Designation: D4737 – 21

Standard Test Method for Calculated Cetane Index by Four Variable Equation[1]

This standard is issued under the fixed designation D4737; 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 The calculated Cetane Index by Four Variable Equation provides a means for estimating the ASTM cetane number (Test Method D613) of distillate fuels from density and distillation recovery temperature measurements. The value computed from the equation is termed the Calculated Cetane Index by Four Variable Equation.

1.2 The Calculated Cetane Index by Four Variable Equation is not an optional method for expressing ASTM cetane number. It is a supplementary tool for estimating cetane number when a result by Test Method D613 is not available and if cetane improver is not used. As a supplementary tool, the Calculated Cetane Index by Four Variable equation must be used with due regard for its limitations.

1.3 Procedure A is to be used for Specification D975, Grades No. 1–D S15, No. 1–D S500, No. 1–D S5000, No. 2–D S15, No. 2–D S5000, and No. 4–D. This method for estimating cetane number was developed by Chevron Research Co.[2] Procedure A is based on a data set including a relatively small number of No. 1–D fuels. Test Method D4737 Procedure A may be less applicable to No. 1–D S15, No. 1–D S500, and No. 1–D S5000 than to No. 2–D grade S5000 or to No. 4–D fuels.

1.3.1 Procedure A has been verified as applicable to Grade No. 2–D S15 diesel fuels.[3]

1.4 Procedure B is to be used for Specification D975, Grade No. 2–D S500.

1.5 The test method "Calculated Cetane Index by Four Variable Equation" is particularly applicable to Grade 1–D S5000, Grade No. 1–D S500, Grade No. 2–D S5000 and Grade No. 2–D S500 diesel fuel oils containing straight-run and cracked stocks, and their blends. It can also be used for heavier fuels with 90 % recovery points less than 382 °C and for fuels containing derivatives from oil sands and oil shale.

NOTE 1—Sxx is the designation for maximum sulfur level specified for the grade. For example, S500 grades are those with a maximum sulfur limit of 500 ppm (µg/g).

1.6 Biodiesel blends are excluded from this test method, because they were not part of the datasets use to develop either Procedure A or B.

1.7 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

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:*[4]

D86 Test Method for Distillation of Petroleum Products and Liquid Fuels at Atmospheric Pressure
D613 Test Method for Cetane Number of Diesel Fuel Oil
D975 Specification for Diesel Fuel
D1298 Test Method for Density, Relative Density, or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method
D2887 Test Method for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography
D4052 Test Method for Density, Relative Density, and API Gravity of Liquids by Digital Density Meter
D4175 Terminology Relating to Petroleum Products, Liquid

[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.E0 on Burner, Diesel and Non-Aviation Gas Turbine Fuels.

Current edition approved Nov. 1, 2021. Published November 2021. Originally approved in 1987. Last previous edition approved in 2016 as D4737 – 10 (2016). DOI: 10.1520/D4737-21.

[2] Ingham, M. C., et al., "Improved Predictive Equations for Cetane Number," SAE Paper No 860250, Society of Automotive Engineers (SAE), 400 Commonwealth Dr., Warrendale, PA 15096-0001.

[3] Supporting data (the analysis leading to the use of Procedure A for No. 2-D S15 diesel fuels and to Procedure B) have been filed at ASTM International Headquarters and may be obtained by requesting Research Report RR:D02-1699. Contact ASTM Customer Service at service@astm.org.

[4] 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

Fuels, and Lubricants

D6751 Specification for Biodiesel Fuel Blend Stock (B100) for Middle Distillate Fuels

D6890 Test Method for Determination of Ignition Delay and Derived Cetane Number (DCN) of Diesel Fuel Oils by Combustion in a Constant Volume Chamber

D7170 Test Method for Determination of Derived Cetane Number (DCN) of Diesel Fuel Oils—Fixed Range Injection Period, Constant Volume Combustion Chamber Method (Withdrawn 2019)[5]

2.2 *CEN Standards:*[6]

EN 14214 Automotive fuels — Fatty acid methyl esters (FAME) for diesel engines — Requirements and test methods

3. Terminology

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

4. Summary of Test Method

4.1 Two correlations in SI units have been established between the ASTM cetane number and the density and 10 %, 50 %, and 90 % distillation recovery temperatures of the fuel. Procedure A has been developed for diesel fuels meeting the requirements of Specification D975 Grades No. 1–D S15, No. 1–D S500, No. 1–D S5000, No. 2–D S5000, and No. 4–D. It has been found to be applicable to Grade No. 2–D S15. The relationship is given by the following equation:

$$CCI = 45.2 + (0.0892)(T_{10N}) + [0.131 + (0.901)(B)][T_{50N}] + [0.0523 - (0.420)(B)][T_{90N}] + [0.00049][(T_{10N})^2 - (T_{90N})^2] + (107)(B) + (60)(B)^2 \tag{1}$$

where:

CCI = Calculated Cetane Index by Four Variable Equation,
D = Density at 15 °C, g/mL determined by Test Methods D1298 or D4052,
DN = D - 0.85,
B = $[e^{(-3.5)(DN)}] - 1$,
T_{10} = 10 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure,
T_{10N} = T_{10} - 215,
T_{50} = 50 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure,
T_{50N} = T_{50} - 260,
T_{90} = 90 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure, and
T_{90N} = T_{90} - 310.

