Performance and Emissions

Each of the test fuels was run in the VCR engine at five different conditions, representative of rated torque, rated power, and part loads at the rated power speed. The basis for selection of these conditions was an extensive engine mapping done early in this project to define the rated torque point, rated power point, and the timing settings for both the best torque and for the equivalent of a 5-gM/hp-hr NOx level. To review, the test conditions were defined as follows:

Mode 1	Condition is representative of rated torque speed and overall equivalence ratio, using an injection timing (3° BTDC) for the controlled NO_x condition on a baseline diesel fuel.
Mode 2	Includes the same speed and load conditions as Mode 1, but using the best torque injection timing for each test fuel.
Modes 3-5	Rated power and part load conditions at the rate power speed, using a fixed timing of 3° BTDC.

The engine settings for the five modes were given in Table 6.

Normally, the results of engine studies of fuel effects on performance and emissions are dominated by variations in the engine test conditions — in particular, speed, load, and ignition timing. The data obtained in this study are separated into five data sets that can be treated independently, thereby eliminating the dominance of the engine conditions in the results.

Preliminary Examination – We initially developed scatter plots showing the relationships among the dependent variable and each of the independent variables. Statistical analysis of the data sets indicated that fuel properties do play a role in most of the engine performance and emissions characteristics measured. In some cases, the majority of the variation of these characteristics could be related to the fuel properties. In many other cases, however, only a portion of the variations were accounted for in the fuel properties, and the rest of the variations were due to the fact that the effects were small and experimental error becomes a more significant factor.

Power – Our analysis of the power in a given data set (Mode) indicated that the power was not a very strong function of the fuel properties. The scatter plots did indicate that the power within a Mode was directly related to the combustion efficiency of the fuel, as shown in Figure 28 for Mode 1. These results, indicated graphically and in linear regression analysis, showed that the variations in power within a given mode were not highly correlated with the fuel properties.

CO Results – The behavior of CO emissions was very similar to the power data, at least in the higher power modes, where the emissions levels were related more strongly to the combustion parameters than to the fuel properties, within the data sets for each Mode. The power in these experiments was fixed within some range of variation that depended on minor variations in the combustion process. The power settings were defined based on fixed overall air-fuel ratios held constant for all tests within the given Mode. It appears that of the fuels that would actually run in the engine, the properties of the fuel must be within a range of acceptability that produces similar results in the global performance parameters, such as the power and the CO emissions. At the lighter load conditions, the initial statistical analysis indicated that the fuel properties did play a role in the CO emissions, with the boiling-point distribution and the aromatic structure playing the most important roles.

