Standard Test Method for Calculated Cetane Index by Four Variable Equation

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. Scope

1.1 The calculated Cetane Index by Four Variable Equation provides a means for estimating the ASTM cetane number of distillate fuels from density and 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 used with due regard for its limitations.

1.3 The test method “Calculated Cetane Index by Four Variable Equation” is particularly applicable to Grade I-D and Grade 2-D diesel fuel oils containing straight-run and cracked stocks, and blends of the two. 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 sands and oil shale.

1.4 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
D 613 Test Method for Cetane Number of Diesel Fuel Oil
D 1298 Test Method for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method
D 4052 Test Method for Density and Relative Density of Liquids by Digital Density Meter

3. Summary of Test Method

3.1 A correlation in SI units has been established between the ASTM cetane number and the density and 10 %, 50 %, and 90 % recovery temperatures of the fuel. The relationship is given by the following equation:

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

where:

CCI = Calculated Cetane Index by Four Variable Equation,
D = Density at 15°C, determined by Test Method D 1298,
\(DN = D - 0.85\),
B = \[e^{-3.5xDN} \] - 1,
\(T_{10\%}\) = 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,
\(T_{90\%} = T_{90} - 310\).

3.2 The empirical equation for 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 sands, shale, and coal. The analysis also accounted for bias amongst the individual sets of data comprising the data base.

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. 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 would be...
Part 1 – Estimate Based on Density and D 86 50% Recovery Temperature

Example:

\[ D = 0.885 \text{ kg/L} \]
\[ T_{50} = 274°C \]

Part 1 Estimate = 34.0

Part 2 – Correction for Deviations in Density and D 86 90% Recovery Temperature from Average Values

Example:

\[ D = 0.885 \text{ kg/L} \]
\[ T_{50} = 323°C \]

Part 2 Corr. = +0.6

Part 3 – Correction for Deviations in D 86 10% and 90% Recovery Temperatures from Average Values

Example:

\[ T_{10} = 5°C \]
\[ T_{90} = 323°C \]

Part 3 Corr. = +0.5

5. Procedure

5.1 Determine the density of the fuel at 15°C to the nearest 0.0001 kg/L, 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. The calculation is more easily performed using a computer or programmable hand calculator. Round the value obtained to the nearest one-tenth.

6.1.1 Calculated Cetane Index by Four Variable Equation can also be easily determined by means of the nomographs appearing in Figs. 1 through 3. Figure 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. Figure 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 Figs. 2 and 3 are summed algebraically with the cetane number estimate from Fig. 1 to find the Calculated Cetane Index by Four Variable Equation. The recommended range of application.

4.2 Within the range from 32.5 to 56.5 cetane number, the expected error of prediction 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

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 of that fuel, provided the fuel's source and mode of manufacture remain unchanged.
method of using these nomographs is indicated by the illustrative example shown below and on Figs. 1 through 3.

Measured Fuel Properties

<table>
<thead>
<tr>
<th>Test Method</th>
<th>Property Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>D 613</td>
<td>Cetane Number</td>
<td>37.0</td>
</tr>
<tr>
<td>D 1298</td>
<td>Density at 15°C, kg/L</td>
<td>0.885</td>
</tr>
<tr>
<td>D 86</td>
<td>10% Recovery Temp, °C</td>
<td>234</td>
</tr>
<tr>
<td>D 86</td>
<td>50% Recovery Temp, °C</td>
<td>274</td>
</tr>
<tr>
<td>D 86</td>
<td>90% Recovery Temp, °C</td>
<td>323</td>
</tr>
</tbody>
</table>

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. Precision and Bias

7.1 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.

7.2 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 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.

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

8. Keywords

8.1 cetane; cetane index; diesel fuel