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Engine Systems Division

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ABSTRACT

The effects of cetane number, total aromatic content and density of diesel fuels on diesel NOx emissions were investigated. Over 20 fuels were studied in a DI diesel engine running steady-state simulation of the U.S. EPA transient test. The composite NOx emissions showed a decrease of about 5% when the cetane number was increased from 44 to 64. The cetane number affected NOx emissions mainly at light load conditions, by reducing the amount of fuel burned in the premixed burning. At the same cetane number rating, the composite NOx emissions increased when total aromatic content and fuel density were increased. The effects of total aromatic content and density were more apparent at heavy load conditions. Higher flame temperatures associated with higher aromatic content and advanced injection caused by higher fuel densities are two possible reasons for the higher NOx emissions.

INTRODUCTION

To meet the progressively more stringent emission regulations, increasing attention has been devoted to the effect of fuel properties on exhaust emissions in diesel engines. It is generally accepted that engine efficiency and exhaust emissions are defined by engine design and operation, but influenced by fuel properties. A knowledge of the interaction between engine operation and diesel fuel properties will benefit both engine designers and fuel producers in their effort to produce engines and fuels that can work together to meet new emission standards.

The general approach in fuel property study is to blend fuels so that a single fuel property can be varied in a large range while maintaining the other fuel properties within a narrow span. This task is always challenging and sometimes impossible. Consequently, most of the studies to investigate the influence of fuel properties on diesel emissions are biased by the specific fuel matrix design and by the inter-correlation between the fuel properties. The key to avoid this problem is a careful fuel matrix design and the ability to blend and test a large number of fuels. In this study, over 20 fuels in three fuel matrices were investigated. The effects of cetane number, total aromatic content and density on NOx emissions were assessed individually.

One of the disadvantages of running transient emission tests is that it is not possible to differentiate the contributions of different operating conditions to exhaust emissions. Some of the engine operating conditions are more sensitive to fuel properties than some others. In this study, a steady state simulation of the U.S. EPA transient test procedure was used. The emission test results were therefore linked to the results obtained from the U.S. EPA transient test. At the same time, the engine test results from different engine operating conditions offered detailed information so that the influence of each fuel property on NOx formation at different engine operating conditions can be investigated.

EXPERIMENTAL

Engine and Operating Conditions

The engine used in this study is a single-cylinder research version (Ricardo Proteus) of a Volvo TD123 heavy-

Table 1 Research engine configuration

Engine Type	Ricardo Proteus (replicates one cylinder of Volvo D123)
Bore	130.2 mm
Stroke	150.0 mm
Number of Cylinders	1
Displacement	1.997 litres
Combustion Chamber Type	Toroidal Bowl
Compression Ratio	17:1
Number of Valves/Cylinder	2
Injection Type	Direct Injection
Fuel Injection Pump	Bosch PE6P 120A 320RS8011
Injection Pressure (Typical)	120 MPa
Fuel Injection Nozzle	Bosch DLLA 152 P 285
Maximum Power Output	44.67 kW (60 bhp) @ 1900 rev/min

Table 2 AVL 8-mode steady-state simulation of U.S. EPA transient test procedure

Mode	Speed (rpm)	Load (%)	Weighting Factor
1	600	0	35.01
2	743	25	6.34
3	873	63	2.91
4	1016	84	3.34
5	1900	18	8.40
6	1835	40	10.45
7	1835	69	10.21
8	1757	95	7.34

duty truck engine. The engine is a direct injection type and has a displacement volume of 2 litres. Major engine configuration data are shown in Table 1. The research engine incorporates many features of contemporary medium- to heavy-duty diesel engines. It is tuned to meet the U.S. EPA 1994 emission standards. Detailed information on the test engine can be found in [2] and [3].

The test procedure used in this study was an eight-mode steady-state simulation of the U.S. EPA transient test procedure. This test procedure was developed by AVL [1]. The engine operating conditions and the weighting factors are listed in Table 2.

For all test fuels, the speed and the load at each mode were kept the same. Therefore, discrepancies in the amount of fuel per cycle supplied to the engine should be eliminated for fuels having different densities. It was noticed in the experiments that fuels having different densities still had slightly different injection timing and duration due to the differences in density and bulk modulus of elasticity.