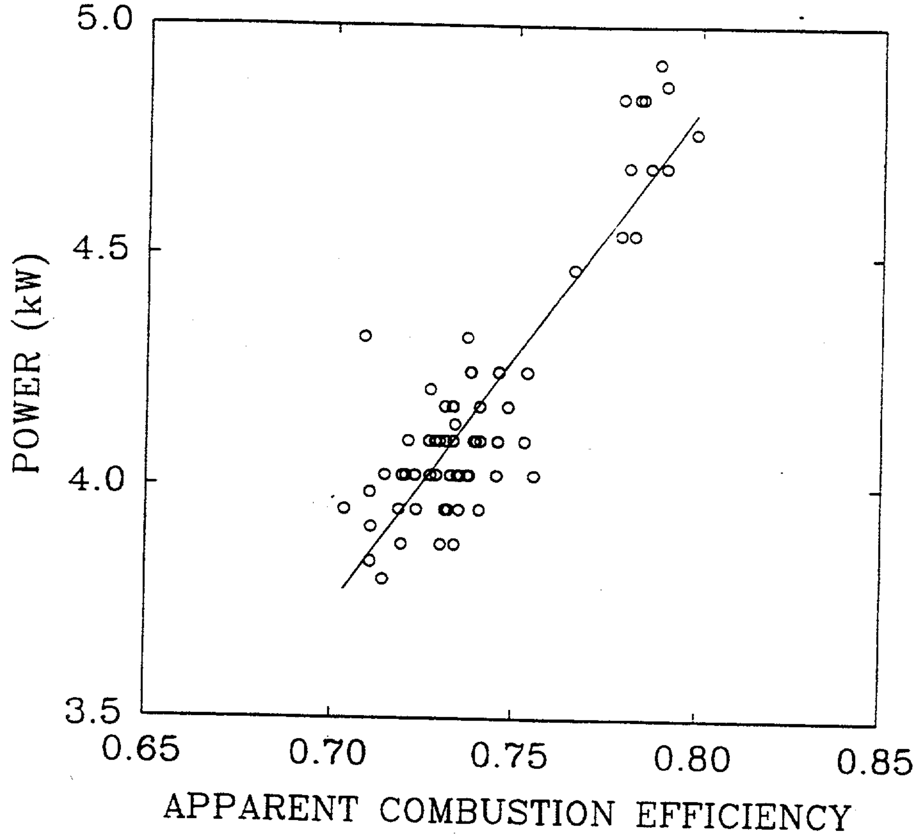

Figure 28. Power variations in Mode 1 versus apparent combustion efficiency

Hydrocarbons – Scatter plots of the hydrocarbon emissions indicated that the fuel physical properties dominated the results within each mode. Figure 29 shows the hydrocarbon emissions plotted versus the viscosity for the Mode 1 test condition. Similar results were obtained for the other test conditions. The preliminary statistical analysis indicated that the relationships between the hydrocarbon emissions and the fuel properties were, in fact, dominated by the boiling-point distribution and the viscosity for all test conditions.

Smoke – Statistical analysis of the smoke data indicated that fuel properties play a significant role in controlling these emissions. Fuel structure appears to dominate these relationships, with total aromatic content an important factor at all test conditions. Other important fuel properties are the sulfur content, the aromatic ring structure, and the boiling-point distribution. The order of importance of these properties varies somewhat as the engine load is reduced: the boiling-point distribution and viscosity become more important at the lighter loads, where the injection process might be more affected by these properties than at the higher load conditions.

NOx Results – Scatter plots of the NOx data indicated dominant effects of fuel composition and cetane number at all but the lightest load condition. These trends are demonstrated in the scatter plots of these fuel variables, presented in Figures 30 and 31 for the Mode 1 condition. The preliminary statistical analysis indicated that the aromatic content and structure, and the structure of the alkyl groups are important.

