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PAUL'S COLUMN ON MIC

"Analyte" is frequently used as synonym for "measurand": is that correct?

Paul De Bièvre

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In a measurement, a most basic concept is "measurand."

When starting to draft a plan for a process called measurement, we must clearly specify the goal of the process. That goal must have been discussed with the end user (frequently called the customer) on beforehand. Agreeing on such a goal and respecting this agreement will ensure that the result obtained at the end of the process as carried out by the analyst, is fit for the intended use [1] of the result by the end user. The product of a discussion between the end user of the result and the analyst is about *what* is the goal of the process. Thereby the end user should not have to worry about *how* the analyst performs the process: that is what the end user pays the analyst for. Thus, the analyst must make sure that the measurement result (s)he obtains at the end of the process is clearly related to the goal (s)he has agreed with the end user. All intermediate steps that need to be taken during the process, including whatever chemical operations such as weighings, dissolutions, separations, chemical transformations, preparation of samples suitable for introduction into whatever type of spectrometer, measurements of other input quantities (see entry 2.50 in [2]) into the measurement function (see entry 2.49 in [2]), etc., deemed necessary by the analyst to reach the goal agreed with the end user, ultimately are the analyst's choice and decision, not the end user's. The analyst is in control of assigning the value (with associated measurement uncertainty) to the measurement result [3]. The intermediate steps, important as they may—or because sometimes they are so important—pertain to the answer to the question *how* the goal agreed with the end user, is attained by the analyst.

This logic is the rationale for the fundamental change in the definition of "measurand" in the 3rd edition of the International Vocabulary of Metrology—VIM [2].

It is important to note that the "quantity subject to measurement," the former definition of "measurand" in the VIM, 2nd edition [4], was very different from the new definition in the 3rd edition of the VIM: "quantity intended to be measured." The definition in the 3rd edition is of great help in chemistry, as chemistry-specific intermediate steps now become part of the process of measurement, possibly including measurements performed on intermediate chemical species showing up in the process (in clinical chemistry, such species is called component or chemical substance [6] and its meaning is considered to be overlapping with the meaning of the term analyte). That has the consequence that all chemical preparation work on a sample in view of obtaining a measured value (with associated uncertainty) for the intended measurement result of an a priori specified quantity (the measurand) in the original material as well as any desired transformation of a chemical species and measurements of its properties, become an inherent part of the planned process. That also has the consequence that the uncertainty naturally associated with each step in that chemical preparation work as well as with any transformation process will have to be included in the uncertainty budget (see entry 2.33 in [2]) of the final measurement result for the measurand. That will increase this final uncertainty, making it larger than just, for example, the measurement of electric current(s) in an instrumental measuring system (see entry 3.2 in [2]). But such a measurement uncertainty will correspond to a more realistic measure of "doubt" [5] about the measurement

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P. De Bièvre (✉)
Kasterlee, Belgium
e-mail: paul.de.bievre@skynet.be

result. This is all the more important in the light of the observation that a measurand "may not be directly accessible to measurement" [7].

Where does that leave us with analyte, a term frequently used to designate a measurand?

Despite the broad usage in the literature of the term, analyte cannot designate a measurand, because analyte is not a quantity.

Several different chemical species and their transformation can occur in the process of measuring a specified "measurand" as a result of the chosen strategy to arrive at a measured quantity value (with associated uncertainty) (see entry 2.10 in [2]) for the chosen measurand. They can introduce (sometimes large) systematic errors in the process, and adequate correction will have to be made for such effects, each of which carry an associated uncertainty which will have to be accounted for in the final measurement uncertainty of the measured value of the measurand. There may be a need to measure the concentration, or amount content, or mass fraction, of intermediate species in order to obtain a value for the measurand via a more complex chemical "route." And all of these will contribute to the total uncertainty budget of the end result, but their necessity in the chosen process, useful or unavoidable as it may be, does not change the a priori chosen "measurand."

In a recent editorial of ACQUAL, aspects of the choice of a measurand [7] are described. In the example given, the specification of the measurand is "mass fraction of total protein in a foodstuff." Although that is the final goal of the measurement, that is the "quantity to be measured," the quantity *subject to measurement* may be the nitrogen content in a food sample as measured by the so-called Kjeldahl method. Careful consideration of various chemical operations is required when using the Kjeldahl method, before a conclusion can be drawn about the value obtained for the measurand as defined before starting the measurement. In the example given, one has to select a suitable measurement process to obtain results directly related to the chosen measurand. It may have been the choice of the analyst to do that via the route passing through measuring, e.g., the "nitrogen content in the food sample as measured by the so-called Kjeldahl method." Of course, any introduction of nitrogen from another source will constitute a systematic effect for which the method must be investigated on beforehand, and which must be compensated for in any subsequent measurement of a measurand using this method. That will, of necessity, bring in an uncertainty of its own, thus increasing the total uncertainty budget. But not investigating the effect will bring in an even greater uncertainty, namely one for a potentially very large unknown systematic error. A lack of having investigated that would disqualify the chosen method.

Crucial here is to clearly understand what happens during the process of measurement and not to use a measurement procedure (see entry 2.6 in [2]) without that detailed understanding. Otherwise, the claim of having obtained a trustworthy value for the measurand is not realizable.

The current definition of measurand contrasts with a long-standing tradition in the literature where the term analyte is so frequently used to designate a "quantity intended to be measured." We usually say that we measure, e.g., Cd in a solution, whereas we mean Cd concentration (expressed in mmol/L, or so). Cd by itself is not a measurand. Cd is an analyte, occasionally called "target species" as in [7].

It is worthwhile to note again that once the 'measurand' has been defined before the measurement, that is by a decision, it cannot be changed anymore during the process of measurement. A goal for a measurement must not become a moving target in the course of that process.

The VIM 3rd edition definition of the concept "measurand", as well as a precise identification of the analyte, prevents imprecise or erroneous formulations, unavoidably leading to imprecise thinking and lack of (intercontinental) understanding. However, it is imperative that the chemical species be indicated (e.g., Cd) when a property of that analyte (e.g., the concentration of Cd) is planned to be measured.

Whatever the route the analyst is following in the measurement plan and its execution, a chemical species is not a quantity and can, therefore, not be a "quantity intended to be measured" i.e, a measurand.

As usual, any comment, question, or amendment is welcome, preferably as a contribution to the Discussion Forum of this Journal.

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