Quality, measurement and communication

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Editor's introduction

In recent editions of *SE* I have asked searching questions about the evolution of ISO 17025 and the role of accreditation bodies. By chance, I received a copy of an article by Gary Price which suggested that here was someone else who wasn't convinced by the *status quo*. I contacted him and found that he is a metrology specialist who has advised Australian governments on the measurement infrastructure requirements of modern chemical measurement. I felt that the readers of this column would enjoy and may like to comment on his views. I asked him to produce the following short review of the arguments presented in the main articles.[1]

Introduction

Basic to every quality system is measurement capability and simple, accurate, concise communication of results to all who make decisions on their basis. This includes the client. It is sometimes a tricky matter. The users of measurements seldom share the technical background of the makers of measurements, yet somehow sufficient understanding and meaning must be conveyed in an extremely short phrase, part numerical, part linguistic. A co-founder of modern information theory, Warren Weaver in a famous editorial in *Science*, proposed to the scientist struggling with communication problems the concept of communicative accuracy. It rests on the fact that the effective accuracy of any communication depends primarily on the interpretation given to it by the audience. Weaver suggested two conditions for communicative accuracy:

"First, taking into account what the audience does and does not know, it must take the audience closer to a correct understanding…"

"Second, its inaccuracies (as judged at a more sophisticated level) must not mislead…"

"Both of these criteria must be applied from the point of view of the audience, not from the more informed and properly more critical point of view of an expert."

On all of these criteria, we have had a serious problem since 1971, when a "mole" was included in the International System (SI) of measurement units. A mole of one form or another had been in practical use in analysis since the end of the 19th century. It was a perfectly simple concept, based on the fundamental fact that the aim of most chemical measurement was to estimate numbers of entities identified and specified according to the purpose of the particular measurement. It is the chemical properties of things that poison us, nourish us, destroy our environment and power our industry. That means numbers of entities. They are the measurand we wish to estimate, by whatever means may be available. The chemical mole was simply a counting unit, like a huge dozen. We didn't need to know the actual number of things represented by the precise "bunch" because we could reliably reproduce it, whatever it was, in an infinity of ways tailored to the situation at hand. It was simply an Avogadro number of things. Specifying, identifying and finding ways to compare and count the things was the hard part of such measurement, but the actual unit, based on the simple everyday practical concepts of number and arithmetic was something common to everyone. It was ideal for the communication of chemical measurement results.

The thermodynamic mole

In 1971 a new and quite different "mole" was conjured into existence by committee decree. We should stop pretending. The "mole" that is defined in the International System of measurement units (SI) is not the mole I have briefly described above and nor is it the mole used in most chemical analysis. It does not even refer to the same quantity, for a new quantity was also invented by the same process. It was called "amount of substance", a little used, *ad hoc*, redundant, artificial and ill named thermodynamic property of ensembles. We should be absolutely clear: "amount of substance" is something quite different to a number of things. To begin with, the first is officially continuous but the second is quantised. There are no fractions of atoms or half hydrocarbons. It is sometimes said that "amount of substance" is proportional to a number of things. That is true. It is also true that pressure is proportional to temperature. Reporting chemical measurement results in official SI thermodynamic moles is like reporting pressure in degrees Celsius, with the added confusion of the same name for two different units of the two different quantities. We need to be utterly clear: the unit that is called the "mole" in the SI has little to do with chemical measurement. It is explicitly a thermodynamic unit. We have the authoritative word of the architect of the SI and his successors on that. Chemical measurements do not come into it. We have two different quantities (number of things and "amount of substance") with two different units (the chemical mole and the thermodynamic "mole"). They have the same name. They are very easily confused. This is not best practice communication.

Consequences

No credible arguments have ever been offered to justify the official preference of complex thermodynamic artifice over common counting for the purpose of reporting chemical measurement results. It is a semantic confusion with very serious consequences.

When measurements leave the laboratory and enter the world, whether it be a production process, a health, environmental or regulatory process, or just to the general polity debating the future of the planet, misunderstandings of these kinds can have alarming and unanticipated consequences. The analyst herself may have a clear idea of what is measured but a politician seeking to make a point will naturally rely on the official definition which points toward the measurement of some continuous cosmic ectoplasm permeating all creation called "substance". It is a concept borrowed directly from medieval theology, not from modern science and a large number of differing conceptions are still attached to it in many cultures. Consider the potential in our world of high technology trade for technical barriers to trade arising from the ambiguities between the chemical mole and the thermodynamic mole and the widely held misunderstanding, due to the SI definition, that they are some variation on the idea of mass. Then add lawyers. Confusions as to pounds and kilograms are as nothing compared to this.

Inside the laboratory, ease and economy of transparently establishing appropriate, fit for purpose calibration and traceability are the essential anchors enabling communication and comparison of measurements across space and time. Using the concept of a number of things, calibration and traceability to an Avogadro number of things is straightforward and relatively simple in concept, dependent vitally on the measurement problem at hand. Many of us remember systems of standard solutions and the like, carefully prepared from materials of known identity and purity, values expressed in chemical moles. This was part of the basic skill set of the analyst. But how do you achieve calibration and traceability to an "amount of substance"? No one really knows because no one has yet explained in common and simple terms exactly what is an "amount of substance". All we really know about it is that it is not a number of things.

This is a dilemma solved by a burgeoning industry. We now rely on reference materials and the veracity and appropriateness of their certificates. The problem is "contracted out", at some expense. We are told that we must use externally sourced "certified" reference materials. But the industrial capacity does not exist to supply all reference materials appropriate to all analytes and matrices. In some situations, reference materials can be convenient and appropriate means of establishing basic metrological control, but they are by no means the only way. Sometimes it is far more appropriate to use do-it-yourself, in-house means of establishing calibration and this can be done in many ways (e.g., the controlled production of a transient species, electrochemical methods, primary methods, intrinsic standards, reference instruments etc). These are options that make sense to the measurer of a number of things. They are far more difficult to conceive if the analyst is measuring an "amount of substance". Important options for flexible metrological control are increasingly ruled out. Often, it is far easier to simply report results in terms of mass, even though it is itself a complex and misleading way of reporting analytical results (because chemical identity does not necessarily correlate with mass).

Conclusion

Measurement units are first and primarily instruments for the linguistic communication of measurement results. The principles of simplicity and clarity are indispensable. Units that cannot be understood by a general audience of their users, that are inconsistent, ambiguous, incoherent with common practice, confused in their conception of what is being measured, or simply not what they purport to be are very much worse than useless.

The SI has evolved in the direction of complexity, obfuscation, inexplicability and irrelevance. It is up to analysts themselves to clearly restate their own simple and effective means to communicate results.

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