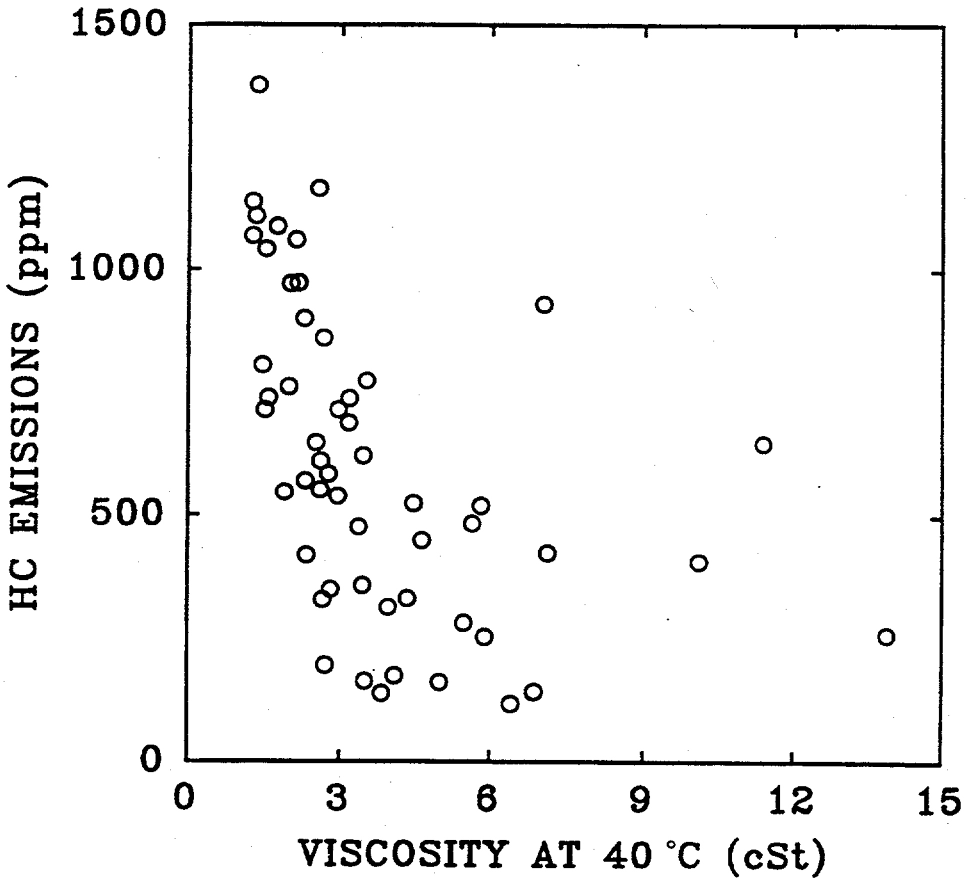

Figure 29. Hydrocarbon emissions versus viscosity for the Mode 1 test condition

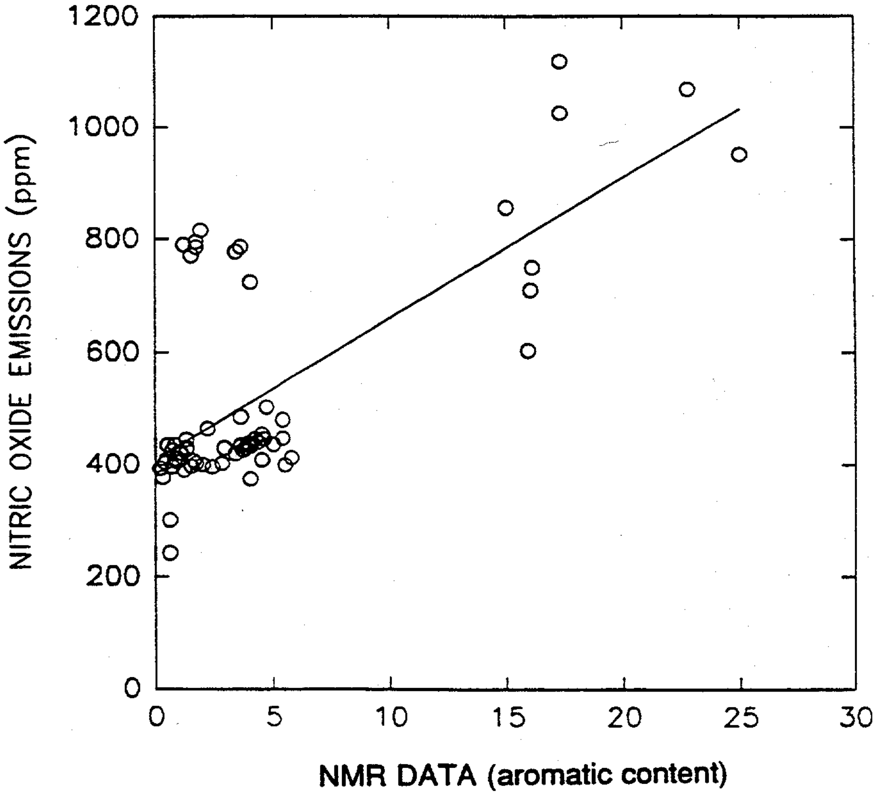

Figure 30. NOx emissions versus NMR aromatic content for Mode 1

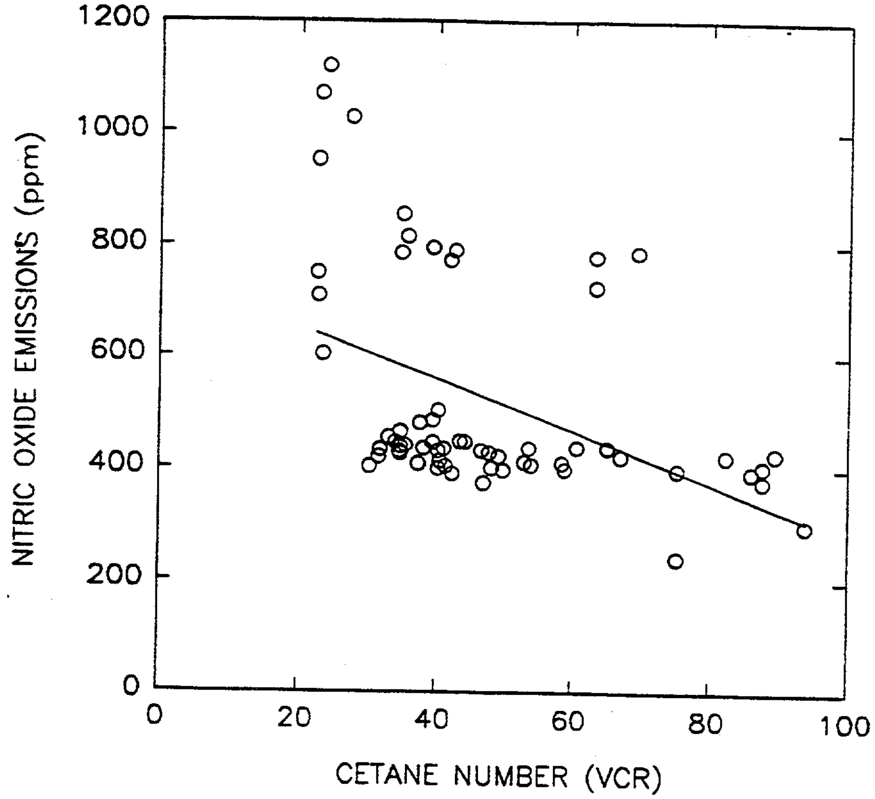

Figure 31. NOx versus cetane number (VCR) for Mode 1

Statistical Analysis – The results of the statistical analysis verified that Mode 2 represented the best test condition for examining the fuel composition and property effects on the NOx, smoke and HC emissions. The stepwise analysis was first performed using three subsets of the independent variables. The subsets were defined to include the combustion parameters, the physical properties, and the chemical properties. Although different properties could have been included in each subset, the goal was to determine where, or if, the physical properties or chemical properties, or combustion parameters dominated the emissions characteristics. For instance, one result was that power and CO emissions did not display significant fuel dependence at any combination of test conditions.

The ***combustion*** properties include the air-fuel ratio, peak combustion pressure, peak heat-release rate, the angles of occurrence of these peak values, beginning of injection, indicated and brake power, energy input, cumulative heat release, and the combustion efficiency. NOx emissions were highly correlated with the combustion characteristics at the rated power and rated torque conditions, with R^2 in the range of 0.97. The R^2 value dropped dramatically at the part-load conditions. The other emissions were not highly correlated with the combustion parameters, based on R^2 values below 0.5.

The fuel ***physical properties*** include average boiling point, heating value, initial boiling point, T50, T95, specific gravity, viscosity, cetane number, vol% aromatics, olefins, and saturates, and wt% carbon, hydrogen, and sulfur. The NOx emissions displayed dependence on T50, specific gravity, the heating value, and vol% aromatics at all but the lightest load condition. The smoke number correlated mainly with boiling point distribution and viscosity across the load range (R^2 in the range 0.5 – 0.75), indicating a dominance of the physical processes on the soot formation and oxidation.

The stepwise regression analysis included a very broad range of ***chemical composition*** variables. In stepwise regression, the computer method substitutes a succession of regression models into the data to determine the best fit each model can obtain, thereby exploring several functional forms for the correlation. The initial analysis included both the NMR characterizations and the GC/MS hydrocarbon-type breakdowns. As expected, the NMR and GC/MS data were highly colinear. The NMR data provide a great deal of structural information regarding the location and environment of the hydrogen within the fuel molecules, and in that sense provide more information regarding the structure of the fuel. The statistical analysis