CORRELATIONS BETWEEN DIESEL FUEL PROPERTIES AND ENGINE EMISSIONS

E. LOIS and S. STOURNAS
Fuels and Lubricants Laboratory, National Technical University,
157 73 Zografou, Athens, Greece

ABSTRACT

The oil industry and motor manufacturers are currently facing
similar problems with diesel engines, namely restrictions on fuel
quality for environmental reasons. It would thus be of value if
some of the most important pollutants, such as NOx and particulate
matter (PM), could be predicted from basic fuel properties. This
paper presents expressions from which the cetane number of the
diesel fuel (without additives) and its aromatic content, are
evaluated from the distillation curve and density, with very good
accuracy, the correlation coefficient in the first case being 0.98
and in the latter 0.99. Subsequently NOx and PM emitted for two
types of engines are evaluated, both for hot and cold conditions,
from the fuel aromaticity. This gives a direct measure of the
pollutants as the fuel cetane number varies in the range 25-65,
making it possible to adjust the fuel distillation curve to meet
emission standards.

INTRODUCTION

In diesel fuels the cetane number is a property measured in a
standard CFR engine (1) and for calculation purposes it can be
approximated by methods such as the Calculated Cetane Index (2) or
the Diesel Index (3), both of which are computed from the API
gravity and either the mid-boiling point or the aniline point of
the fuel. More recently, ASTM has introduced a method (4) that
employs three points of the distillation curve, whereas numerous
reports have appeared in the literature (5-7) that rely on
instrumental methods such as NMR and HPLC for the estimation of
cetane number. The reason for this approximation is the necessity
of a rather cumbersome and expensive engine test for   the
measurement of the cetane number, which describes accurately the
fuel ignition behavior. It would thus be of value if a simple
method is developed to calculate the actual cetane number of a
gasoil from other characteristics less troublesome to measure. A
simple method was developed here, which accurately predicts the
cetane number from five points of the distillation curve, i.e. the
initial boiling point, the 10%, the 50%, 90% and end point, the density
and aromaticity of the fuel.
An effort was also made to predict the fuel aromaticity from
the distillation curve and the density, making the evaluation of
the cetane number dependent only on these two properties. The fuel
aromaticity is important since it influences directly or indirectly
many other specifications. If one examines the nature of the
aromatic components found in gasoils (8), it is easy to see the
diverse nature of the various aromatic, alkylaromatic or poly-
aromatic components, whose molecular weights and structures are
such that they span the entire boiling point range of the middle

distillate fuels. The concentrations of each aromatic family also varies in each distillation fraction without following a specific pattern. The conclusion of this approach was that the prediction of the aromatic content depends on the method used to evaluate it. Accurate predictions were made following this method, whereas a global prediction effort was less successful.

Finally, we have attempted to correlate the cetane number with engine emissions. The emittants are directly dependent not only on the fuel specifications, but also on the type of engine used and the running conditions (9-12). Our effort was to correlate some of the most important emittants, i.e. NOx and particulate matter for hot and cold conditions, for two types of engines, a Detroit diesel engine of 315 hp (9), and a Cummins diesel engine of 400 hp (9). NOx and particulate emission values were obtained from the fuel aromatic content and the 90% point of the distillation curve, from equations refering to the above engines (5). The value of such correlations lies in the fact that given the level of the emittants set by regulations, and the dependence of the cetane number on the distillation curve and density, the refinery can adjust the distillation curve to meet these regulations for specific types of engines.

CETANE NUMBER

The parameters chosen to predict the cetane number were the fuel aromaticity, the distillation curve and the density. Other parameters such as viscosity, sulfur content etc., were excluded from the calculation since they did not seem to affect the results further.

For this reason a matrix of 26 fuels was analysed, Table 1. None of the fuels considered contained any additives and the distillation characteristics were measured either according to the IP or the ASTM standards (8, 13-15).