To check the repeatability of the emission measurements, the fuel Ref2 (Table A-2) was run in the engine periodically. The results showed that the standard deviation of NOx emission measurements was 0.92% of the mean. The difference between the maximum and the minimum NOx emission measurements was 2.84% of the mean. The error was of a random nature. Therefore, the experimental data obtained with all other test fuels were not adjusted for engine shift or experimental system error.

Test Fuels

Among the three fuel matrices tested, two of them were blended using refinery streams and fuel additives. One fuel matrix was blended by adding cetane improvers into the base fuel Ref1 (Table A-2). The maximum amount of cetane improver used was 1% by volume, achieving the maximum cetane number of 64.1. In this fuel matrix, cetane number rating was the only fuel property that was varied. The other fuel properties such as total aromatic content and density remained virtually the same.

The second fuel matrix were blended using refinery streams (Table A-1). A total of 22 components obtained from seven refineries were used in this fuel matrix. The parameters controlled in this fuel matrix were:

- total aromatics (10, 20 and 30% by mass)
- sulphur content (<500 ppm by weight)
- cetane number (42 to 46)
- viscosity, cloud point and distillation properties (within the typical range of current commercial diesel fuels in Canada).

In this second fuel matrix, total aromatic content was varied intentionally in a wide range. Subsequently, the density of the blended fuels also varied. Cetane number was controlled in a narrow range. The properties of these fuels are listed in the appendix together with the reference fuels Ref1 and Ref2.

To investigate the effect of aromatics on exhaust emissions, it is crucial to measure aromatics accurately. In this study, four different methods were used to characterise the test fuels. These methods include Supercritical Fluid Chromatography (SFC), High Performance Liquid Chromatography (HPLC), Hot Fluorescent Indicator Analysis (FIA) and Gas Chromatography/Mass Spectroscopy (GC/MS).

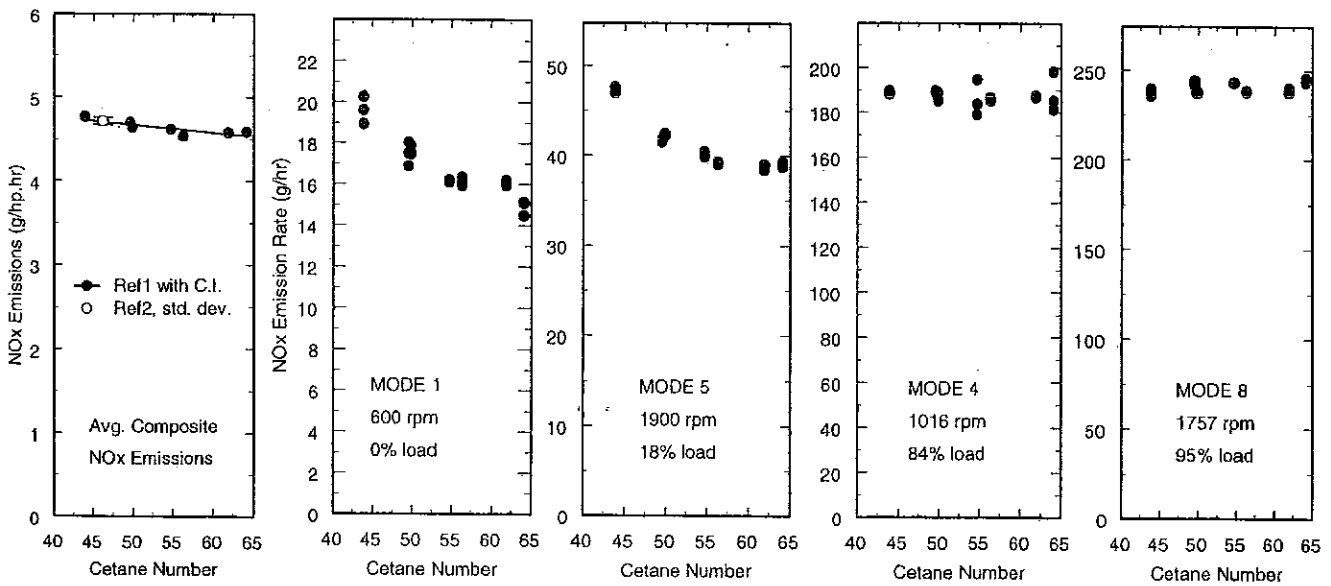

Figure 1 The NOx emissions versus cetane number, averaged composite emissions and emission rates at four individual modes