indicated that both the NMR and GC/MS data provided nearly equivalent representations of the results. We believe that NMR analyses is less routine than GC/MS; therefore, the subsequent statistical analysis included only the component hydrocarbon composition data obtained by GC/MS. NOx emissions displayed a strong dependence, (across the speed and load range of the engine) on the hydrocarbon-type data, with R^2 in the range 0.6 – 0.8. The ignition quality, in terms of the engine-based cetane number, was also highly correlated with the chemical composition.

Following the stepwise regression analysis, we calculated linear fits using all possible combinations of those fuel variables found to be important in one or more of the fits for each subset. We used these results as the basis for selecting the best linear models for each independent variable at each test condition. Although scatter plots of the residuals (degree of statistical fit of each dependent variable) were indicative of linear behavior, we tried to improve the linear models by using natural-log-transformed, curvilinear, and interactive terms. The R^2, or fit, of the model was not improved by the inclusion of these nonlinear terms.

We developed the final models for each of the emissions at each speed-load condition. The results of these analyses for the Mode 2 test condition appear to present the best indication of the effects of the fuel properties and composition on the cetane number and the emissions. We discussed the Mode 2 models in detail in the following paragraphs, and definitions of the terms are presented in Appendix B.

NOx – The NOx emissions were highly correlated with the combustion parameters, reflecting the kinetic nature of the NOx formation mechanism. The Zeldovich kinetic model for NOx relates the formation process to the concentrations of the nitrogen and oxygen species in the flame zone and the time and temperature of reaction (Zeldovich, 1946; Hanson & Salimian, 1984). The local adiabatic flame temperature is appropriate for use in the Zeldovich mechanism. The adiabatic flame temperature and the overall combustion rate are directly related to the chemical composition of the fuel. These dependencies are reflected in the regression equation that was developed for NOx:

$$\begin{aligned} \text{NOx} = \; & A_1 + A_2 \times (\text{AlkylNaphthalenes}) \\ & + A_3 \times (\text{Indenes}) + A_4 \times (\%\ \text{Carbon}), \end{aligned}$$

where concentrations are in wt% and the coefficients are:

$A_1 = -96.34$ $R^2 = 0.82$
$A_2 = 0.22$
$A_3 = 0.24$
$A_4 = 1.17$

The regression analysis included several variables describing the aromatic structure:

- Alkyl benzenes
- Indanes/Tetralin
- Indenes
- Naphthalene
- Alkylnaphthalene
- Acenaphthylenes
- Acenaphthenes
- Tricyclics

The results indicate that two-ring structures lead to higher NOx levels, while the level of unsaturation indicated by the indenes tends to lower levels of NOx. The importance of the total aromatic nature of the fuel is reflected in the carbon content.

