Designation: D4737 – 04

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 Low Sulfur, No. 1–D, No. 2–D, 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 may be less applicable to No.1–D, No. 1–D Low Sulfur and No. 4–D grades than to No. 2–D grade.

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

1.5 The test method "Calculated Cetane Index by Four Variable Equation" is particularly applicable to Grade 1-D, Grade No. 1–D Low Sulfur and Grade 2-D 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.

1.6

1.7 *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.*

2. Referenced Documents

2.1 *ASTM Standards:*[3]

D86 Test Method for Distillation of Petroleum Products at Atmospheric Pressure
D613 Test Method for Cetane Number of Diesel Fuel Oil
D975 Specification for Diesel Fuel Oils
D1298 Test Method for Density, Relative Density (Specific Gravity), 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 and Relative Density of Liquids by Digital Density Meter

3. Summary of Test Method

3.1 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 1-D Low Sulfur, Nos. 1-D, 2-D, and 4-D. The relationship is given by the following equation.

$$CCI = 45.2 + (0.0892)(T_{10N}) + [0.131 + (0.901)(B)][T_{50N}] \quad (1)$$

$$+ [0.0523 - (0.420)(B)][T_{90N}] \quad (1)$$

$$+ [0.00049][(T_{10N})^2 - (T_{90N})^2] \quad (1)$$

$$+ (107)(B) + (60)(B)^2 \quad (1)$$

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} = $T_{10} - 215$,

[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products and Lubricants and is the direct responsibility of Subcommittee D02.E0 on Burner, Diesel, Non-Aviation Gas Turbine, and Marine Fuels.

Current edition approved Dec. 1, 2004. Published December 2004. Originally approved in 1987. Last previous edition approved in 2003 as D4737 – 03. DOI: 10.1520/D4737-04.

[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] 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.

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.

3.2 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.

3.3 Procedure B has been developed for diesel fuels meeting the requirements of Specification D975 Grade 2-D Low Sulfur. The relationship is given by the following equation:

$$CCI = -386.26(D) + 0.1740\,(T_{10}) + 0.1215\,(T_{50}) + 0.01850\,(T_{90}) + 297.42 \tag{2}$$

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
T_{90} = 90 % recovery temperature, °C, determined by Test Method D86 and corrected to standard barometric pressure

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

$$CCI = -386.26(D) + 0.09668\,(T_{10}) + 0.06751\,(T_{50}) + 0.01028\,(T_{90}) + 291.83 \tag{3}$$

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
T_{90} = 90 % recovery temperature, °F, determined by Test Method D86 and corrected to standard barometric pressure

3.4 The empirical equation for Procedure B of the Calculated Cetane Index by Four Variable Equation was derived from National Exchange Group data for 87 No. 2 Low Sulfur diesel fuels with sulfur level between 16 and 500 ppm using a Partial Least Squares technique. A 2-principal component model was chosen. The model was validated with a set of 980 diesel fuels with sulfur levels in the same range.

4. Significance and Use

4.1 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 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.

4.2 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.

5. Procedure

5.1 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.

5.2 Determine the 10 %, 50 %, and 90 % recovery temperatures of the fuel to the nearest 1°C, as described in Test Method D86.

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

5.3.1 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.

5.3.2 Provision for use of test Method of D2887 data in this Test Method is intended to facilitate its use in determining compliance with Specification D975D1298 requirements. If this test method is used for purposes other than Specification D975D1298 compliance, the use of estimated Test Method D86 data should be reviewed to ensure it is acceptable.

6. Calculation or Interpretation of Results

6.1 Compute the Calculated Cetane Index by Four Variable Equation using the equation given in 3.1 (Procedure A) for Grades 1-D Low Sulfur, 1-D, 2-D, 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 3.3. (Procedure B) for Grade 2-D Low Sulfur.

6.1.1 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