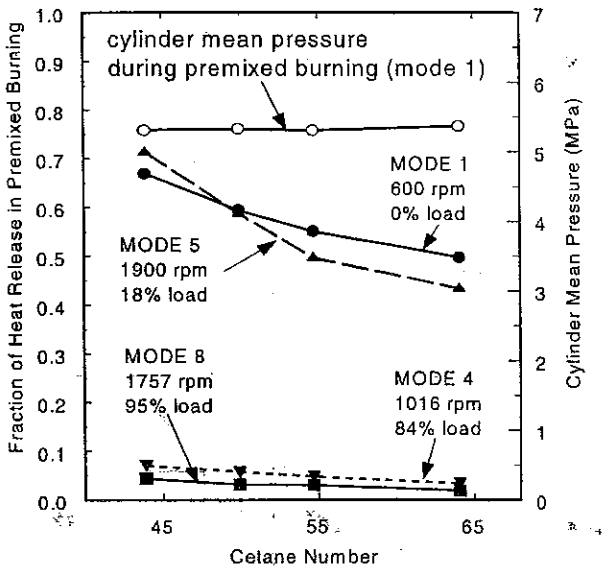

Figure 2 Fraction of heat release during the "premixed burning" period at light and heavy load conditions

The four methods yielded total aromatic contents that correlated well with each other. The correlation coefficients ranged from 0.996 to 0.999. Using total aromatic contents measured by any of the methods should yield the same conclusion when assessing the impact of total aromatics on engine emissions. In this paper, SFC data were used for all the analyses.

The third fuel matrix contained fuels obtained from different sources (Table A-2). These fuels were used to test the regression models generated using the fuel blends listed in Table A-1.

RESULTS AND DISCUSSIONS

Effect of Cetane Number

In the first fuel matrix, the only fuel property that changed widely is the cetane number. Figure 1 shows the averaged composite NOx emissions and the NOx emission rates at four different modes as functions of cetane number. These four modes represent typical operating conditions at the extremes of the speed and the load.

When the cetane number of the reference fuel Ref1 was increased from 44 to 64 by adding cetane improvers, the composite NOx emissions were reduced by about 5%. The NOx reduction occurred at light load engine operations, such as mode 1, 2 and 5 (modes 1 and 5 are shown in Figure 1). At medium and heavy load conditions, modes 3, 4, 6, 7, and 8, cetane number had no effect on NOx emissions regardless of the speed (modes 4 and 8 are shown in Figure 1).

The ignition delays at all modes were reduced when cetane number was increased from 44 to 64. However, the effect of cetane number on the heat release curve differed for the light-load and the heavy-load conditions. Figure 2 shows the fraction of heat release during the "premixed burning" period for individual modes. It should be noted that the heat release analysis did not consider heat loss to the cylinder walls [4]. At light load conditions, the major heat release occurred in the premixed burning period, contributing more than 50% to the total heat release. At heavy load conditions, the premixed burning comprised only about 5% of the total heat release.

Nitrogen oxides form in high temperature regions. During the premixed burning period, the rapid heat release inevitably generates regions with high temperatures. The NOx emission from the test engine at light load conditions came mainly from the premixed burning. When fuel cetane number was increased, the averaged pressure during the premixed burning changed less than 1% (Figure 2 shows the mean pressure for mode 1). This indicates that the combustion event did not change substantially even though its timing relative to crank angle position was shifted about two degrees. What changed substantially was the amount of fuel that was consumed in the premixed burning period. When the cetane number was increased from 44 to 64, the NOx emissions can be reduced by as much as 20% at light load conditions (Figure 1).

When cetane number was increased, the premixed fraction of heat release was reduced substantially at heavy load conditions. Since the NOx formed during this period constitutes only a small portion of the total NOx emissions at these conditions, the effect of cetane number becomes insignificant.

