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Standard Practice for Use of Terms Relating to the Development and Evaluation of Methods for Chemical Analysis[1]

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INTRODUCTION

ASTM methods for determining the chemical composition of materials usually are developed in four stages: (*1*) experimental development of procedures and techniques, (*2*) translation of research into text suitable for analysts (in ASTM format), (*3*) demonstration of performance in an interlaboratory study (ILS), and (*4*) acceptance as a method published for use in laboratories. Details of the development processes may be complex, but the common concepts and terms needed to discuss them are relatively simple. The concepts must be carefully defined and terms selected to represent them unambiguously in the intended contexts.

A list of terms and definitions does not guarantee clear communication. Many terms have different common and technical meanings while representing different concepts when used in various contexts. The use of important terms and concepts in the context of methods of chemical analysis is illustrated by descriptions and by examples to help task group and subcommittee members communicate clearly.

1. Scope

1.1 This document covers terms and concepts used in developing and evaluating the performance of methods for determining chemical composition. Although useful with many types of methods, they are dealt with in this document in the context of chemical analysis of metals and related materials.

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E 135 Terminology Relating to Analytical Chemistry for Metals, Ores, and Related Materials

E 1601 Practice for Conducting an Interlaboratory Study to Evaluate the Performance of an Analytical Method

E 1763 Guide for Interpretation and Use of Results from Interlaboratory Testing of Chemical Analysis Methods

3. Terminology

3.1 *Definitions Relating to Analytical Methods:*

3.1.1 *accuracy*, *n—of methods of chemical analysis*, a characteristic manifested by agreement between average results and true analyte contents.

3.1.2 *analyte*, *n—in methods of chemical analysis*, the component determined by a method.

3.1.3 *matrix*, *n—in methods of chemical analysis*, all components in a material except the analyte.

3.1.4 *method*, *n*—instructions used to produce a numerical result which are detailed in a document also referred to as "the method."

3.1.5 *precision*, *n—of methods of chemical analysis*, a characteristic manifested by agreement among individual results at a given analyte content.

3.1.6 *result*, *n*—value representing the quantity of analyte that is obtained by applying a method one time to a test material.

3.1.7 *sample*, *n—in methods of chemical analysis*, a portion of a material selected and processed to render its composition representative of the composition of the whole. (Contrast *specimen*.)

3.1.8 *specimen*, *n—in methods of chemical analysis*, a piece of material selected to be typical of the whole under the assumption that the whole is composed of pieces of similar composition. (Contrast *sample*.)

3.2 *Definitions Referring to Statistics:*

3.2.1 *b-value*, *n—in statistics*, the difference between the mean of a set of results on a material and its accepted reference value. (Compare *error*.)

[1] This practice is under the jurisdiction of ASTM Committee E01 on Analytical Chemistry for Metals, Ores and Related Materials and is the direct responsibility of Subcommittee E01.22 on Statistics and Quality Control.

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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.

3.2.2 *between-laboratory standard deviation,* s_R, *n*—the standard deviation of results obtained on the same material in different laboratories (Synonym: *reproducibility*).

3.2.3 *detection limit*, *n—for an analytical instrument*, the minimum quantity of analyte expected to yield a response greater than zero.

3.2.4 *error*, *n—of a result*, the difference between a result obtained on a material and its accepted reference value. (Compare *b-value*.)

3.2.5 *interlaboratory study, ILS*, *n*—a study undertaken to demonstrate the precision and accuracy of a method.

3.2.6 *minimum standard deviation,* s_M, *n*—the standard deviation of results on a test material obtained under conditions of minimum variability.

3.2.7 *repeatability*, *n*—see *within-laboratory standard deviation.*

3.2.8 *repeatability standard deviation*, *n*—see *within-laboratory standard deviation.*

3.2.9 *repeatability index, r*, *n*—an estimate of the maximum difference expected for results on the same test material on different days in the same laboratory, a difference not expected to be exceeded an average of more than once in 20 comparisons (95 % probability.)