The relationship found to describe the cetane number best is the following:

$$\text{Cetane Number} = a.IP + b.D10 + c.D50 + d.D90 + e.(1/EP)$$
$$+ f.(1/DENS^2) + g.(1/AROM^4) + h \qquad (1)$$

where, IP = Initial boiling point, $^\circ$C
Dn = n% vol. recovered, $^\circ$C
EP = End boiling point, $^\circ$C
DENS = Specific gravity, 15/4 $^\circ$C
AROM = Aromatics, wt%
and,
a = -0.011
b = 0.092554
c = 0.119366
d = 0.130821
e = 7083.031
f = 110.258
g = 16096.35
h = -219.705

The correlation obtained between the measured and the calculated cetane number (r = 0.983) was good, where in over 92% of the cases the error was less than 5%, and for the rest 8% of the

points the error was less than 6%. In absolute numbers, the calculated cetane number of 24 of the fuels was within two units of the experimentally determined value, i.e within the accuracy limits of the measuring method; the maximum error in the other two fuels was 2.9 units. It is worth noting that ASTM D-976 estimations of the same 26 fuels fall within two units in only eleven of the cases, and the maximum error is in excess of five cetane number units. The results are depicted in Figure 1.

FUEL AROMATICITY

The aromaticity of fuels 1-8, Table 1, was measured using the FIA method (IP Method No 156/70) (8) whereas the aromatic content of fuels 9-16 was evaluated using the HPLC method (14); the method employed for the rest of the fuels was not specified (15). The equation found to fit best the data of the 26 fuels was the following:

$$AROM = a.IP + b.D10 + c.(d50)^{0.5} + d.D90 + e.EP + f.(1/DENS^2) + g \qquad (2)$$

where, a = -0.25931
       b = 0.514474
       c = -13.157
       d = -0.03947
       e = 0.059787
       f = -166.654
       g = 400.452

The results are shown in Figure 2, and the correlation coefficient between the measured and the calculated aromatic fuel content would not exceed 0.91, regardless of the number of points selected from the distillation curve. The high degree of scatter of the results does not allow an accurate estimate of the aromatic content.
However, much better results were obtained if one considers the results of each individual method separately, even in the case that only one point was selected to represent the distillation curve, Figure 3. The equations used to evaluate the aromaticity content are the following:

$$AROM\ wt\% =\ \ 236.323x10^{-3}xD50 + 396.9xDENS \qquad (3)$$
$$AROM\ wt\% = -144.17\ x10^{-3}xD50 + 583.6xDENS \qquad (4)$$

It is worth mentioning that in both cases very good results were obtained, irrespective of the point selected from the distillation curve, the correlation coefficients being always at least 0.99.

ENGINE EMISSIONS

The equations set forward for two types of engines (9), a Cummins NTCC 400, six cylinder engine, 14 liter displacement, direct-injection, in-line, turbocharged, intercooled, rated power 400 hp at 2100 rpm, and fuel consumption of 153 lb/hr and a Detroit diesel DDC 60-11-315, six cylinder engine, 11 liter displacement, in-line, direct injection, turbocharged, intercooled, rated power

315 hp at 1800 rpm, and fuel consumption of 105 lb/hr, were utilized in this analysis:

Cummins   PMCS(g/hp-hr) = 0.436563 + 5.375x10^{-3}x(%Aromatics) (5)
           PMHS(g/hp-hr) = 0.370001 + 3.947x10^{-3}x(%Aromatics) (6)
           NOxCS(g/hp-hr)= 3.911810 + 11.89x10^{-3}x(%Aromatics) (7)
           NOxHS(g/hp-hr)= 4.28257 + 12.7932x10^{-3}x(%Aromatics) (8)

DDC   NOxCS(g/hp-hr)= 9.3563 + 28.5266x10^{-3}x(%Aromatics)
                        -88.5758x10^{-4}x(90% Boiling point)   (9)
           NOxHS(g/hp-hr)= 6.45922 + 26.8833x10^{-3}x(%Aromatics)
                        -43.0576x10^{-4}x(90% Boiling point)   (10)

where   PMCS = Particulate Matter Cold-Start
        PMHS = Particulate Matter Hot-Start
        NOxCS = NOx Cold-Start
        NOxHS = NOx Hot-Start
        g/hp-hr = gram per brake horsepower-hour