Effects of Total Aromatic Content and Fuel Density

In the second fuel matrix, cetane number of the 12 fuels were controlled in a narrow range, whereas the total aromatic content of the fuels varied substantially. The densities of the test fuels in this matrix were not controlled. The correlation coefficient between density and the total aromatic content is 0.67.

The averaged composite NOx emissions and the NOx emission rates are shown in Figure 3 versus total aromatic content and fuel density. The results at modes 1 and 5 are typical of those obtained with light load conditions, and results at modes 4 and 8 are typical of those obtained with medium to heavy load conditions. The composite NOx emissions increased with the increase in total aromatic content and fuel density. This increase occurred mostly at medium to heavy load conditions. The effect of total aromatics or fuel density on NOx emissions at light load conditions was not significant.

The fuel density generally affects the fuelling rate when conducting transient tests. If all the test fuels are run using the same power curve that is generated from a reference fuel, the fuel with a higher density will run at a higher fuelling rate on mass basis. This fuelling discrepancy can bias emission comparison between fuels. In this study, steady-state tests were conducted, and the power outputs of all the fuels were kept the same. This minimised the fuelling discrepancy between the test fuels. The specific fuel consumption changed less than 1% and was not a function of density.

The fuel density, however, affects the fuel injection timing and rate. At the same timing setting, the start of injection of the fuel with a higher density is slightly advanced. In this study, an advance of about 0.5 crank angle degree was observed among the 12 fuels. An injection advance of 0.5 crank angle degree corresponds to a change of 3% in composite NOx emissions between the heaviest and the lightest fuels [5].