3.2.10 *reproducibility*, *n*—see *between-laboratory standard deviation.*

3.2.11 *reproducibility standard deviation*, *n*—see *between-laboratory standard deviation.*

3.2.12 *reproducibility index, R*, *n*—an estimate of the maximum difference expected for results on the same material in two laboratories, a difference not expected to be exceeded an average of more than once in 20 comparisons (95 % probability.)

3.2.13 *set*, *n—of results*, a group of results collected under specified conditions for statistical analysis.

3.2.14 *standard deviation, between-laboratory*, *n*—see *between-laboratory standard deviation.*

3.2.15 *standard deviation, minimum*, *n*—see *minimum standard deviation.*

3.2.16 *standard deviation, within-laboratory*, *n*—see *within-laboratory standard deviation.*

3.2.17 *within-laboratory standard deviation,* s_r, *n*—the standard deviation of results collected on the same material in the same laboratory on different days (Synonym: *repeatability*).

3.3 The terms *mean, standard deviation, random* (as in random error), and *systematic error*, in their statistical senses, are adequately defined in Webster's Collegiate Dictionary, Tenth Edition.

4. Analytical Science and Analytical Methods

4.1 Analytical science deals with the development and use of methods for determining chemical composition of materials. Chemical analysis is the application of written analytical methods.

4.2 Analytical method development consists of selecting chemical and physical systems that respond to a specific analyte in a defined suite of material types. The purpose is to define a process that produces a physical change proportional to analyte content unaffected by other sample components. The measurement system (instrument) yields a numerical result that represents the quantity of analyte. A good analytical method has the following desirable properties:

4.2.1 *Accuracy*—When a method is applied to materials containing various quantities of analyte, it has the property of accuracy if results equal the numerical values of the analyte contents. This property relates solely to a method's average response at each analyte level, ignoring random statistical fluctuations of individual results. Actual methods are never known to be perfectly accurate and this term is usually used in a relative sense to compare different methods or the behavior of a single method under different conditions.

4.2.2 *Precision*—When a method is applied a number of times to a homogeneous sample, it has the property of precision if the result is always the same. This property relates solely to time-related variations in the response of a method and ignores systematic (averaged) differences between results and analyte content that may occur at various analyte levels. Actual methods are never perfectly precise and this term is usually used in a relative sense to compare different methods or the behavior of a single method under different conditions.

4.3 Written methods must satisfy two criteria: (*1*) they shall have the form and editorial style specified in the latest edition of Form and Style for ASTM Standards, and (*2*) the technical content shall be stated in terms that convey precise meanings to laboratory personnel using the method. The language used in the method must direct users (who may not have the same technical knowledge or experience as the developer) to repeat the procedural steps in the manner that produced satisfactory results in the development laboratory. Unless the method conveys this information, users will not achieve the potential accuracy and precision of the method.

4.4 The ILS demonstrates the performance of the method in a group of laboratories typical of those expected to use the method; whereas the accuracy and precision of the analytical techniques and procedures employed are defined by the statistics obtained in the development laboratory. ILS statistics are influenced by three additional factors: (*1*) the success of the translation of the research findings into the method tested in the ILS, (*2*) the care with which the ILS experimental design was followed, and (*3*) the quality of the test materials employed during the ILS.

4.5 The published method contains a summary of the ILS statistics that a user may interpret, based upon the user's own experience. A task group observing a relationship between the method's precision and analyte content as described in Guide E 1763E 1763, may choose to provide more detailed descriptions of the method's performance, for example, an equation or table predicting approximate standard deviations at various analyte levels.

5. Statistics and Statistical Methods

5.1 Statistics deals with the collection, analysis, interpretation, and presentation of numerical data sets. The mathematical procedures employed in these processes are statistical methods. Statistic is a generic term for the variable represented by a statistical procedure, but it also refers to the numerical value obtained when a statistical procedure is applied to a data set. For example, mean is a statistic, but the value 6 is the mean of