    The data from Table 1 were applied to the above equations, and the results obtained are depicted in Figures 4-6. It can be seen that for the two engines, as the cetane number increases in the range 25-65, both NOx and particulate matter decrease, irrespective of hot or cold conditions. An equation of the type

$$y = a.exp(-b.CN) \tag{11}$$

where CN is the fuel cetane number, was found to fit reasonably well the points of the above figures. The values of a and b for the various emittants are listed in Table 2.

CONCLUSIONS

    Equations were presented which predict the gasoil aromatic content from the density and the distillation curve, and its cetane number from the density, aromaticity and the distillation characteristics.
    Subsequently the cetane number was correlated to NOx and particulate emittants for two types of engines, making it thus possible to adjust the fuel characteristics to meet current or future legislation.

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TABLE 1. THE FUEL MATRIX

NO OF FUEL	CETANE NUMBER	AROM wt%	DENSITY gr/cm³	IP °C	D10 °C	D50 °C	D90 °C	EP °C
1	50.6	19.43	0.8438	197	230	279	329	355
2	65.1	8.18	0.8170	220	253	274	308	322
3	47.9	25.70	0.8557	214	245	292	346	364
4	47.2	34.94	0.8727	220	248	297	346	364
5	38.0	44.63	0.8917	220	257	299	345	368
6	37.3	54.87	0.9137	220	266	303	349	368
7	28.1	66.36	0.9471	257	280	310	351	368
8	45.0	32.00	0.8722	231	257	286	330	351
9	56.0	23.80	0.8230	191	219	255	322	348
10	57.0	28.20	0.8392	192	243.5	295.5	349	369
11	57.0	34.60	0.8570	211	270	320.5	366.5	393
12	58.0	37.80	0.8647	230	288.5	329	369	398
13	30.0	65.30	0.8996	175	236	273	312.5	335
14	34.0	59.70	0.8884	180	239	275	315	337
15	40.0	54.20	0.8764	184	241.5	276.5	317	338
16	44.0	45.00	0.8640	193	245	279.5	318	340
17	34.3	48.40	0.8486	83	165	221	304	350
18	39.7	31.70	0.8331	112	166	220	303	346
19	44.8	15.50	0.8181	138	166	220	302	346
20	35.0	53.00	0.8683	71	176	251	328	359
21	39.1	40.10	0.8532	72	178	250	328	359
22	44.6	26.80	0.8380	76	177	250	328	359
23	35.1	58.90	0.8931	107	201	285	340	358
24	39.8	47.70	0.8825	126	211	285	342	368
25	44.2	38.90	0.8641	108	209	291	341	367
26	45.5	24.70	0.8522	172	221	263	312	340

TABLE 2. VALUES OF THE CONSTANTS a and b

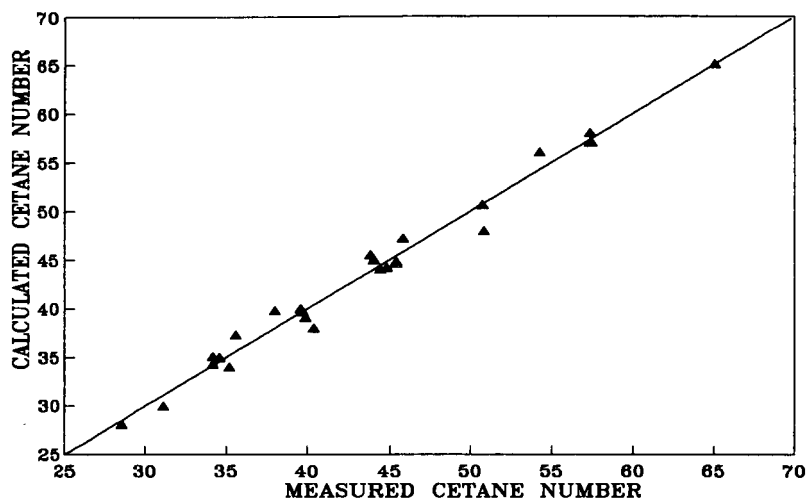|		**a**	**b**
Cummins	PMCS	1.127440	0.0118222
	PMHS	0.876955	0.0109310
	NOxCS	5.27345	0.0039207
	NOxHS	5.74554	0.0038658
DDC	NOxCS	7.69730	0.0096137
	NOxHS	7.21377	0.0086266

