SUPPLEMENTAL DOCUMENT SD-3
FOR PART IVC – Quality Assurance/Uncertainty

Measurement Uncertainty for Weight Determinations in Seized Drug Analysis

Introduction

The following demonstrates the application of an uncertainty budget approach for weight determinations. The factors described in Part IV C, Section 4, are considered. It is assumed that the value being reported is the conventional mass and final results are rounded to the precision of the balance. The term "weight" is used interchangeably with "conventional mass," the quantity typically reported. Definitions for the statistical terms used can be found in the glossary or references listed below. The references also contain additional examples and detailed information regarding estimation of uncertainty.

Multiple approaches exist for estimating combined uncertainties. In these examples, the elements used to calculate the standard uncertainties contain correlated and uncorrelated factors. The methods illustrated represent a conservative approach in which the uncertainty is likely to be overestimated.

The following examples should not be directly applied to methodology used without first considering the specific purpose of a method and its relevant operational environment and the operational capabilities and parameters of the balance.

A   Example 1:

Scenario: A laboratory must determine the net weight of a white powder, which appears to weigh approximately 30 g, received in a plastic bag. The decision is made to weigh the material using a balance with a maximum capacity of 3100 g. The following conditions apply: the operator is competent on the use of the balance; the balance is calibrated and certified as per established laboratory protocols; the balance is being used above the defined minimum balance load; and the balance is performing within the manufacturers' specifications. The balance operates in a controlled environment using a draft shield with ambient temperature varying ±5 °C (range of 10 degrees total).

The weight is determined as follows: A weigh vessel is placed on the balance and tared. It is then removed from the balance and the powder is transferred to the vessel, which is placed on the balance and reweighed. The taring of the weighing vessel and the weighing are considered as two weighing events.

The net weight obtained for the powder is 30.03 grams.

A.1   Factors contributing to weight measurement uncertainty

The factors considered in estimating the measurement uncertainty include readability; repeatability; linearity; buoyancy; sensitivity; uncertainty from balance calibration report; number of weighing events; and sample loss in transfer. The uncertainty associated with sample loss is, for practical purposes, indeterminate.

Buoyancy is considered to be a small systematic error that can contribute as much as 0.1% bias to the weight. Buoyancy is difficult to account for in seized drug cases because the density of the object being weighed must be known. However, for objects that have a lower density than steel (8.0 g/cm^3), the bias imparted is always negative and the weight displayed by the balance will be less than the true weight of the object.

Based on the current calibration and performance certification for the balance and given that the balance is operating within specifications, other factors (e.g. environmental, static, corner loading) are deemed insignificant in this example. Laboratories should examine their balances, calibration reports, methods, circumstances, and applications to determine which factors are significant and which are insignificant for their particular application.

The factors deemed significant in this example are expressed in the table to follow.

A.2 Uncertainty Budget Table

Factors	Value (x)	Standard uncertainty (u), g	Distribution	Index (Relative contribution)[a]
Readability[b]	0.01 g	$\dfrac{x}{\sqrt{3}} = \dfrac{0.01}{\sqrt{3}} = 0.00577$	Rectangular	$\dfrac{0.00577^2}{0.000313} *100 = 10.6\%$
Repeatability (s)[c]	0.0101 g	0.0101	Normal	32.5%
Linearity[d]	0.0201 g	$\dfrac{x}{\sqrt{3}} = \dfrac{0.0201}{\sqrt{3}} = 0.0116$	Rectangular	42.9%
Temperature coefficient[e]	6 ppm/°C (6×10^{-6} g /°C)	$\dfrac{x}{\sqrt{3}} = \dfrac{\dfrac{6x10^{-6}\,g}{^{\circ}C} *10\,^{\circ}C * 30.03\,g}{\sqrt{3}}$ $= 0.00104$	Rectangular	0.3%
Uncertainty from balance calibration report (U, coverage factor k=2)	0.0131 g	$\dfrac{U}{k} = \dfrac{0.0131}{2} = 0.00655$	Normal	13.7%
Subtotal ($\sum u_n$):	0.0350			
Subtotal ($\sum \left(u_n \right)^2$):	0.000313			

---

[a] $\dfrac{u^2}{\displaystyle\sum_{i=1}^{k} u_i^2} *100$ This value is used to determine which terms are significant.