As indicated in the stepwise regressions discussed under "Statistical Analysis", the fuel physical properties provided a good indication of the NOx trends when they alone were used in the regression analysis. The final regression equation did not include fuel physical properties, however, because the stepwise analysis indicated that the physical properties added little to the prediction of the NOx emissions when the chemical composition parameters are included in the analysis. This finding is related to the fact that the physical properties and the chemical composition are colinear in many cases, that is, they tend to change in the same way if a fuel blend is varied, i.e., aromatic content increases with boiling point.

Smoke – The smoke number reflects the soot fraction of the particulate emission. Soot emissions depend on the difference between the soot formation and the soot oxidation rates in the engine. A great deal of soot is formed during combustion in diesel-engine cylinders, but most of this soot is oxidized prior to exhaust. The soot formation mechanism is dependent on fuel composition, the thermodynamic state in the combustion chamber, and the mode of combustion (premixed versus diffusion). The soot oxidation mechanism is dependent mostly on the thermodynamic state and the physical processes associated with mixing. Regression of the Bosch smoke data indicated that only a part of the variation could be accounted for in the fuel properties. This probably reflects the fact that the soot oxidation mechanism depends more on the physical processes than on the chemical composition of the fuel. That portion of the smoke emissions that can be accounted for in the final properties is best modeled using the following equation:

$$\begin{aligned}\text{Bosch Smoke} = {} & A_1+A_2\times(\text{Acenaphthylenes}) \\ & +A_3\times(\text{Alkylbenzenes})+A_4\times(\text{Tricyclic aromatic}) \\ & +A_5\times(\text{Total aromatics})+A_6\times(\text{vol\% aromatics}),\end{aligned}$$

where concentrations are in wt% except as indicated, and where:

A_1 = 2.24 R^2 = 0.61
A_2 = – 0.065
A_3 = – 0.029
A_4 = 0.08
A^5 = 0.027
A^6 = – 0.013

Most of the combustion event in the test engine occurred in diffusion burning of the fuel jets. Palmer and Curtis (1965) indicate that the tendency for soot formation in diffusion flames decreases in the order: naphthalenes>benzenes>diolefins> monolefins>paraffins, where the tendency to form soot decreases in each group with increasing molecular weight (except the paraffins) and increasing compactness.

The results of the regression analysis indicate a direct relationship with the total aromatic content and the concentration of three-ring aromatics. We expected this effect based on the conclusions of Palmer and Curtis. The inverse relationship with the acenaphthylenes and the alkyl benzenes may be related to the decreased stability of the tertiary carbon atoms in these structures, the increased molecular weight, or the compactness of these groups of compounds. Inclusion of the vol% aromatics provides a marginal improvement in the R^2 and may reflect an interaction with the density.

It should be noted that the Bosch smoke number is not an accurate measurement of the total mass of particulate emissions. The regression equations generated using these data reflect this limitation, and the resulting discussion should be considered in light of this limitation. Future experiments should consist of total mass measurements, with actual breakdown between the soot and the soluble fraction

HC – Surprisingly HC emissions decreased with increasing boiling point at all speed-load conditions. This relationship is demonstrated in Figure 32 for the Fischer-Tropsch fuels, where the HC emissions are plotted versus the fuel fraction or average boiling point. Figure 33 is a similar plot of the Mode 2 smoke data, showing that the smoke tends to increase with fraction number. The regression equation for the HC emissions reflected this inverse relation with the boiling-point distribution, as reflected in the T50 coefficient. As indicated above, the regression equations for smoke did not include boiling-point information. They did indicate, however, that boiling-point data could be used in lieu of some of the composition data to account for some variation of smoke. The regression equation for the HC emissions is:

$$\begin{aligned} HC = {} & A_1+A_2\times(\text{Alkylbenzenes})+A_3\times(\text{T50}) \\ & +A_4\times(\text{Indenes})+A_5\times(\text{Monocycloparaffins}) \\ & +A_6\times(\%\ \text{Carbon}) \end{aligned}$$

where concentrations are mass percentage, and where:

$A_1 = 21.61$ $R^2 = 0.83$

$A_2 = 0.095$

$A_3 = -0.004$

$A_4 = -0.15$

$A^5 = 0.029$

$A^6 = -0.21$

The unburned hydrocarbon emissions from diesel engines are dependent on both the physical processes that occur in the engine and the fuel properties that affect combustion efficiency. The physical processes include fuel atomization, vaporization, mixing and impingement, as well as quenching in the bulk gas due to over-rich or over-lean conditions and thermal quenching in the boundary layers; all these processes result in incomplete burning. If the HC emissions are in fact dominated by the physical processes that lead to incomplete combustion, the properties that lead to increased soot production will likely produce reduced HC emissions. One possibility is that the total mass of unreacted carbon is accounted for in either the HC or the smoke emission, with the distribution also dependent on the conditions in the engine and on the fuel properties.