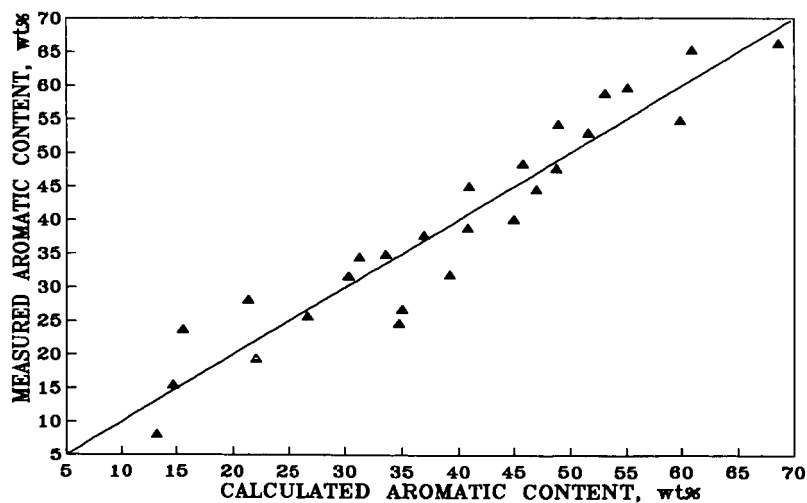**FIGURE 1.** *Calculated vs. Experimental Cetane Number*

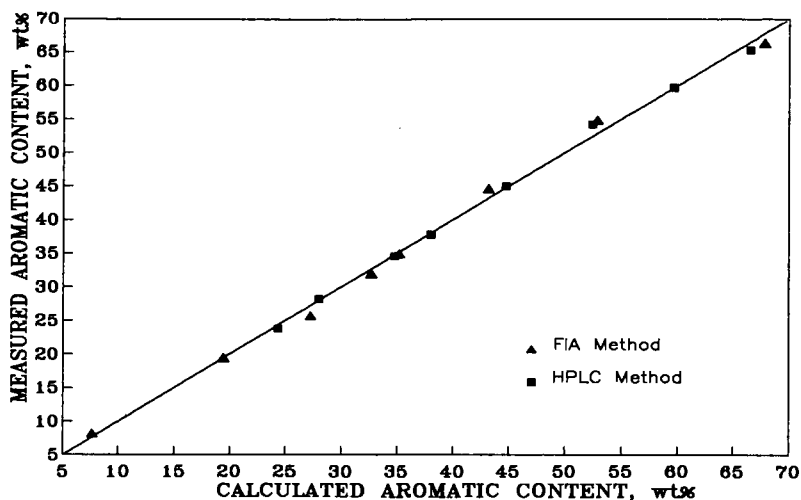**FIGURE 2.** *Calculated vs. Experimental Aromaticity*

