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PRACTITIONER'S REPORT

A comparison in the evaluation of measurement uncertainty in analytical chemistry testing between the use of quality control data and a regression analysis

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Abstract The evaluation of measurement uncertainties has been widely applied to the calibration of measurement instruments, whereas its application to tests, despite increasing requirements, is a more recent phenomenon. The generalization of the evaluation of measurement uncertainties to tests has been a gradual process, in line with changes in the requirements of the normative framework that regulates the accreditation of tests laboratories and also as the perceived good practices have evolved. The sole identification of the relevant sources of uncertainty was followed by the requirement to provide a simplified estimate of the measurement uncertainty, and it is now an accepted requirement to properly evaluate the expanded measurement uncertainty associated with any tests. In this study, the evaluation of measurement uncertainty associated with the determination of sulfate in water will be attempted using a procedure that includes linear regression, with the regression parameters provided with associated uncertainties, and a Monte Carlo method applied as a validation tool of the conventional mainstream evaluation method, concerning the approximations in terms of linearization of the model and the assumed shape of the output distribution introduced by this approach.

Keywords Measurement uncertainty · Chemical metrology · Regression analysis · Monte Carlo method · GUM uncertainty framework

Introduction

The gradual process of measurement uncertainty evaluation being applied to testing, from the sole identification of sources of uncertainty to the full evaluation of the expanded measurement uncertainty, was naturally also extended to chemical metrology, where accredited tests laboratories now fully comply with the requirement of evaluating the measurement uncertainty for each chemical parameter being tested [1].

As a consequence, guides have been published [2], in an attempt to provide a common ground to the evaluation of uncertainty in chemistry, mainly to comply with the views expressed in the Guide to the Expression of Uncertainty in Measurement [3] (GUM), and it is still very common in analytical chemistry to find evaluation methods based on different uncertainty frameworks depending on the information available, for example on data from collaborative studies, measurements on certified reference materials (CRM) and recovery tests, as the main indicators. Thus, it is relevant to compare different approaches commonly used in chemical laboratories to evaluate measurement uncertainties, and to validate some of these procedures with an accepted validation tool as specified in the Supplement 1 to the GUM [4].

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