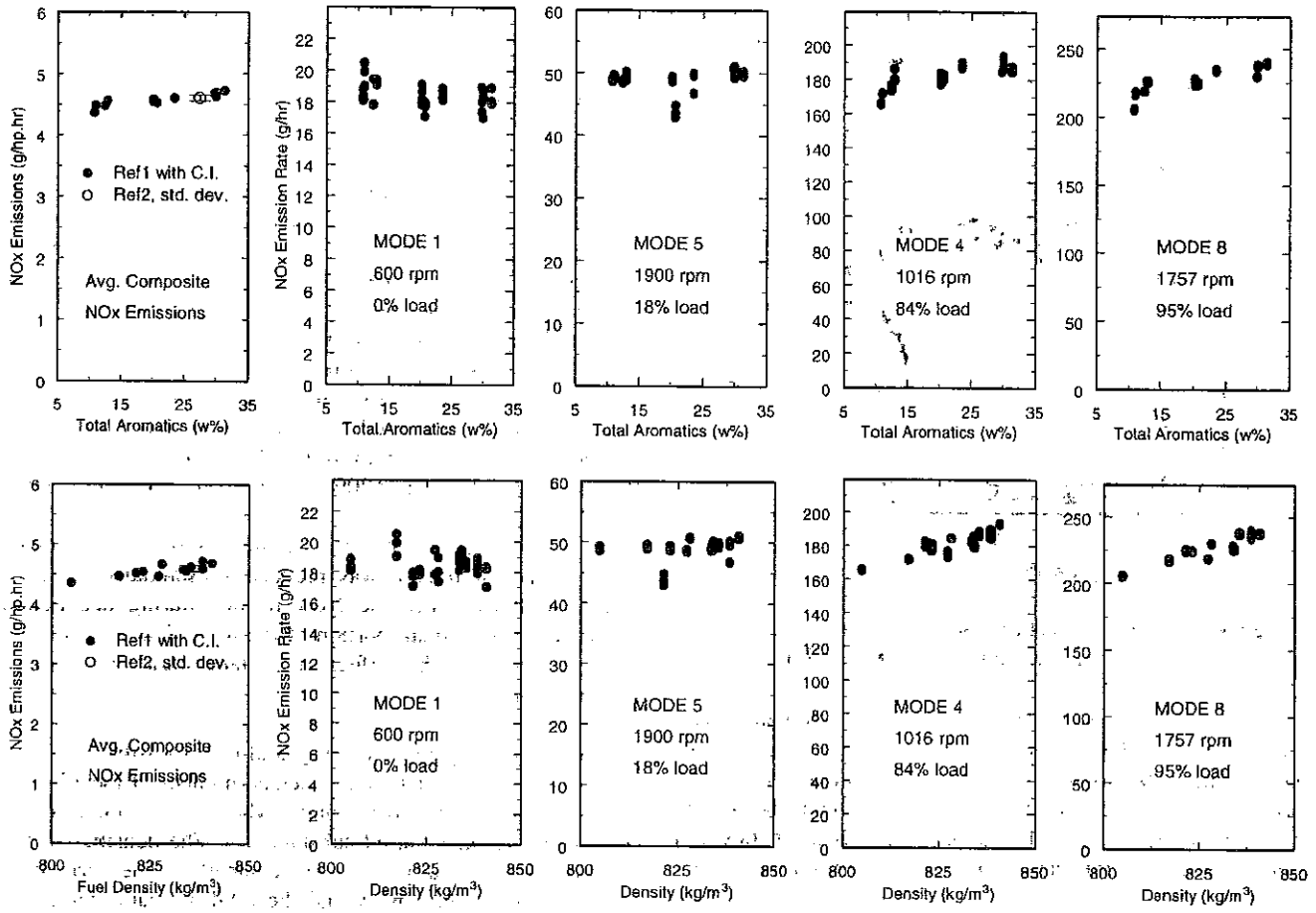

Figure 3 Effects of total aromatics and density on NOx emissions

The fuel injection rate on a mass basis for a heavier fuel is higher, but the duration is shorter. This becomes more significant at heavy load condition due to the longer injection duration. At heavy load conditions, a major part of the fuel was injected and consumed during the mixing controlled burning period. Between the heaviest and the lightest fuels, a 4% difference was observed in the mean cylinder pressure that was averaged from the start of mixing controlled burning to the end of fuel injection. This indicates that a higher injection rate causes more fuel to be injected into the high temperature region, leading to higher NOx emissions. However, the extend of this effect could not be assessed from the available data.

The composite NOx emissions increased when the total aromatic content in the fuel was increased. The correlation between fuel aromatic content and the NOx emissions is more evident at medium to heavy load conditions (see Figure 3). At these conditions, major portion of the fuel was burned at fuel-rich locations where the chemical composition of the fuel is likely to have an impact on the local gas temperature. The fuel with a higher total aromatic content can be expected to generate a higher temperature in these fuel-rich regions because the adiabatic temperatures of the hydrocarbons with ring structures tend to be higher. A higher local peak temperature could be the cause for higher NOx emissions for fuels having higher total aromatic contents.

To estimate the effects of fuel density and total aromatic content, regression analysis was performed on the corrected composite NOx emissions. Small differences on NOx emissions were corrected for the cetane number (reference 44) and the injection timing (reference fuel C20B) [5]. The fuel properties considered in the regression analyses were: density, viscosity, T90, T50, T10, total aromatic content, and poly-aromatic content (di+-aromatics). The highest correlation of these fuel properties, 0.776, is between T50 and viscosity. Some degree of correlation between total aromatic content and poly-aromatic content is also observed with a coefficient of 0.714.

The total aromatic content and the fuel density are found to be the two significant variables in the regression analysis. Between the two variables, total aromatic content contributes more than the fuel density to the changes observed in NOx emissions among the 12 fuels (see Table 3). The combined effects of these two variables account for 93% of the changes in NOx emissions.

Table 3 Regression analysis of corrected composite NOx emissions

Variable	Standard Error	Standard Coefficient	F-Value	Probability	R^2
Total Aromatics	0.0016	0.5964	24.48	0.0008	0.93
Density	0.0012	0.4559	14.31	0.0043	

