Designation: D7215 – 22

Standard Test Method for Calculated Flash Point from Simulated Distillation Analysis of Distillate Fuels[1]

This standard is issued under the fixed designation D7215; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope*

1.1 This test method covers the calculated flash point formula, which represents a means for directly estimating the flash point temperature of distillate fuels from Test Method D2887 data. The value computed from the equation is termed the "calculated flash point." The calculated flash point formula is applicable to diesel fuel samples based on a correlation to Test Method D93 over the range from 47 °C to 99 °C, and to jet fuel samples based on a correlation to Test Method D56 and Test Method D3828 over the range from 35 °C to 67 °C.

1.2 The calculated flash point formula is valid for diesel and jet fuels with an IBP between 90 °C and 162 °C (194 °F and 324 °F), Test Method D2887 5 % recovery temperature between 136 °C and 207 °C (277 °F and 405 °F), and Test Method D2887 10 % recovery temperature between 142 °C and 222 °C (288 °F and 432 °F). For each flash point test method (Test Method D56, Test Method D93, and Test Method D3828) a separate equation has been established. See 4.4 for a detailed overview of the simulated distillation IBP, 5 %, and 10 % ranges per equation.

1.3 A calculated diagnostic parameter, not exceeding a given threshold value, is a prerequisite for acceptance of the calculated flash point.

1.4 The diagnostic parameter $MSPE_X$ (Mean Summed Prediction Error) checks the sample compliance, based on reconstruction of T_{IBP}, $T_{5\,\%}$, and $T_{10\,\%}$ of the sample, via a calculation procedure. A value for $MSPE_X$ not exceeding the threshold level of 1.9 °C is a prerequisite for accepting the calculated flash point, CFP.

NOTE 1—It is important to note that calculated flash point results, at this time, are not recognized by regulatory organizations in verifying conformance to applicable regulations.

NOTE 2—The calculated flash point derived from simulated distillation data depends upon the accuracy of determination of the IBP temperature and the 5 % and 10 % recovery temperatures.

NOTE 3—If the user's specification requires a defined flash point test method other than this test method, neither this test method nor any other test method should be substituted for the prescribed test method without obtaining comparative data and an agreement from the specifier.

1.5 The values stated in SI units are to be regarded as the standard.

1.5.1 *Exception*—The values given in parentheses are for information only.

1.6 *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.*

1.7 *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]

D56 Test Method for Flash Point by Tag Closed Cup Tester

D93 Test Methods for Flash Point by Pensky-Martens Closed Cup Tester

D975 Specification for Diesel Fuel

D1655 Specification for Aviation Turbine Fuels

D2887 Test Method for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography

D3828 Test Methods for Flash Point by Small Scale Closed Cup Tester

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

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

3. Terminology

3.1 *Definitions:*

[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products, Liquid Fuels, and Lubricants and is the direct responsibility of Subcommittee D02.04.0K on Correlative Methods.

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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.

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

TABLE 1 Overview

	IBP		5 %		10 %	
	Min temp	Max temp	Min temp	Max temp	Min temp	Max temp
Test Method D93 Diesel	103 °C (217 °F)	163 °C (326 °F)	144 °C (291 °F)	210 °C (410 °F)	159 °C (318 °F)	236 °C (457 °F)
Test Method D56 Jet Fuel	101 °C (213 °F)	136 °C (277 °F)	135 °C (275 °F)	169 °C (337 °F)	141 °C (285 °F)	183 °C (362 °F)
Test Method D3828 Jet Fuel	101 °C (213 °F)	136 °C (277 °F)	135 °C (275 °F)	169 °C (337 °F)	141 °C (285 °F)	183 °C (362 °F)

3.1.1 For definitions of terms used in this test method, refer to Terminology D4175.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *calculated flash point (CFP), n*—flash point calculated using this test method from the IBP, 5 %, and 10 % recovery temperature obtained from simulated distillation according to Test Method D2887.

