



## Standard Test Method for Calculated Cetane Index by Four Variable Equation<sup>1</sup>

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 reappraisal. A superscript epsilon ( $\epsilon$ ) indicates an editorial change since the last revision or reappraisal.

### 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.<sup>2</sup> Procedure A is based on a data set including a relatively small number 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 for 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 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 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<sup>3</sup>
- D 613 Test Method for Cetane Number of Diesel Fuel Oil<sup>4</sup>
- D 975 Specification for Diesel Fuel Oils<sup>3</sup>
- D 1298 Test Method for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method<sup>3</sup>
- D 4052 Test Method for Density and Relative Density of Liquids by Digital Density Meter<sup>5</sup>

### 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 D 975 Grades 1–D Low Sulfur, No. 1–D, 2–D and 4–D. The relationship is given by the following equation.

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

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

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

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

where:

$CCI$  = Calculated Cetane Index by Four Variable Equation,

$D$  = Density at 15°C, g/mL determined by Test Methods D 1298 or D 4052,

$DN$  =  $D - 0.85$ ,

$B$  =  $[e^{(-3.5)(DN)}] - 1$ ,

$T_{10}$  = 10 % recovery temperature, °C, determined by Test Method D 86 and corrected to standard barometric pressure,

<sup>1</sup> 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 July 10, 2003. Published August 2003. Originally approved in 1987. Last previous edition approved in 2001 as D 4737–96a (2001).

<sup>2</sup> 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.

<sup>3</sup> Annual Book of ASTM Standards, Vol 05.01.

<sup>4</sup> Annual Book of ASTM Standards, Vol 05.05.

<sup>5</sup> Annual Book of ASTM Standards, Vol 05.02.

$$\begin{aligned}
 T_{10N} &= T_{10} - 215, \\
 T_{50} &= 50 \% \text{ recovery temperature, } ^\circ\text{C, determined by} \\
 &\quad \text{Test Method D 86 and corrected to standard baro-} \\
 &\quad \text{metric pressure,} \\
 T_{50N} &= T_{50} - 260, \\
 T_{90} &= 90 \% \text{ recovery temperature, } ^\circ\text{C, determined by} \\
 &\quad \text{Test Method D 86 and corrected to standard baro-} \\
 &\quad \text{metric pressure, and} \\
 T_{90N} &= T_{90} - 310.
 \end{aligned}$$

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 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 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:

$$\begin{aligned}
 CCI &= \text{Calculated Cetane Index by Four Variable Equation} \\
 D &= \text{Density at } 15^\circ\text{C, g/mL determined by Test Methods} \\
 &\quad \text{D 1298 or D 4052} \\
 T_{10} &= 10 \% \text{ recovery temperature, } ^\circ\text{C, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure} \\
 T_{50} &= 50 \% \text{ recovery temperature, } ^\circ\text{C, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure} \\
 T_{90} &= 90 \% \text{ recovery temperature, } ^\circ\text{C, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure}
 \end{aligned}$$

3.3.1 The equation for Procedure B when  $T_{10}$ ,  $T_{50}$ , and  $T_{90}$  are in  $^\circ\text{F}$  is:

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

where:

$$\begin{aligned}
 CCI &= \text{Calculated Cetane Index by Four Variable Equation} \\
 D &= \text{Density at } 15^\circ\text{C, g/mL determined by Test Method} \\
 &\quad \text{D 1298 or D 4052} \\
 T_{10} &= 10 \% \text{ recovery temperature, } ^\circ\text{F, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure} \\
 T_{50} &= 50 \% \text{ recovery temperature, } ^\circ\text{F, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure} \\
 T_{90} &= 90 \% \text{ recovery temperature, } ^\circ\text{F, determined by Test} \\
 &\quad \text{Method D 86 and corrected to standard barometric} \\
 &\quad \text{pressure}
 \end{aligned}$$

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  $\pm 2$  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  $15^\circ\text{C}$  to the nearest 0.0001 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  $1^\circ\text{C}$ , 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  $15^\circ\text{C}$  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.