4.2 The empirical equation for Procedure A of the Calculated Cetane Index by Four Variable Equation was derived using a generalized least squares fitting technique which accounted for measurement errors in the independent variables (fuel properties) as well as in the dependent variable (cetane number by Test Method D613). The data base consisted of 1229 fuels including; commercial diesel fuels, refinery blending components and fuels derived from oil sands, shale, and coal. The analysis also accounted for bias amongst the individual sets of data comprising the database.

4.3 Procedure B has been developed for diesel fuels meeting the requirements of Specification D975 Grade No. 2–D S500. The relationship is given by the following equation:[3]

$$CCI = -399.90(D) + 0.1113\,(T_{10}) + 0.1212\,(T_{50}) + 0.0627\,(T_{90}) + 309.33 \tag{2}$$

where:

CCI = Calculated Cetane Index by Four Variable Equation,
D = Density at 15 °C, g/mL determined by Test Methods D1298 or D4052,
T_{10} = 10 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure,
T_{50} = 50 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure, and
T_{90} = 90 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure.

4.3.1 The equation for Procedure B when T_{10}, T_{50}, and T_{90} are in °F is:[3]

$$CCI = -399.90(D) + 0.06183\,(T_{10}) + 0.06733\,(T_{50}) + 0.03483\,(T_{90}) + 304.09 \tag{3}$$

where:

CCI = Calculated Cetane Index by Four Variable Equation,
D = Density at 15 °C, g/mL determined by Test Method D1298 or D4052,
T_{10} = 10 % recovery temperature, °F, determined by Test Method D86 and corrected to standard barometric pressure,
T_{50} = 50 % recovery temperature, °F, determined by Test Method D86 and corrected to standard barometric pressure, and
T_{90} = 90 % recovery temperature, °F, determined by Test Method D86 and corrected to standard barometric pressure.

4.4 The empirical equation for Procedure B of the Calculated Cetane Index by Four Variable Equation was derived from National Exchange Group data for 111 No. 2–D S500 diesel fuels with sulfur level between 16 and 500 ppm using a Partial Least Squares technique. A 3-principal component model was chosen. The model was validated with a set of 980 diesel fuels with sulfur levels in the same range.

5. Significance and Use

5.1 The Calculated Cetane Index by Four Variable Equation is useful for estimating ASTM cetane number when a test engine is not available for determining this property directly and when cetane improver is not used. It may be conveniently employed for estimating cetane number when the quantity of

[5] The last approved version of this historical standard is referenced on www.astm.org.

[6] Available from the National CEN members listed on the CEN website (www.cenorm.be) or from the CEN/TC 19 Secretariat (astm@nen.nl).

sample available is too small for an engine rating. In cases where the ASTM cetane number of a fuel has been previously established, the Calculated Cetane Index by Four Variable Equation is useful as a cetane number check on subsequent batches of that fuel, provided the fuel's source and mode of manufacture remain unchanged.

NOTE 2—Test Methods D6890 and D7170 may be used to obtain a Derived Cetane Number (DCN) when the quantity of sample is too small for an engine test. These methods do measure the effect of cetane improver.

5.2 Within the range from 32.5 to 56.5 cetane number, the expected error of prediction of Procedure A of the Calculated Cetane Index by Four Variable Equation will be less than ±2 cetane numbers for 65 % of the distillate fuels evaluated. Errors may be greater for fuels whose properties fall outside the recommended range of application.

6. Procedure

6.1 Determine the density of the fuel at 15 °C to the nearest 0.0001 g/mL, as described in Test Method D1298 or Test Method D4052.

6.2 Determine the 10 %, 50 %, and 90 % recovery temperatures of the fuel, as described in Test Method D86.

6.3 Test Method D2887 maybe used as an alternative to Test Method D86 to determine the 10 %, 50 %, 90 % recovery temperatures of the fuel.

6.3.1 If Test Method D2887 is used, convert the Test Method D2887 data to estimated Test Method D86 data following Appendix X5, Correlation of Jet and Diesel Fuel, of Test Method D2887 and use the estimated Test Method D86 data in place of actual Test Method D86 data in the calculations.

