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An American National Standard

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

This standard is issued under the fixed designation D 4737; 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] 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.

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1. Scope

1.1 The calculated Cetane Index by Four Variable Equation provides a means for estimating the ASTM cetane number (Test Method D 613) 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 D 613 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 D 975, 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]

~~1.2 The Calculated Cetane Index by Four Variable Equation~~ Procedure A is ~~not an optional method for expressing ASTM cetane number. It is~~ based on a ~~supplementary tool for estimating cetane~~ data set including a relatively small number ~~w~~ of No. 1–D fuels. Test Method D 4737 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 ~~with due regard~~ for ~~its limitations.~~

~~1.3 The~~ Specification D 975, 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 ~~blends of the two.~~ their blends. It can also be used for heavier fuels with 90 % recovery points less than 382°C and for fuels containing ~~non-petroleum~~ derivatives from ~~tar~~ oil sands and oil shale.

1.~~4~~6 The values stated in SI units are to be regarded as the standard. The values given in parentheses are for information only.

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:*

D 86 Test Method for Distillation of Petroleum Products[3]

D 613 Test Method for Cetane Number of Diesel Fuel Oil[4]

D 975 Specification for Diesel Fuel Oils[3]

D 1298 Test Method for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method[3]

D 4052 Test Method for Density and Relative Density of Liquids by Digital Density Meter[5]

~~[2] This method of estimating cetane number was developed by Chevron Research Co. See Ingham,~~

[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] *Annual Book of ASTM Standards*, Vol 05.01.

[4] *Annual Book of ASTM Standards*, Vol 05.05.

[5] *Annual Book of ASTM Standards*, Vol 05.02.

3. Summary of Test Method

3.1 ~~A~~Two correlations in SI units ~~has~~ 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 D 975 Grades 1-D Low Sulfur, No. 1-D, 2-D and 4-D. The relationship is given by the following equation:.

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

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

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

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

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

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

~~$+ (107)(B) + (60)(B)^2$~~ (1)

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

~~where:~~
~~CCI~~
where:
CCI = Calculated Cetane Index by Four Variable Equation,
D = Density at 15°C, g/mL determined by Test Methods D 1298 or D 4052,
DN = ~~D – 0.85,~~ *D* - 0.85,
B = $[e^{(-3.5)(DN)}]$ ~~—~~ - 1,
T10~~*10*~~ = 10 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure,
T10N~~*10N*~~ = ~~*T*~~T_{10} ~~– 215,~~ - 215,
T50~~*50*~~ = 50 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure,
T = T_{50} ~~– 260,~~ - 260,
~~*50N*~~*50N* ~~*T*~~
T90~~*90*~~ = 90 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure, and
T = ~~*T*~~T_{90} ~~– 310.~~- 310.
~~*90N*~~*90N*

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 D 613). The data base consisted of 1229 fuels including; commercial diesel fuels, refinery blending components and ~~non-petroleum~~ fuels derived from ~~tar~~ 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 D 975 Grade 2-D Low Sulfur. The relationship is given by the following equation:

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

where:
CCI = Calculated Cetane Index by Four Variable Equation
D = Density at 15°C, g/mL determined by Test Methods D 1298 or D 4052
T~~*10*~~ = 10 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure
T~~*50*~~ = 50 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure
T~~*90*~~ = 90 % recovery temperature, °C, determined by Test Method D 86 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:

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

where:
CCI = Calculated Cetane Index by Four Variable Equation
D = Density at 15°C, g/mL determined by Test Method D 1298 or D 4052
T~~*10*~~ = 10 % recovery temperature, °F, determined by Test Method D 86 and corrected to standard barometric pressure
T~~*50*~~ = 50 % recovery temperature, °F, determined by Test Method D 86 and corrected to standard barometric pressure
T~~*90*~~ = 90 % recovery temperature, °F, determined by Test Method D 86 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 ~~samples~~ 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 ~~k~~ g/mL, as described in Test Method D 1298 or Test Method D 4052.

5.2 Determine the 10 %, 50 %, and 90 % recovery temperatures of the fuel to the nearest 1°C, as described in Test Method D 86.

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 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.