[b] Obtained from the current calibration and performance certification for the balance and assumes that the balance has a single readability range.

[c] Determined empirically in the laboratory.

[d] This value is the maximum permitted deviation across the mass range of the balance.

[e] Value obtained from manufacturer specifications.

A.3 Calculation of combined standard uncertainty

Considering all factors noted above (A.2) as uncorrelated, the combined standard uncertainty per weighing event in this example can be expressed mathematically as:

$$u_c = \sqrt{u(read)^2 + u(repeat)^2 + u(linear)^2 + u(bal\ cal)^2}$$

where u is the standard uncertainty and u_c is combined standard uncertainty. The term $u(temperature\ coefficient)$ is not included in the combined uncertainty due to its minimal relative contribution to the total standard uncertainty.

The combined standard uncertainty is:

$$u_c = \sqrt{(0.00577)^2 + (0.0101)^2 + (0.0116)^2 + (0.00655)^2} = 0.0176\ g$$

A.4 Calculation of expanded uncertainty

The expanded uncertainty per weighing event (U) is expressed mathematically as:

$$U = k^* u_c$$

Using a coverage factor (k) = 2 (confidence level of approximately 95%):

$$U = 2^*0.0176\ g = 0.0352\ g$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U^* \text{number of weighing events}$$

$$U_{final} = 0.0352\ g^*2 = 0.0704\ g$$

Using a coverage factor (k) = 3 (confidence level of approximately 99%):

$$U = 3^*0.0176\ g = 0.0528\ g$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U^* \text{number of weighing events}$$

$$U_{final} = 0.0528\ g^*2 = 0.1056\ g$$

Measurement Uncertainty for Weight Determinations in Seized Drug Analysis
Supplemental Document SD-3

A.5 Results

A.5.1 *Net Weight: 30.03 g ± 0.07 g (k=2)*

A.5.2 *Net Weight: 30.03 g ± 0.11 g (k=3)*

B Example 2

Scenario: In this example, the measurement uncertainty is calculated using control chart data obtained from a measurement quality assurance process that mimics casework samples as closely as possible. All other conditions are the same as Example 1.

The control chart should capture uncertainty deemed appropriate to the specific laboratory and procedure and could include factors such as environmental conditions, analysts, and sample types. A conservative approach is to select the largest standard deviation if a range of masses is charted.

B.1 Factors contributing to weight measurement uncertainty

As the control chart is well established, it is expected to capture all of the factors described in Example 1 except linearity and balance calibration uncertainty.

B.2 Uncertainty Budget Table

Factors	Value (x)	Standard uncertainty (*u*), g	Distribution	Index (Relative contribution)
Control chart standard deviation (*s*)[a]	0.0110 g	0.0110	Normal	40.6%
Linearity[b]	0.0201 g	$\dfrac{x}{\sqrt{3}} = \dfrac{0.0201}{\sqrt{3}} = 0.0116$	Rectangular	45.1%
Uncertainty from balance calibration report (*U*, coverage factor *k*=2)	0.0131 g	$\dfrac{U}{k} = \dfrac{0.0131}{2} = 0.00655$	Normal	14.3%
Subtotal ($\sum u_n$):	0.0291			
Subtotal ($\sum \left(u_n \right)^2$):	0.000298			

---

[a] $s = \sqrt{\dfrac{\sum \left(x - \bar{x} \right)^2}{\left(n - 1 \right)}}$

[b] This value is the maximum permitted deviation across the mass range of the balance.