6.3.2 Provision for use of Test Method D2887 data in this test method is intended to facilitate its use in determining compliance with Specification D975 requirements. If this test method is used for purposes other than Specification D975 compliance, the use of estimated Test Method D86 data should be reviewed to ensure it is acceptable.

7. Calculation or Interpretation of Results

7.1 Compute the Calculated Cetane Index by Four Variable Equation using the equation given in 4.1 (Procedure A) for Grades 1–D S15, 1–D S500, 1–D S5000, 2–D S15, 2–D S5000, and 4–D. The calculation of Procedure A is more easily performed using a computer or programmable hand calculator. Round the value obtained to the nearest one-tenth. Compute the Calculated Cetane Index by Four Variable Equation using the equation given in 4.3. (Procedure B) for Grade No. 2–D S500.

7.1.1 Calculated Cetane Index by Four Variable Equation (Procedure A) can also be easily determined by means of the nomographs (applicable to Procedure A only) appearing in Figs. 1-3. Fig. 1 is used to estimate the cetane number of a fuel based on its density at 15 °C and its 50 % recovery temperature. Fig. 2 is used to determine a correction for the estimate from Fig. 1 to account for deviations in the density and the 90 % recovery temperature of the fuel from average values. Fig. 3 is used to determine a second correction for the estimate from Fig. 1 to account for deviations in the 10 % and the 90 % recovery temperatures of the fuel from average values. The corrections determined from Fig. 2 and Fig. 3 are summed algebraically with the cetane number estimate from Fig. 1 to find the Calculated Cetane Index by Four Variable Equation (Procedure A). The method of using these nomographs is indicated by the illustrative example shown below and on Figs. 1-3.