3.2.2 *mean sum of prediction errors of variable X ($MSPE_X$), n*—mean of summed prediction errors of the predictor variables, that is, the recovery temperatures.

3.2.3 *partial least squares (PLS) regression, n*—extension of the multiple linear regression model, specifying a linear relationship between a dependent variable and a set of predictor variables.

4. Significance and Use

4.1 The flash point temperature is one measure of the tendency of the test specimen to form a flammable mixture with air under controlled laboratory conditions. It is only one of a number of properties that must be considered in assessing the overall flammability hazard of a material.

4.2 Flash point is used in shipping and safety regulations to define flammable and combustible materials. Consult the particular regulation involved for precise definitions of these classifications.

4.3 Flash point can indicate the possible presence of highly volatile and flammable materials in a relatively non-volatile or non-flammable material.

4.4 In cases where Test Method D2887 data are available, that is, for determination of boiling range distribution or calculation of other physical properties, this test method provides a calculation method for flash point without performing an additional analysis. Table 1 shows the ranges for the IBP, 5 %, and 10 % results for each equation.

4.5 In the case where the flash point of a fuel has been initially established, the calculated flash point is useful as a flash point check on subsequent samples of that fuel, provided its source and mode of manufacture remain unchanged.

5. Procedure

5.1 Obtain the IBP, 5 % and 10 % recovered temperatures of the specimen by performing a simulated distillation according to Test Method D2887.

5.2 Calculate reconstruction values of T_{IBP}, $T_{5\,\%}$, and $T_{10\,\%}$ recovery temperatures according to Eq 1-3:

$$\hat{T}_{IBP} = 2.75 + 0.944 \cdot T_{IBP} + 0.163 \cdot T_{5\,\%} - 0.124 \cdot T_{10\,\%}\,[^\circ C] \quad (1)$$

$$\hat{T}_{5\,\%} = 2.21 + 0.163 \cdot T_{IBP} + 0.363 \cdot T_{5\,\%} + 0.455 \cdot T_{10\,\%}\,[^\circ C] \quad (2)$$

$$\hat{T}_{10\,\%} = -3.71 - 0.124 \cdot T_{IBP} + 0.455 \cdot T_{5\,\%} + 0.694 \cdot T_{10\,\%}\,[^\circ C] \quad (3)$$

5.3 Compute the sample compliance mean sum of prediction errors of the recovery temperatures, $MSPE_X$ of the specimen according to Eq 4:

$$MSPE_X = \frac{1}{3}\sqrt{\left[T_{IBP} - \hat{T}_{IBP}\right]^2 + \left[T_{5\,\%} - \hat{T}_{5\,\%}\right]^2 + \left[T_{10\,\%} - \hat{T}_{10\,\%}\right]^2}\,[^\circ C] \quad (4)$$

where T_{IBP}, $T_{5\,\%}$, and $T_{10\,\%}$ refer to the experimental sample boiling point temperatures.

5.4 Compare $MSPE_X$ to the critical value of 1.9 °C. If $MSPE_X$ exceeds this critical value, then the sample is not suitable for calculation of flash point according to this test method. Do not proceed with this test method.

6. Calculation

6.1 Calculation of the CFP using the appropriate Eq 5-7:

6.1.1 For correlation to Test Method D56:

$$CFP_{D56} = -55.5 + 0.164 \cdot T_{IBP} + 0.095 \cdot T_{5\,\%} + 0.453 \cdot T_{10\,\%}\,[^\circ C] \quad (5)$$

6.1.2 For correlation to Test Method D93:

$$CFP_{D93} = -51.7 + 0.403 \cdot T_{IBP} + 0.163 \cdot T_{5\,\%} + 0.214 \cdot T_{10\,\%}\,[^\circ C] \quad (6)$$

