What are the simpler workable approaches for measurement uncertainty in chemical analysis?

In addition to the widely known master GUM (Guide to the Expression of Uncertainty in Measurement) approach for evaluating measurement uncertainty, there are other schools of thought suggesting to view the overall performance of a test method instead of looking into the uncertainty components of each step of the procedure. In chemical analysis, the GUM approach has been found to be troublesome and tedious because one has to evaluate each and every uncertainty contribution in the test method and then combine them as variances. GUM is acknowledged as the master document on measurement uncertainty for calibration laboratories where the uncertainty components are fewer with systematic effects discouraged.

Those alternative approaches (so-called "top-down" approaches), some still debatable, are fully compliant with the GUM principles, and capitalize in fully utilizing the existing quality control data which should have been in store for an accredited laboratory under the global standard ISO/IEC 17025. Hence, the pre-requisite for such alternative approaches is to have a proven robust quality system in place for a prolonged period before one can confidently adopt them. The basic components of uncertainty in the "top-down" methods for a routine test procedure are precision, reproducibility and trueness.

The precision parameter is concerned with the within-laboratory data which can be in the form of intermediate reproducibility standard uncertainty obtained as the standard deviation of a series of repeated testing carried out by different anlaysts with different analytical equipment over a period of time on a stable sample in the same laboratory. However certain significant effects on variations of test samples and test conditions may not have been captured in this precision data.

The reproducibility estimates are best obtained by taking part in a reputable proficiency testing (PT) program regularly or a collaborative method performance exercise with satisfactory outcome. A good PT program should have got a good number of laboratory participants and collated test data generated from a standardized test method instead of allowing the laboratories to report their results on any test method of their own choice. Method difference is a significant effect on the final statistical outcome of such PT program.

Trueness is a measure of method bias after taking corrective actions to remove or reduce such bias to the greatest possible extent. Such bias-related uncertainty estimate therefore reflects the potential residual bias after correction, and we may call it a corrected method bias. We can determine such bias by analyzing certified reference materials or comparing the test with a reference measurement procedure.

By experience, the following alternative top-down approaches are workable and would save much time in evaluating measurement uncertainty instead of adopting the GUM:

- Study of laboratory precision and reproducibility (EUROLAB Technical Report No. 1/2006; EUROLAB Technical Report No. 1/2007; EURACHEM/CITAC (2000); NORTEST Technical Report 537 (2003).)
- Adopting the inter-laboratory validation approach (ISO 21748:2010; EUROLAB Technical Report No. 1/2007; NORTEST Technical Report 537(2003); EA 4/16 (2004).)
- Use of control chart moving range data (ASTM D6299:2008)
- Use of linear calibration of reference materials (ISO 11095:1996 Reconfirmed in 2014)

It is a matter of practice to understand their simple principles and master the application of these “top-down” approaches. Some electronic templates prepared would be beneficial in keeping the measurement uncertainty data of the test method current because its quality control data are dynamic in routine testing.