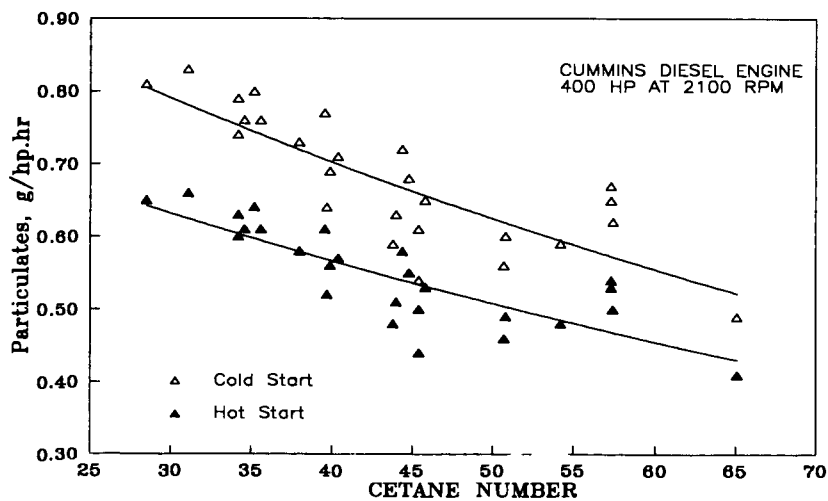**FIGURE 3.** *Calculated vs. Experimental Aromaticity, with the method of measurement taken into account*
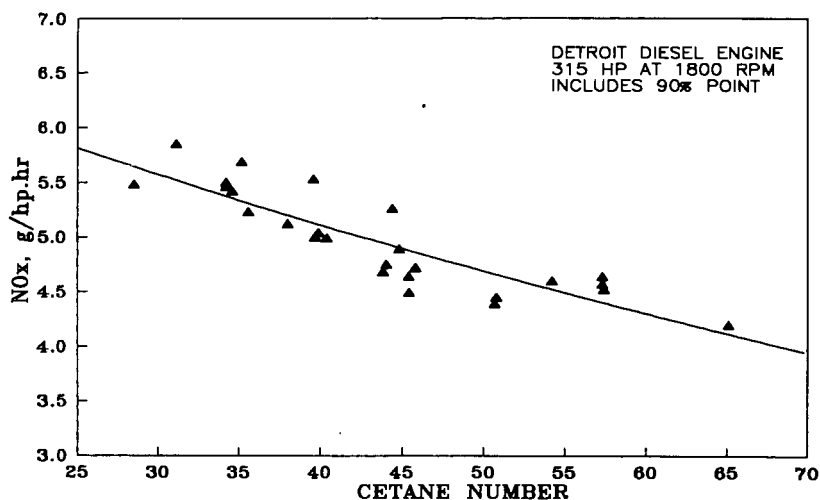

FIGURE 4. *Particulate Emissions*
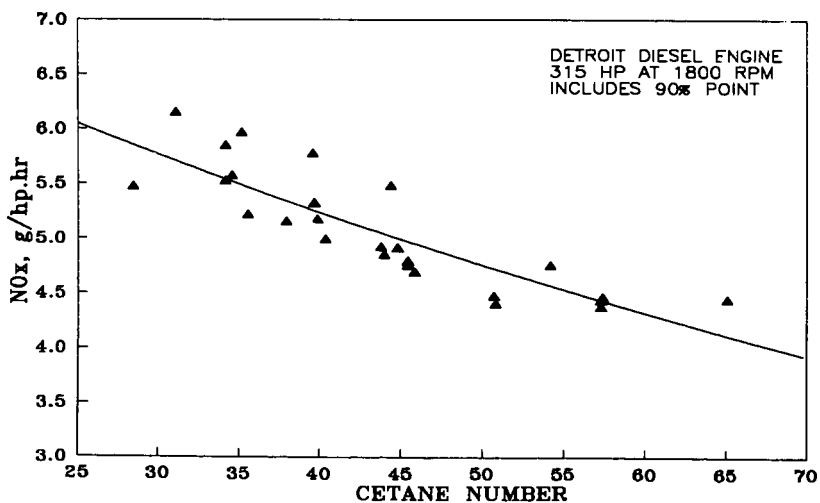
FIGURE 5. *NOx Emissions (Hot Start)*

FIGURE 6. *NOx Emissions (Cold Start)*