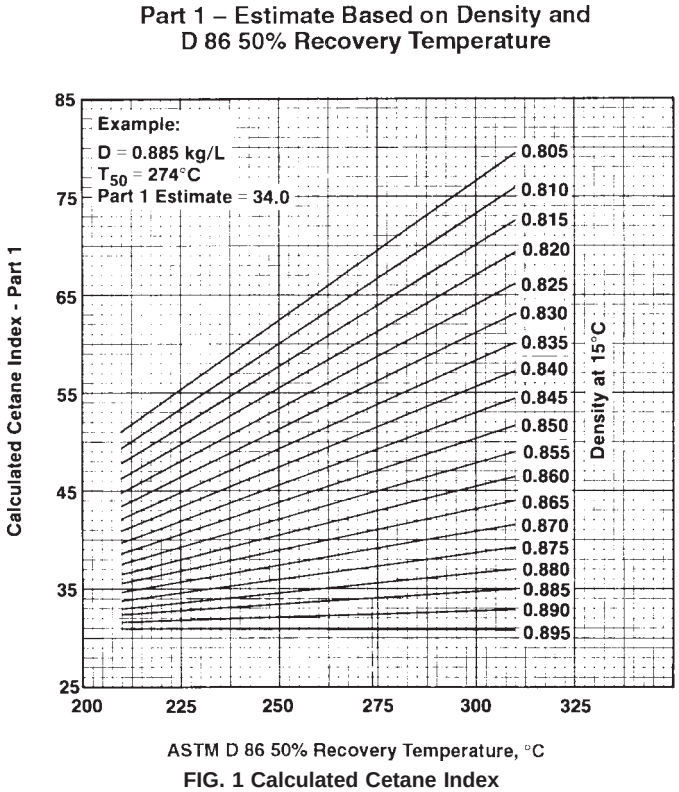

FIG. 1 Calculated Cetane Index

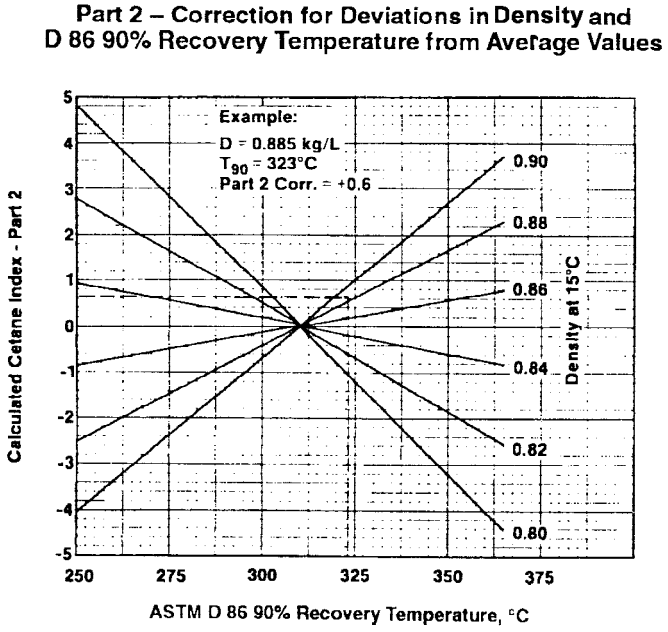

FIG. 2 Calculated Cetane Index

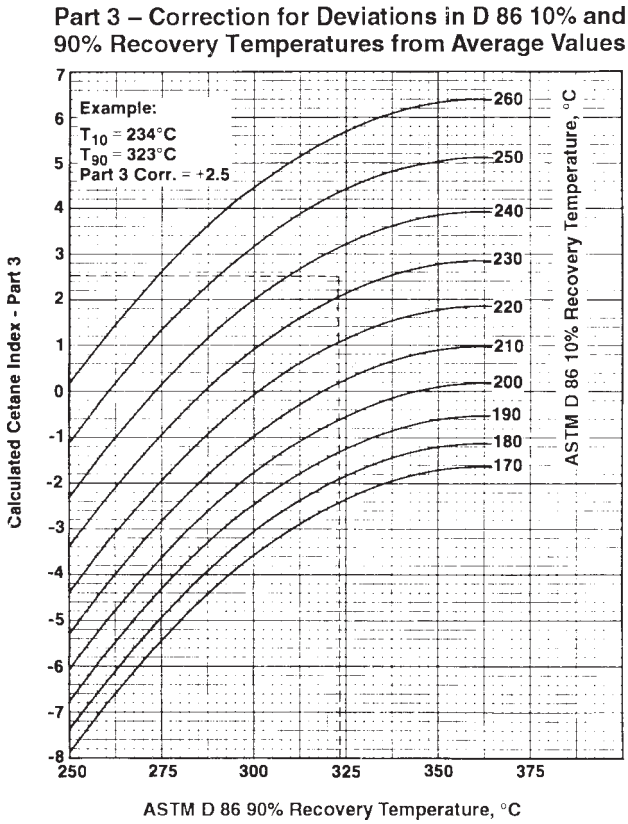

FIG. 3 Calculated Cetane Index

Measured Fuel Properties	
Test Method D 613 Cetane Number	37.0
Test Method D 1298 Density at 15°C, kg/L	0.885
Test Method D 86 10 % Recovery Temperature, °C	234
Test Method D 86 50 % Recovery Temperature, °C	274
Test Method D 86 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

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

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

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

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

7. Report

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

$$\text{Cetane Index by D 4737 (Procedure A or B)} = \_\_\_\_\_ \quad (4)$$

8. Precision and Bias

~~7~~8.1 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.

~~7~~8.2 *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 D 1298 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 D 4052 has a stated repeatability of 0.0001 g/mL and reproducibility of 0.0005 g/mL. Test Method D 86 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 D 86 for details.

~~7~~8.3 *Bias*—No general statement is made on bias of this test method since a comparison with accepted reference values is not available.

~~8~~9. Keywords

~~8~~9.1 cetane; cetane index; diesel fuel