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Standard Practice for Estimating Uncertainty of Test Results Derived from Spectrophotometry[1]

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1. Scope

1.1 This practice describes a protocol to be utilized by measurement laboratories for estimating and reporting the uncertainty of a measurement result when the result is derived from a measurand that has been obtained by spectrophotometry.

1.2 This practice is specifically limited to the reporting of uncertainty of color measurement results that are reported as color-differences in ΔE format, even though the measurement itself may be reported in other units such as percent reflectance or transmittance.

1.3 The procedures defined here are not intended to be applicable to national standardizing laboratories or transfer laboratories.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.* ~~*Some specific hazards statements are given in Section 7 on Hazards.*~~

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D2244 Practice for Calculation of Color Tolerances and Color Differences from Instrumentally Measured Color Coordinates

E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

E284 Terminology of Appearance

2.2 *ISO Standards:*[3]

ISO 9001 Quality Management Systems—Requirements

ISO/IEC 17025 General Requirements for the Competence of Calibration and Testing Laboratories

2.3 *Other Standard:*[4]

QS 9000 Quality Systems Requirements Chrysler Corporation, Ford Motor Company, General Motors Corporation

3. Terminology

3.1 *Definitions:* For definitions of terms used in this standard refer to Terminology E284.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *uncertainty, n*—a parameter associated with a measurement result or test result that reasonably characterizes the dispersion of results attributable to the particular quantity being measured of the particular characteristic being tested.

3.2.2 *instrument uncertainty conditions, n—of a measurement*, conditions wherein the measurements are made repetitively and carefully over a short timescale, without replacement of the specimen being measured in the specimen port of the instrument.

NOTE 1—Instrument uncertainty conditions always include potential specimen drift due to causes such as theromchromism, photochromism, or bleaching of the specimen. While these may be thought of as characteristics of the specimen, their effects will be picked up here under instrument uncertainty conditions.

[1] This practice is under the jurisdiction of ASTM Committee E12 on Color and Appearance and is the direct responsibility of Subcommittee E12.04 on Color and Appearance Analysis.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.

[4] Available from Automotive Industry Action Group (AIAG), 26200 Lahser Rd., Suite 200, Southfield, MI 48033, http://www.aiag.org.

3.2.3 *operator uncertainty conditions, n—of a measurement*, conditions wherein the measurements are made repetitively and carefully over a short timescale, with replacement of the specimen being measured by the operator completely withdrawing the specimen from the specimen port and replacing the specimen back in the specimen port prior to the ensuing measurement so that the specimen aperture samples the same location on the specimen, and the specimen has the same orientation as previous, to the best of the operator's ability to accomplish.

3.2.4 *uniformity uncertainty conditions, n—of a measurement*, conditions wherein the measurements are made repetitively and carefully over a short timescale, with replacement of the specimen being measured to an entirely new location on the face of the specimen with the intent of sampling the entire surface of the specimen, or as much of the surface as is practical, by the end of the repetitive sampling run.

3.2.5 *instrument uncertainty, n*—the results of an uncertainty analysis of a measurement system made under instrument uncertainty conditions.

3.2.6 *operator uncertainty, n*—the results of an uncertainty analysis of a measurement system made under operator uncertainty conditions.

3.2.7 *uniformity uncertainty, n*—the results of an uncertainty analysis of a measurement system made under uniformity uncertainty conditions.

3.2.8 *expanded uncertainty, n*—uncertainty reported as a multiple of the standard uncertainty.

3.2.9 *measurement system, n*—the entirety of variable factors that could affect the precision, accuracy, or uncertainty of a measurement result. These include the instrument, the operator, the environmental conditions, the quality of the transfer standard, the specimen aperture size, as well as other factors.

3.2.10 *standard uncertainty, n*—uncertainty reported as the standard deviation of the estimated value of the quantity subject to measurement.

3.2.11 *95 % confidence interval, n*—the 95 percentile value of an ascending-ordered distribution of differences between multiple measurement results of a derived parameter characterized by a color measurement system.

3.2.11.1 *Discussion—*

This value is the cumulative distribution between zero and the stated value of the measurand that contains 95 % of all the measurement results made by this procedure.

4. Summary of Practice

4.1 This practice establishes a protocol for measurement laboratories to assess the uncertainty of their measurement system from test specimens or from control samples of materials similar in both first-surface characteristics and color to those being measured and reported.

4.2 Where control samples are used, the process will be to establish control samples representative of the type of materials to be measured. Control samples will be processed to assess the various uncertainty components of measurement results, the results retained in a control chart, and the rolling average of the uncertainty components of the control samples used as a surrogate for assessing the uncertainty of a similar specimen.

4.3 Some of the components of uncertainty for color measurement result are instrument uncertainty, operator uncertainty, and uniformity (of the specimen) uncertainty.