Measurement Uncertainty for Weight Determinations in Seized Drug Analysis
Supplemental Document SD-3

B.3   Calculation of combined standard uncertainty

Considering all factors noted above (B.2) as uncorrelated, the combined standard uncertainty per weighing event in this example can be expressed mathematically as:

$$u_c = \sqrt{u(control\ chart)^2 + u(linearity)^2 + u(cal\ cal)^2}$$

where u is the standard uncertainty and u_c is combined standard uncertainty. The combined standard uncertainty is:

$$u_c = \sqrt{(0.0110)^2 + (0.0116)^2 + (0.00655)^2} = 0.0172\ g$$

B.4   Calculation of expanded uncertainty

The expanded uncertainty per weighing event (U) is expressed mathematically as:

$$U = k*u_c$$

Using a coverage factor (k) = 2 (confidence level of approximately 95%):

$$U = 2*0.0172\ g = 0.0344\ g$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U*\text{number of weighing events}$$

$$U_{final} = 0.0344\ g*2 = 0.0688\ g$$

Using a coverage factor (k) = 3 (confidence level of approximately 99%):

$$U = 3*0.0172\ g = 0.0516\ g$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U*\text{number of weighing events}$$

$$U_{final} = 0.0516\ g*2 = 0.1032\ g$$

B.5 Results

B.5.1 *Net Weight: 30.03 g ± 0.07 g (k=2)*

B.5.2 *Net Weight: 30.03 g ± 0.10 g (k=3)*

C Example 3

Scenario: In this example, the laboratory must determine the net weight of a white powder, received in 15 similar plastic bags, which appear to weigh approximately 30 g each. All other conditions are the same as Example 2.

The total net weight obtained for the powder, determined by individually placing the material from each plastic bag inside 15 separate tared weighing vessels, is 458.37 grams.

C.1 Factors contributing to weight measurement uncertainty

As the control chart is well established, it is expected to capture all of the factors described in Example 1, except linearity and balance calibration uncertainty.

C.2 Uncertainty budget table: Same as Example 2.

C.3 Calculation of combined standard uncertainty: Same as Example 2.

C.4 Calculation of expanded uncertainty

The expanded uncertainty per weighing event (U) is expressed mathematically as:

$$U = k^*u_c$$

Using a coverage factor (k) = 2 (confidence level of approximately 95%):

$$U = 2^*0.0172 \text{ g} = 0.0344 \text{ g}$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U^*\text{number of weighing events}$$

$$U_{final} = U^*(15^*2) = U^*30$$

$$U_{final} = 0.0344 \text{ g*}30 = 1.032 \text{ g}$$

Using a coverage factor (k) = 3 (confidence level of approximately 99%):

$$U = 3\text{*}0.0172 \text{ g} = 0.0516 \text{ g}$$

Considering all weighing events as correlated, the final expanded uncertainty for the net weight is expressed mathematically as:

$$U_{final} = U\text{*}\text{number of weighing events}$$

$$U_{final} = 0.0516 \text{ g*}30 = 1.548 \text{ g}$$

C.5   Results

C.5.1 *Net Weight: 458.37 g ± 1.03 g (k=2)*

C.5.2 *Net Weight: 458.37 g ± 1.55 g (k=3)*

D   References

D.1   Books:

D.1.1 Dieck, R.H. 2007. *Measurement Uncertainty: Methods and Applications.* 4th ed. Research Triangle Park, NC: The Instruments, Systems, and Automation Society (ISA).

D.1.2 Jones, F. E., and R. M. Schoonover. 2002. *Handbook of Mass Measurement.* Boca Raton, FL: CRC Press.

D.1.3 Kimothi, S.K. 2002. *The Uncertainty of Measurements: Physical and Chemical Metrology: Impact and Analysis.* Milwaukee, WI: ASQ Press (American Society for Quality).

D.1.4 Kirkup, L., and R. B. Frenkel. 2006. *An Introduction to Uncertainty in Measurement.* Cambridge, UK: Cambridge University Press.

D.1.5 Lawn, R., R. Lawn, and E. Pritchard. 2003. *Measurement of Mass Practical Laboratory Skills Training Guides Series*: Royal Society of Chemistry.

D.1.6 Pavese, F., and A.B. Forbes, eds. 2009. *Data Modeling for Metrology and Testing in Measurement Science.* Edited by N. Bellomo, *Modeling and Simulation in Science, Engineering, and Technology.* Boston: Birkhauser.