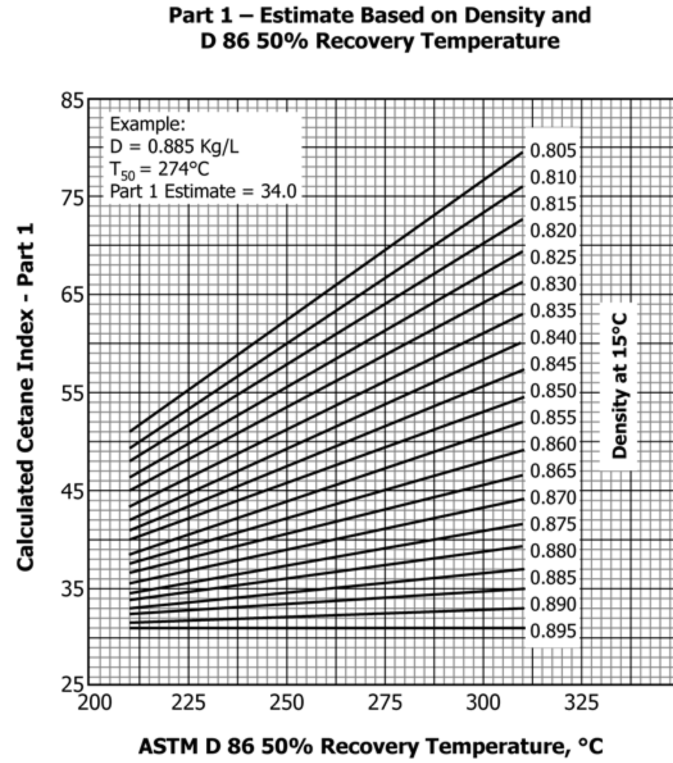

FIG. 1 Calculated Cetane Index

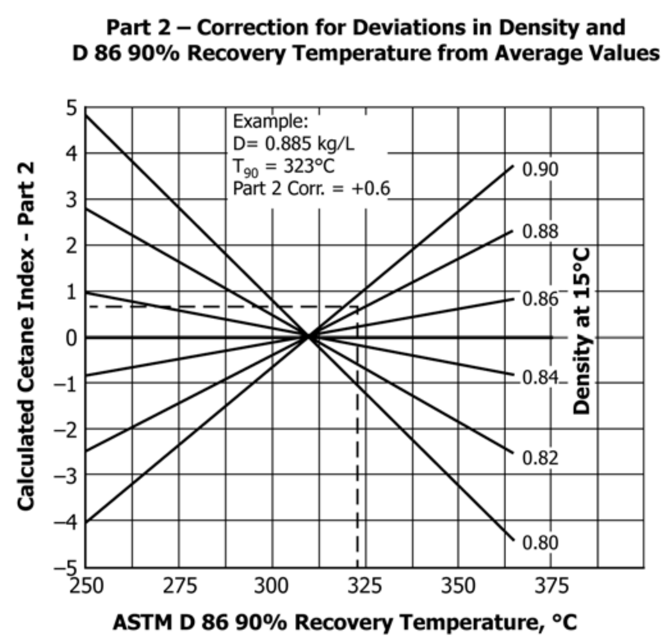

FIG. 2 Calculated Cetane Index

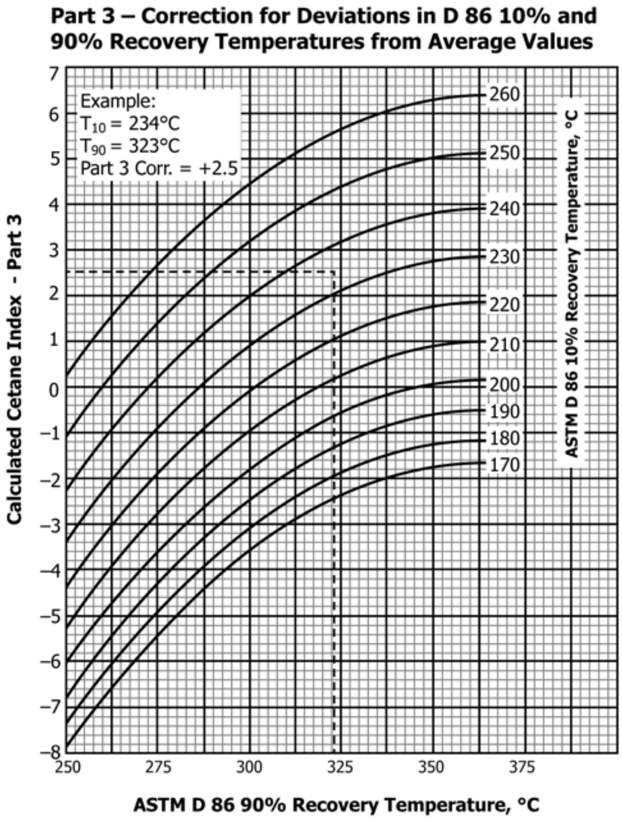

FIG. 3 Calculated Cetane Index

Measured Fuel Properties	
Test Method D613 Cetane Number	37.0
Test Method D1298 Density at 15 °C, kg/L	0.885
Test Method D86 10 % Recovery Temperature, °C	234
Test Method D86 50 % Recovery Temperature, °C	274
Test Method D86 90 % Recovery Temperature, °C	323

Calculated Cetane Index	
Estimate from Fig. 1	34.0
Correction from Fig. 2	+0.6
Correction from Fig. 3	+2.5
	CCI = 37.1

7.2 The Calculated Cetane Index by Four Variable Equation possesses certain inherent limitations which must be recognized in its application. These are as follows:

7.2.1 It is not applicable to fuels containing additives for raising the cetane number.

7.2.2 It is not applicable to pure hydrocarbons, nor to non-petroleum fuels derived from coal.

7.2.3 It is not applicable to fuels containing biodiesel as defined by Specification D6751 or CEN Specification EN 14214.

7.2.4 Substantial inaccuracies in correlation may occur if the equation is applied to residual fuels or crude oils.

8. Report

8.1 Report the result of Procedure A or Procedure B to one decimal place (XX.X) as:

$$\text{Cetane Index by D4737 (Procedure A or B)} = \_\_\_\_\_\_\_\_ \quad (4)$$

9. Precision and Bias

9.1 The determination of Calculated Cetane Index by Four Variable Equation from measured density at 15 °C and measured 10 %, 50 %, and 90 % recovery temperatures is exact.

9.2 *Precision*—The precision of the Calculated Cetane Index by Four Variable Equation is dependent on the precision of the original density and recovery temperature determinations which enter into the calculation. Test Method D1298 has a stated repeatability limit of 0.0006 kg/L and a stated reproducibility limit of 0.0015 kg/L at 15 °C. Test Method D4052 has a stated repeatability of 0.0001 g/mL and reproducibility of 0.0005 g/mL. Test Method D86 has stated repeatability and reproducibility limits which vary with the rate of change of recovery temperature. See Figs. 2 through 7 and Tables 7 through 10 of Test Method D86 for details.

9.3 *Bias*—No general statement is made on bias of this test method since a comparison with accepted reference values is not available.

10. Keywords

10.1 cetane; cetane index; diesel fuel

SUMMARY OF CHANGES

Subcommittee D02.E0 has identified the location of selected changes to this standard since the last issue (D4737 – 10 (2016)) that may impact the use of this standard. (Approved Nov. 1, 2021.)

(1) Added Terminology D4175 to Section 2.

(2) Added Section 3, Terminology.