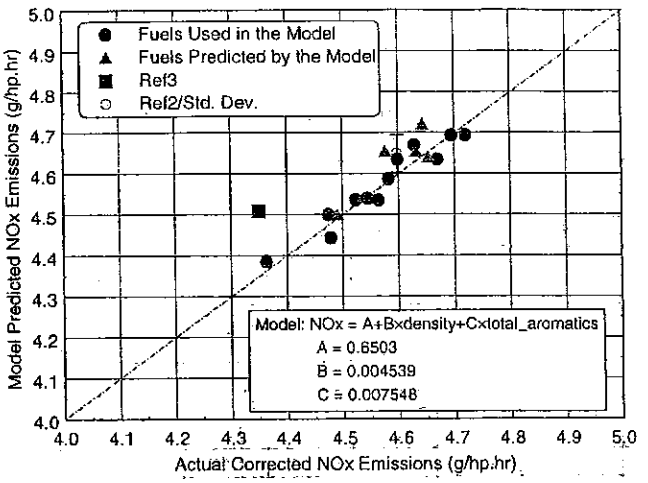

Figure 4 Regression model for NOx emissions

To further evaluate the regression results, the model was used to predict the NOx emissions of seven test fuels that was not included in generating the regression model (Table A-2). The results are shown in Figure 4. The model predicts the NOx emission results well for six of the seven fuels that have similar properties with the 12 test fuels. The model prediction is 3.8% higher for fuel Ref3. This fuel had substantially different properties including higher density, higher cetane number and lower total aromatic content. The fact that the regression model is able to predict the NOx emissions for other fuels indicates that total aromatic content and fuel density are indeed two important fuel properties affecting NOx emissions.

It should be noted that density and total aromatic content in this test fuel matrix are correlated to a certain degree (correlation coefficient 0.67). Their individual effects on NOx emissions are not certain. Further studies where fuel density is de-coupled from the total aromatic content are in progress.

CONCLUSIONS

In this work, we investigated the effects of cetane number, total aromatic content and density of diesel fuels on NOx emissions. Our results lead to the following conclusions:

- Different fuel properties influence NOx emissions at different engine operating conditions. Increasing cetane number reduced NOx emission at light load conditions, whereas increasing fuel density and total aromatic content increased NOx emissions at medium to heavy load conditions.
- The effect of cetane number is mainly physical. Increasing cetane number reduced the amount of fuel burned in the premixed burning. At medium to higher loads, NOx emissions were not affected by cetane number. At light loads, NOx emissions could be reduced by as much as 20% when cetane number was increased from 44 to 64.
- Fuel density changes the injection timing and the mass injection rate. Even under steady-state engine tests, density was found to correlate with NOx emissions.
- The effect of total aromatic content on NOx emissions is likely to be a chemical one. The higher flame temperature associated with aromatics in the fuel-rich regions could be a cause for higher NOx emissions. Reducing total aromatic content from 30% to 10% without changing other fuel properties could reduce NOx emissions by about 5%.