The direct relationship between the HC and the alkylbenzenes and monocycloparaffins most probably reflects the stability of these structures relative to the other hydrocarbon groups. This hypothesis is supported by the inverse relationship with the less stable indenes. The relationship to the wt% carbon probably reflects the propensity of the fuels to form soot rather than HC.

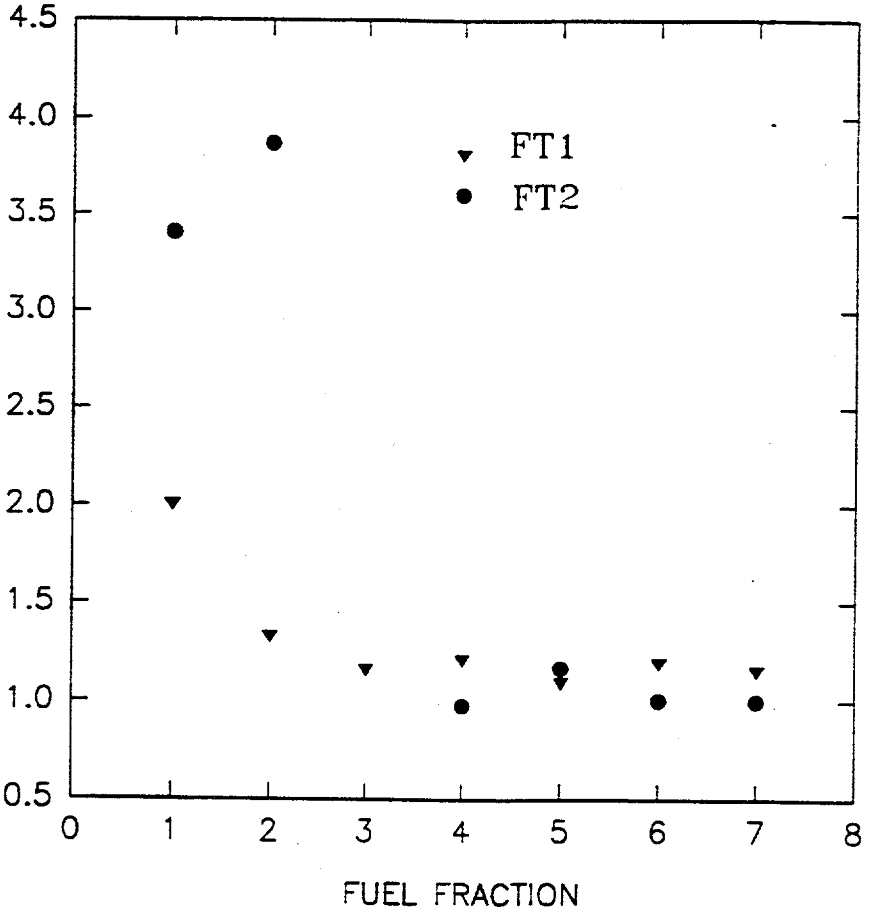

Figure 32. HC emissions versus fuel fraction for the F-T fuels at Mode 2

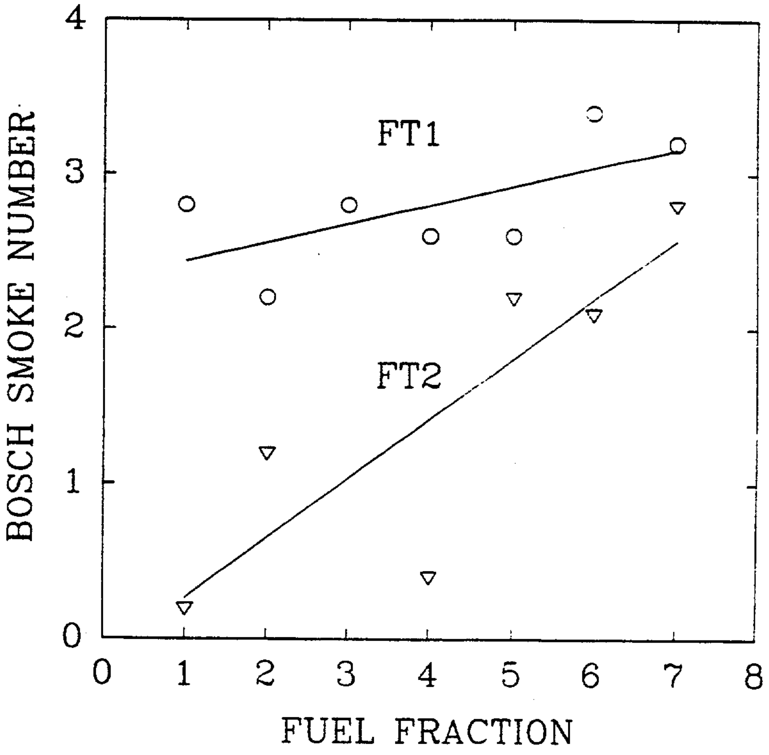

Figure 33. Bosch smoke number versus fuel fraction for the F-T fuels at Mode 2

TASK 3 CLEAN-FUEL STUDY

The goal of Task 3 was to study the results of the fuel fraction analyses and the emissions measurements to recommend methods to produce reduced-emissions diesel fuels. During the foregoing studies, the concepts of aromatics identity, aromatics concentration, and ignition quality (cetane number) emerged as the central variables for emissions control for a given boiling range. The comparisons with the F-T materials showed that the aromatics in the petroleum blendstocks are a crucial determining factor for emissions. With these observations in mind, we developed an approach to the Clean Fuel Study in which we would use the emissions measurements for the samples to select a formulation via linear programming for the lowest-emission test fuel meeting possible future diesel specifications — with and without F-T material. Continuing this approach, we used linear programming to formulate three fuels spanning the range of aromatics concentrations likely to be encountered at about 55 CN. The complementary set of three formulations spanning the likely cetane range at 15% aromatics were also developed by linear programming. These levels of aromatics content and cetane number are representative of those used in fuels certified as reformulated diesel fuels in California. (Nikanjam, 1993).

We processed enough of the selected materials to perform performance and emission tests similar to those in Table 6, which were obtained for the sample fractions. This testing was carried out on the same engine configuration and with the same standard diesel fuel as before. We then compared these results with the predicted values and the values of the correlations.

Determining Blend Compositions for Low-Emissions Fuels

The preliminary statistical analysis of the engine performance and emissions data indicated the dominant effects of the aromatic content, aromatic type, and cetane number, on the emissions. However, much more detailed analysis is required to develop relationships between the various fuel properties and the emissions. A simplified approach was therefore taken in the design and formulation of "low emissions" diesel fuels. The approach consisted of including the emissions data for each cut as properties that could be modeled using linear programming techniques.

