Top down approaches for measurement uncertainty evaluation – basic principles

We see many advantages in the holistic top down approaches for evaluating measurement uncertainty in chemical and microbiological analyses in terms of much simpler evaluation processes and offering dynamic or current uncertainty level in the test results offered. The traditional GUM method is known to be tedious and complicated in the evaluation.

However, the following important points of the top down approaches are to be noted:

a. All laboratory quality control (QC) and quality check (CS) processes are based on the validity of QC samples and check samples used. The important pre-requisites are that these samples must be homogeneous and stable with their matrices and the analyte-of-interest levels to be as close to that of the actual sample analysis as possible.

b. The top down approaches adopt the results of intermediate precision standard deviation, $s_{R'}$ and the reproducibility standard deviation, s_R of the laboratory method concerned over a period of time.

c. The monitoring data collected for $s_{R'}$ and/or s_R must be continuous throughout the adoption of the test method, covering most of the possible sample variations. The data are to be random (i.e. normally distributed) and independent as evidenced by the Anderson Darling (AD) statistic test.

d. We can use the control chart method to evaluate the intermediate precision standard uncertainty $u_{R'}$ or its relative standard uncertainty. The reliability of this $u_{R'}$ follows the following order: stable reference sample, prepared standard solution and basing on past experiences. Its reliability is also judged on the number of data collected with a minimum number of 20.

e. If the test method covers a wide range of matrices and analyte levels which might lead to bigger variations of $s_{R'}$ or s_R, we may have to consider using different reference standard samples for these top down approaches.

f. There is another element component of uncertainty for consideration: bias standard uncertainty, u_b

g. The bias standard uncertainty, u_b is to be evaluated from a sample with an acceptable reference value (ARV) and its reliability decreases from bias of a stable check sample CS, to that of a consensus value from a proficiency testing (PT) program, to inter-laboratory comparison (ILC) outcome and to laboratory recovery testing.

h. The effectiveness of bias standard uncertainty, u_b also relies on the analyte levels and number of batches studied

i. If the ARV is given by PT or ILC studies, its standard uncertainty u_{Cref} based on mean value $\bar{x}$ is given by $u_{Cref} = \frac{s_R}{\sqrt{L}}$; its standard uncertainty based on the median value is given by $u_{Cref} = 1.25\frac{s_R}{\sqrt{L}}$ where L is the number of laboratories participated.

j. The standard uncertainty of bias from a laboratory recovery experiment has to consider the standard uncertainties of weight of standard analtye spiked, apparatus and volume, amongst other contributors.

k. If $u_b < \frac{u_{R'}}{3}$, u_b can be neglected; if the results of b（bias）or u_{Cref} significant, they must be separately evaluated，but if u_{Cref} is too large, the estimation of u_b is considered failed.

l. When the whole analytical process is satisfied with no other significant uncertainty contributors, we can then combine both $u_{R'}$ and u or their relative values as combined standard uncertainty before proceeding to reported the expanded uncertainty result.