5. Significance and Use

5.1 Many competent measurement laboratories comply with accepted quality system requirements such as ISO 9001, QS 9000, or ISO 17025. When using standard test methods, the measurement results should agree with those from other similar laboratories within the combined uncertainty limits of the laboratories' measurement systems. It is for this reason that quality system requirements demand that a statement of the uncertainty of the test results accompany every test result.

5.2 Preparation of uncertainty estimates is a requirement for laboratory certification under ISO 17025. This practice describes the procedures by which such uncertainty estimates may be calculated.

6. Concepts in Reporting Uncertainty of Test Results

6.1 A commonly cited definition (**1, 2**)[5] paraphrased to form a single citation defines uncertainty as "a parameter, associated with the measurement result, or test result, that characterizes the dispersion of values that could reasonably be attributed to the quantity

[5] The boldface numbers in parentheses refer to a list of references at the end of this standard.

subject to measurement or characteristic subject to test." This definition emphasizes uncertainty as an attribute of an individual test result, not as a property defining statistical variation of test results.

6.2 The methodology for classification of uncertainty types has been classified as Type A and Type B as discussed in references (**2**) and (**3**). Type A estimates of uncertainty include estimates based upon knowledge of the statistical character of the measurement results, or estimates based upon statistical analysis of replicate measurement results. The latter may include results from control sample monitoring programs, or proficiency testing. Type B estimates of uncertainty include estimates from calibration certificates and manufacturer's specifications. Type A are evaluated by statistical methods and Type B by non-statistical methods.

6.3 The goal of reporting uncertainty is to account for all potential causes contributing to uncertainty in the measurement result. Uncertainty for a single measurement result is then

$$(s_1^2 + s_2^2 + \ldots + s_n^2)^{1/2}$$

where s_1 is the estimate of the uncertainty of the first factor contributing to variance, s_2 the second, and so on, through all n components of variance.

6.4 Uncertainty in this practice shall be reported as the 95% confidence interval of the largest component of all the components of uncertainty assessed.

6.5 The minimum components contributing to variance shall be the instrument uncertainty, the operator uncertainty, the uniformity uncertainty, and the uncertainty of the traceability scheme.

7. Procedure

7.1 Measure the test specimen a minimum of 20 times, and preferably as many as 30 times, under instrument uncertainty conditions. Make all measurements in compliance with the manufacturer's recommendations including prior standardization of the instrument using a white tile, a black tile, or light trap, and a grey tile, if required.

7.2 There will be $n^* (n - 1) / 2$ possible ~~differences~~color-differences between the n measurement results taken two-at-a-time in all possible combinations.

7.3 Calculate the absolute value of the ~~differences~~color-differences between each of these combinations and retain the results in a list. Calculate these color-differences in accordance with a color-difference equation chosen from Practice D2244.

7.4 Sort the list in ascending order. The member of the sorted list whose index is *Int* [0.95 * n * (n-1) / 2] contains the value of the 95 % confidence interval of the instrument uncertainty s_1. The symbol *Int* means the integer value of the expression in brackets.

7.5 Measure the test specimen a minimum of 20 times, and preferably as many as 30 times, under operator uncertainty conditions. Follow the operations of 7.1 – 7.3 using this data set to calculate the 95 % confidence interval of operator uncertainty s_2.

7.6 Measure the test specimen a minimum of 20 times, and preferably as many as 30 times, under uniformity uncertainty conditions. Follow the operations of 7.1 – 7.3 using this data set to calculate the 95 % confidence interval of uniformity uncertainty s_3.

7.7 Sort the uncertainties obtained from Sections 7.1 – 7.6 s_1, s_2, s_3 in ascending order with the smallest of the three in s_1 and the next larger in s_2, and so forth. Let

~~$$s'_1 = s_1 \quad (1)$$~~

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~~$$s'_2 = (s_2^2 - s_1^2)^{1/2} \quad (2)$$~~

$$s'_2 = (s_2^2 - s_1^2)^{1/2} \quad (2)$$

~~$$s'_3 = (s_3^2 - s_2^2)^{1/2} \quad (3)$$~~

$$s'_3 = (s_3^2 - s_2^2)^{1/2} \quad (3)$$

The value of s_2 used in Eq 3 is the original experimentally assessed value, not that value which results from the calculation of Eq 2 which is ~~s_2~~ s'_2. This isolates the uncertainties, each of which has been until now included in each of the measured uncertainties, into a separate uncertainty contribution attributable to each subsequent type of uncertainty considered. However, consult the cautionary remarks in Appendix X1 to this Practice at X2.1 – X2.4.

7.8 Calculate the combined uncertainty

~~$$U = (s_1'^2 + s_2'^2 + s_3'^2)^{1/2} \quad (4)$$~~

$$U = (s_1'^2 + s_2'^2 + s_3'^2)^{1/2} \quad (4)$$

where the elements s'_1, s'_2, and s'_3 are the uncertainties from 7.4.