Distillation of original components provided a large number of potential blend components. Collectively, they contained a wide range of properties, and in general, several different blend formulations could be determined with properties meeting any particular set of specifications. In general, our goals were to produce full-boiling-range fuels that would either provide the lowest possible emissions, or would indicate the independent effects of aromatic content and cetane number. The blend compositions of 10 different low-emissions fuel concepts were determined using the linear programming (LP) technique for selecting an optimal solution from many acceptable solutions. This process allowed us to rapidly select a blend formulation that was best for each particular concept.

We calculated a blend formulation for each low-emission fuel concept, which differed in the constraints placed on the problem or in the property that was optimized. Table 9 gives a description of each calculated blend. Of the four "minimum-emissions" test fuels, Fuel 1 was designed for the lowest possible emissions, using all of the available components. Fuel 2 had the added constraint of using the most of one of the least valued products — LALCO. Concentrations of LCO and LCGO, typical of actual refinery operation, were used to design the lowest possible emissions in Fuel 9. Fuel 10 had the same constraints as Fuel 1 except that the high-quality Fischer-Tropsch materials were not included in the blend.

Table 9. Low-Emissions Fuels Descriptions

Blend No.	Blend Concept Description
1	Minimum emissions
2	Minimum emissions with maximum use of light-cycle oil product (low-aromatics LCO)
3	Minimum aromatics concentration with CN 55 to 56
4	Maximum aromatics concentration with CN 55 to 56
5	Maximum cetane number with aromatics 15–16%
6	Minimum cetane number with aromatics 15–16%
7	50:50 mixture of blends 3 and 4*
8	50:50 mixture of blends 5 and 6*
9	Minimum emissions with LCO and LCGO products in typical abundance
10	Minimum emissions, F-T products excluded

* Not calculated directly by linear programming

Next, two sets of three test fuels each were devised to test two important trends. Fuels 3 and 4 were designed to examine the effects of aromatic content, at a constant cetane number of 55. Fuels 5 and 6 were designed to examine the effect of cetane number at constant aromatic content of 15%. Fuels 7 and 8 were designed to be the midpoints between Fuels 3 and 4 and Fuels 5 and 6, respectively.