ACKNOWLEDGEMENT

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APPENDIX

Table A-1 Properties of blended diesel fuels

FUEL ID	S10A	S10B	S20A	S20Bn1	S30An5	S30Bn1	C10A	C10B	C20A	C20B	C30A	C30B
Density, kg/m^3 @15°C	827.2	834.2	833.6	838.4	840.8	838.4	804.9	817.1	821.4	823.1	835.4	828.1
Viscosity @40°C, cSt	1.65	2.14	1.7	1.92	1.81	1.73	1.62	2.01	1.97	1.66	2.18	1.70
Cloud Point, °C	-44	-27	-26	-25	-28	-33	<-70	-27	3	-39	-10	-37
Distillation, D86, IBP, °C	155.0	158.5	156.5	156.5	170.5	170.5	189.5	201.5	187.0	173.5	178.5	175.5
T10, °C	175.5	183.0	181.0	179.0	185.0	186.5	200.0	207.5	191.0	194.0	198.5	198.5
T50, °C	217.5	244.0	224.0	232.0	222.5	224.5	212.5	221.5	223.0	219.5	244.0	231.0
T90, °C	286.0	317.0	284.5	323.5	324.0	301.5	242.0	285.5	335.0	272.0	317.0	268.0
EP, °C	313.5	344.5	310.5	348.5	347.5	334.5	284.5	320.5	379.0	315.0	352.0	301.0
Cetane In., D976-80	41.0	46.8	40.9	41.8	37.9	39.5	47.4	46.1	45.0	43.2	46.5	45.1
Cetane No. D613	41.0	43.4	40.2	42.9	42.3	42.0	40.4	41.6	46.5	41.9	43.9	44.2
Sulphur, ppm (mass)	13.2	2.4	28.8	31.1	84.7	3.0	8.1	131	31.4	134.0	270.0	202.0
Hydrogen Content m%	13.75	13.73	13.49	13.42	13.08	13.16	14.18	14.13	13.72	13.68	13.28	13.40
Nitrogen, ppm (mass)	27.9	0.3	56.4	1.5	24.8	2.5	1.0	17.5	4.7	19.7	41.2	21.8
SFC												
Total Aromatics, %m	12.4	12.9	20.2	23.5	30.0	31.4	10.8	11.0	20.7	20.2	30.0	29.8
Mono-Aromatics m%	10.9	9.5	17.9	20.2	25.2	27.4	9.6	7.8	16.0	16.8	22.1	25.1
Di-Aromatics m%	1.5	2.9	2.2	2.7	4.3	3.6	1.1	2.9	4.3	3.2	7.1	4.4
Tri+-Aromatics m%	0.0	0.5	0.1	0.5	0.6	0.3	0.1	0.3	0.3	0.3	0.8	0.3
HPLC												
Total Aromatics, %m	11.7	12.0	20.0	22.8	32.1	31.3	10.4	10.2	20.0	19.8	29.6	30.2
Mono-Aromatics m%	11.2	10.0	19.0	20.9	29.6	28.8	9.7	8.2	16.8	17.4	24.0	26.9
Di-Aromatics m%	0.5	1.5	1.0	1.3	1.9	2.2	0.7	1.7	2.8	2.2	5.0	3.0
Tri+-Aromatics m%	<0.1	0.5	<0.1	0.6	0.6	0.3	<0.1	0.3	0.4	0.2	0.6	0.3
Hot FIA												
Aromatics, %v.	10.3	10.6	17.3	20.8	27.8	27.6	8.7	9.2	17.4	17.7	25.0	25.4
Olefins, %v.	2.0	2.0	1.9	2.3	2.9	2.3	1.9	2.4	1.8	2.4	1.6	2.7
Saturates, % v.	87.7	87.4	80.8	76.9	69.3	70.1	89.4	88.4	80.8	79.9	73.4	71.9
GC/MS												
Total Aromatics m%	11.1	12.3	19.7	22.3	30.5	30.2	10.2	10.2	19.9	19.4	28.8	28.8
Mono-Aromatics m%	9.8	9.3	17.6	19.2	26.4	26.2	9.1	7.3	15.5	15.7	21.6	24.5
Di-Aromatics m%	1.2	2.7	2.0	2.8	3.8	3.9	1.1	2.8	4.3	3.6	6.9	4.2
Tri+-Aromatics m%	0.0	0.2	0.0	0.1	0.1	0.1	0.0	0.1	0.1	0.1	0.3	0.1

Table A-2 Properties of other test diesel fuels

FUEL ID	Ref1	Ref2	Ref3	A	C	E	F
Density, kg/m^3 @15°C	836.2	835.0	842.0	829.7	841.0	836.8	857.3
Viscosity @40°C , cSt	2.135	2.207	4.03	1.752	1.723	1.439	2.464
Cloud Point, °C	-22	-19	-6				
Distillation, D86, IBP,	178.5	172.9	175.5	166	170	170	170
T10, °C	205.6	198.9	244.8	183	185	183	189
T50, °C	245.5	255.9	297.8	220	224	209	245
T90, °C	306.1	311.4	333.8	284	284	251	344
EP, °C	343.3	336.7	352.6	317	313	282	378
Cetane In., D976-80	46.6	49.7	55.5	40.7	38.0	34.2	39.5
Cetane No. D613	43.9	46.2	55.4	45.8	43.5	40.3	43.1
Sulphur, ppm (mass)	287.0	351.0	9.2	466	460	374	299
Hydrogen Content m%	13.38	13.37	13.95	13.78	13.28	13.29	13.19
Nitrogen, ppm (mass)	54.1	42.9	2.5				
SFC							
Total Aromatics, %m	27.3	27.5	4.8	10.8	24.5	25.2	23.5
Mono-Aromatics m%	21.8	19.9	4.0	6.5	17.8	20.4	11.4
Di-Aromatics m%	4.9	6.7	0.7	3.6	6.2	4.7	8.6
Tri+-Aromatics m%	0.5	1.0	0.1	0.7	0.5	0.1	3.6