D.1.7 Taylor, J.R. 1997. *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements*. Sausalito, CA: University Science Books.

D.2 Peer-reviewed journal articles and reviews:

D.2.1 Brown, R. J. C., and M. J. T. Milton. 2007. Developments in accurate and traceable chemical measurements. *Chemical Society Reviews* 36 (6):904-913.

D.2.2 Burns, M. 2004. Current practice in the assessment and control of measurement uncertainty in bio-analytical chemistry. *Trac-Trends in Analytical Chemistry* 23 (5):393-398.

D.2.3 Gonzalez, A. G., and M. A. Herrador. 2007. The assessment of electronic balances for accuracy of mass measurements in the analytical laboratory. *Accreditation and Quality Assurance* 12 (1):21-29.

D.2.4 Kehl, K. G., K. Weirauch, S. Wunderli, and V. R. Meyer. 2000. The influence of variations in atmospheric pressure on the uncertainty budget of weighing results. *Analyst* 125 (5):959-962.

D.2.5 Konieczka, P. 2007. The role of and the place of method validation in the quality assurance and quality control (QA/QC) system. *Critical Reviews in Analytical Chemistry* 37 (3):173-190.

D.2.6 Linsinger, T. P. J. 2008. Use of recovery and bias information in analytical chemistry and estimation of its uncertainty contribution. *Trac-Trends in Analytical Chemistry* 27 (10):916-923.

D.2.7 Meyer, V. R. 2007. Measurement uncertainty. *Journal of Chromatography A* 1158 (1-2):15-24.

D.2.8 Populaire, S., and E. C. Gimenez. 2006. A simplified approach to the estimation of analytical measurement uncertainty. *Accreditation and Quality Assurance* 10 (9):485-493.

D.2.9 Pozivil, M., W. Winiger, S. Wunderli, and V. R. Meyer. 2006. The influence of climate conditions on weighing results. *Microchimica Acta* 154 (1-2):55-63.

D.2.10 Rios, A., and M. Valcarcel. 1998. A view of uncertainty at the bench analytical level. *Accreditation and Quality Assurance* 3 (1):14-19.

D.2.11 Schoonover, R. M., and F. E. Jones. 1981. Air Buoyancy Correction in High-Accuracy Weighing on Analytical Balances. *Analytical Chemistry* 53 (6):900-902.

D.2.12 Wunderli, S., G. Fortunato, A. Reichmuth, and P. Richard. 2003. Uncertainty evaluation of mass values determined by electronic balances in analytical chemistry: a new method to correct for air buoyancy. *Analytical and Bioanalytical Chemistry* 376 (3):384-391.

D.3   On-line resources:

D.3.1 EURACHEM. *Quantifying Uncertainty in Analytical Measurement* 2007. Available from http://www.measurementuncertainty.org/index.html

D.3.2 JCGM. *JCGM 100-2008: Evaluation of measurement data (GUM 1995 with minor corrections)*. JCGM: Joint Committee for Guides in Metrology, 2008 2008. Available from http://www.iso.org/sites/JCGM/GUM/JCGM100/C045315e-html/C045315e.html?csnumber=50461

D.3.3 NIST. 2006. NIST/SEMATECH e-Handbook of Statistical Methods: National Institute of Science and Technology, U.S. Department of Commerce. Available from http://www.itl.nist.gov/div898/handbook

D.3.4 *The NIST Reference on Constants, Units, and Uncertainty* 2009. Available from http://physics.nist.gov/cuu/Uncertainty/index.html

D.3.5 NIST 1994. NIST Technical note 1297Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results. National Institute of Science and Technology, U.S. Department of Commerce.
Available from http://physics.nist.gov/Pubs/guidelines/contents.html

D.3.6 SIM Guidelines on the calibration of non-automatic weighing instruments. 2009. SIM MWG7/cg-01/v.00. (Identical to the original EURAMET/cg-18/v.02). Available from http://www.sim-metrologia.org.br/SIM_MWG7_English_Corrected_9_Feb.pdf

End of Document