone who is interested in knowing more is welcome to participate in the IUPAC/CITAC Workshop and Isranalytica 2023 in Tel Aviv, www.isranalytica.com. The Workshop details are on the IUPAC webpage, https://iupac.org/event/metrology-quality-and-conformity-assessment/, and also on the CITAC webpage, https://www.citac.cc/conferences-and-workshops/.

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