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Standard Practice for Performance-Based Qualification of Spectroscopic Analyzer Systems¹

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INTRODUCTION

Successful use of spectroscopic analyzers involves several activities, including sample introduction, analyzer calibration, and analyzer validation. Many of these activities are covered in separate existing documents, but not necessarily tied together therein. There are also activities not captured in existing documents that are essential for spectroscopic methods. This practice is intended to pull these together for users to employ and show the confidence in an analyzer system.

This practice is not limited to specific analyzers or applications. It does provide certain requirements that analyzers, associated systems, and software must meet.

1. Scope*

1.1 This practice covers requirements for establishing performance-based qualification of vibrational spectroscopic analyzer systems intended to be used to predict the test result of a material that would be produced by a Primary Test Method (PTM) if the same material is tested by the PTM.

1.1.1 This practice provides methodology to establish the lower/upper prediction limits associated with the Predicted Primary Test Method Result (PPTMR) in 1.1 with a specified degree of confidence that would contain the PTM result (if tested by the PTM).

1.1.2 The prediction limits in 1.1.1 can be used to estimate the confidence that product released using the analyzer system based on a PPTMR that meets PTM-based specification limits will meet PTM-based specification limits when tested by a PTM.

1.2 The practice covers the qualification of on-line, at-line, or laboratory infrared or Raman analyzers used to predict physical, chemical, or performance properties of liquid petroleum products and fuels. Infrared analyzers can operate in the near-infrared (NIR) region, mid-infrared (MIR) region, or both.

1.2.1 This practice applies to all analyzer systems that can meet the performance requirements defined within.

1.2.2 This practice is not limited to analyzers designed by any specific instrument manufacturer.

1.2.3 This practice allows for multiple calibration techniques to create a multivariate model which relates the spectra produced by the analyzer to the corresponding property determined by a PTM. Spectra can be used to predict multiple properties, but the analyzer system performance of each predicted property is qualified individually.

1.3 The practice describes procedures for establishing performance requirements for analyzer system applications. The user of this practice must establish written protocols to confirm the procedures are being followed.

1.4 This practice makes use of standard practices, guides, and methods already established in ASTM. Additional requirements are listed within this practice.

1.5 Any multivariate model that meets performance requirements and detects when the spectrum of a sample is an outlier (analysis that represents an extrapolation of the model) or a nearest neighbor distance inlier (a spectrum residing in a gap in the multivariate space) can be used.

1.6 This practice can be used with methods for determining properties of biofuel blends. Three alternative procedures can be used. In all three cases, the qualification of the predicted values for the blend are established and monitored as part of a continual program by application of Practice D6122 or by combined application of Practices D6122 and D3764 (see definition in section 3.1.18).

1.6.1 If the analyzer is used to directly predict a property of the biofuel blend, and both the Primary Test Method Result (PTMR) and Predicted Primary Test Method Result (PPTMR)

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*A Summary of Changes section appears at the end of this standard

are measured on the same material, then the analyzer is validated using Practice **D6122**.

1.6.2 If the analyzer is used to directly predict a property of a blend stock to which a fixed level of biofuel material is added prior to measurement by the PTM, and if the multivariate model correlates the spectrum of the blend stock to the PTMR for the fixed level blend, then the analyzer is validated using Practice **D6122**.

1.6.3 If the analyzer directly predicts a property of a blend stock to which some amount of biofuel material is later added, then Practice **D6122** is used to validate the analyzer performance. If the PPTMR produced by the analyzer is input into a second model to predict the property value for the final blend, based on the PPTMR for the blend stock and the blend level for the biofuel material, then the performance of this second model is validated using Practice **D3764**.

1.7 *Disclaimer of Liability as to Patented Inventions—Neither ASTM International nor an ASTM committee shall be responsible for identifying all patents under which a license is required in using this document. ASTM International takes no position respecting the validity of any patent rights asserted in connection with any item mentioned in this standard. Users of this standard are expressly advised that determination of the validity of any such patent rights, and the risk of infringement of such rights, are entirely their own responsibility.*

1.8 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.9 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 ASTM Standards:²

- D86** Test Method for Distillation of Petroleum Products and Liquid Fuels at Atmospheric Pressure
- D1265** Practice for Sampling Liquefied Petroleum (LP) Gases, Manual Method
- D2699** Test Method for Research Octane Number of Spark-Ignition Engine Fuel
- D2700** Test Method for Motor Octane Number of Spark-Ignition Engine Fuel
- D3700** Practice for Obtaining LPG Samples Using a Floating Piston Cylinder
- D3764** Practice for Validation of the Performance of Process Stream Analyzer Systems
- D4057** Practice for Manual Sampling of Petroleum and Petroleum Products

D4175 Terminology Relating to Petroleum Products, Liquid Fuels, and Lubricants

D4177 Practice for Automatic Sampling of Petroleum and Petroleum Products

D5842 Practice for Sampling and Handling of Fuels for Volatility Measurement

D6122 Practice for Validation of the Performance of Multivariate Online, At-Line, Field and Laboratory Infrared Spectrophotometer, and Raman Spectrometer Based Analyzer Systems

D6299 Practice for Applying Statistical Quality Assurance and Control Charting Techniques to Evaluate Analytical Measurement System Performance

D6596 Practice for Ampulization and Storage of Gasoline and Related Hydrocarbon Materials

D6624 Practice for Determining a Flow-Proportioned Average Property Value (FPAPV) for a Collected Batch of Process Stream Material Using Stream Analyzer Data

D6708 Practice for Statistical Assessment and Improvement of Expected Agreement Between Two Test Methods that Purport to Measure the Same Property of a Material

D6792 Practice for Quality Management Systems in Petroleum Products, Liquid Fuels, and Lubricants Testing Laboratories

D7453 Practice for Sampling of Petroleum Products for Analysis by Process Stream Analyzers and for Process Stream Analyzer System Validation

D7808 Practice for Determining the Site Precision of a Process Stream Analyzer on Process Stream Material

D7825 Practice for Generating a Process Stream Property Value through Application of a Process Stream Analyzer

D8009 Practice for Manual Piston Cylinder Sampling for Volatile Crude Oils, Condensates, and Liquid Petroleum Products

D8321 Practice for Development and Validation of Multivariate Analyses for Use in Predicting Properties of Petroleum Products, Liquid Fuels, and Lubricants based on Spectroscopic Measurements

E131 Terminology Relating to Molecular Spectroscopy

E1866 Guide for Establishing Spectrophotometer Performance Tests

3. Terminology

3.1 Definitions:

3.1.1 For definitions of terms used in this practice, refer to Terminology **D4175**.

3.1.2 For definitions of terms and symbols relating to IR spectroscopy, refer to Terminology **E131**.

3.1.3 For definitions of terms and symbols relating to multivariate calibration, refer to Practice **D8321**.

3.1.4 *accepted reference value (ARV), n*—value that serves as an agreed-upon reference for comparison and that is derived as (1) a theoretical or established value, based on scientific principles, (2) an assigned value, based on experimental work of some national or international organization, such as the U.S. National Institute of Standards and Technology (NIST), or (3) a consensus value, based on collaborative experimental work under the auspices of a scientific or engineering group. **D6596**

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.