6.1.3 For correlation to Test Method D3828:

$$CFP_{D3828} = -61.4 + 0.223 \cdot T_{IBP} - 0.201 \cdot T_{5\,\%} + 0.721 \cdot T_{10\,\%}\,[^\circ C] \quad (7)$$

7. Report

7.1 Report the calculated flash point to the nearest 0.1 °C (0.2 °F), including the correlating subscript.

8. Precision and Bias[3]

8.1 Within the range of 47 °C to 99 °C (117 °F to 210 °F), for diesel fuel samples and within the range of 35 °C to 67 °C (95 °F to 153 °F) for jet fuel samples, the difference between the calculated flash point and the experimental flash point will be less than ±4 °C (7 °F) for 95 % of the distillate fuels evaluated.

8.2 *Precision*—The precision of this test method as determined by the statistical evaluation of the published repeatability and reproducibility of the Test Method D2887 method and the Test Method D56, Test Method D93 and Test Method D3828 correlation models, is as follows:

8.3 *Repeatability*—The difference between successive test results, obtained by the same operator using the same apparatus under constant operating conditions on identical test material,

[3] Supporting data have been filed at ASTM International Headquarters and may be obtained by requesting Research Report RR:D02-1636. Contact ASTM Customer Service at service@astm.org.

TABLE 2 Repeatability

Calculated	Repeatability, r	
	°C	°F
Test Method D56	0.5	0.9
Test Method D93	0.8	1.4
Test Method D3828	0.8	1.4

TABLE 3 Reproducibility

Calculated	Reproducibility, R	
	°C	°F
Test Method D56	2.0	3.6
Test Method D93	4.4	7.9
Test Method D3828	2.9	5.2

would in the long run, in normal and correct operation of this test method, exceed the values in Table 2 in only one case in twenty.

8.4 *Reproducibility*—The difference between two single and independent results obtained by different operators working in different laboratories on identical test material would, in the long run, exceed the values in Table 3 in only one case in twenty.

8.5 *Bias*—Bias between flash points from Test Method D56, Test Method D93, and Test Method D3828 and calculated flash point from simulated distillation data has been evaluated using Practice D6708. No significant bias was found between the calculated flash point and the flash point determined using the above flash point methods.

8.6 *Cross-method Reproducibility*—The difference between two single and independent results obtained by different operators working in different laboratories on identical test material and applying the correlated and reference method respectively, would in the long run, exceed the values in Table 4 in only one case in twenty.

TABLE 4 Cross-Method Reproducibility

Calculated	Cross-method Reproducibility, R_{XY}	
	°C	°F
Test Method D56	4.3	7.7
Test Method D93	5.2	9.9
Test Method D3828	3.6	6.4

8.7 This correlation model and determination of the cross-method reproducibility was validated by an analysis of variance procedure in accordance with Practice D6708.

8.8 The statistical evaluation and validation can be found in the research report.

9. Keywords

9.1 calculated flash point; diesel fuel; flash point; jet fuel; $MSPE_X$; PLS; simulated distillation

ANNEX

(Mandatory Information)

A1. CORRELATION DATA

A1.1 Development of the Correlation

A1.1.1 A database with 117 representative samples was collected and divided into a correlation data set and a validation data set. The complete data set included 56 diesel fuel samples and 61 jet fuel samples. The detailed data set structure is given in Tables A1.1 and A1.2.

A1.1.2 The empirical equation for the calculated flash point correlation was derived using a partial least squares (PLS) regression. Other correlation techniques have been investigated.[3]

A1.1.3 The correlation equations were developed using Test Method D2887 distillation data and Test Method D93 flash point data for diesel fuel and Test Method D56 and Test Method D3828 flash point data for jet fuel.

TABLE A1.1 Number of Samples Used for the Correlation

	Jet Fuel		Diesel Fuel		Total
	Europe	USA/ Canada	Europe	USA/ Canada	
Test Method D56	14	10			24
Test Method D93			13	20	33
Test Method D3828	4	10			14
Total					71