Several preliminary actions facilitated the selection process. The Mode 2 data were selected as the most appropriate for the selection. Because the LP method optimizes on a single property, we defined an "emissions parameter" for each component by normalizing and adding the normalized emissions data in each concept. We normalized the emissions data by dividing the measured or predicted emissions data by the respective target value for each component. If the target emissions levels are achieved exactly for each emission, the emissions parameter (EP) equals 4. Values of EP below 4 indicate emissions levels better than the target, and values greater than 4 indicate that the target levels are not achieved. The EP provides a convenient parameter to compare different fuels, even if the target values are never achieved.

The targets, based on the rated torque condition, were:

4 g/hp-hr for CO,
2 g/hp-hr for HC,
5 g/hp-hr for NOx,
2 for Bosch smoke number.

The LP problem was computerized using the optimization feature of Quattro Pro to include as many components as practical, and preliminary runs were made with the individual distillation cuts. The results showed that adjacent cuts were in general not selected in similar quantities, so more realistic, broad-range cut properties were calculated by linear combination of the individual cuts weighted by their yield. The goal was to select one, or at most two, cut points for a given stock. Accordingly, the LP was provided with artificial stocks comprising adjacent fractions, for example, fractions 1 through 4, or fractions 3 through 5, etc. The possible combinations of adjacent fractions provided the LP problem with about 215 different blendstocks, including the full-boiling-range products.

Two further actions helped reduce the scope to manageable proportions. The component properties were entered in a Quattro Pro spreadsheet library and set up so they could be input to the problem readily, allowing a large number of components to be tried rapidly by manual action. The other action reduced the number of artificial stocks requiring trials. In addition to the blend formulation, the LP solution indicates the relative utility of unused components to the blend. Preliminary LP runs quickly established that similar cuts had similar utilities to the blends. For example, if a blend made of cuts 3 through 5 was not used in a blend and had low utility, a blend made of cuts 3 through 6 of the same product would also have low utility and would not be used. These actions allowed calculation of optimal blends from a set of fuels including the parent stocks, products, and all the practical distillation cuts.

In this way, linear programming computed the blend compositions based on the property and emissions data for each component. The properties of each of the blends were also computed based on the assumptions of linear blending. The results of these calculations for the aromatic content and the cetane number are summarized in Table 10. The measured cetane numbers, also listed in Table 10, are in some cases significantly different than the computed values, indicating the nonlinear nature of the cetane scale.

Table 10. Computed and Measured Properties of the Low-Emissions Fuels

Fuel Number	Aromatics (wt %)	Computed CN	VCR Measured CN
1	10	70	62
2	7.8	66	40
3	0.7	57	43
4	29	63	41
5	15	75	60
6	7.7	63	29
7	15	60	41
8	11.3	69	44
9	8.7	73	56
10	13.9	55	50

Clean-Fuel Experimental Results and Discussion

The Phase III test fuels included the 10 "low emissions" fuels described in the previous section, as well as repeats of the fractions of the Fischer-Tropsch wax material (FT1) and fractions of a straight-run material (FT2) from the Fischer-Tropsch processing of coal.

Linear programming was also used to compute the other properties and compositional data for each of the fuel blends. The statistical models for emissions are based mainly on the composition of the fuels and physical properties that are also linear functions of the composition. It is reasonable, therefore, to assume that the computed values of these properties are appropriate for use in the statistical models of the emissions. The results of the calculations of the properties and compositional data are presented in Table 11. These are linear combinations of component properties and variables such as viscosity which have blending indices were not transformed via a blending index.

Fischer-Tropsch Fuels

The Fischer-Tropsch fuels consisted of two different materials produced from the indirect liquefaction of coal. Each of these materials and seven fractions of both materials were subjected to both CVCA ignition experiments and VCR engine ignition and combustion and emissions testing. Both F-T liquids were added to the project after its inception, but FT2 came at about the time Task 3 was started, so its evaluation was done as part of Task 3 and reported here.

The CVCA and VCR ignition quality ratings of the various materials were in excellent agreement with each other, both demonstrating that the full-boiling-range base materials had relatively high cetane numbers in the range of 65 to 85. The cetane numbers of the fractions of both materials demonstrated strong relationships to the boiling point, as shown in Figure 34 for the VCR cetane ratings. The lower-boiling fractions of each of these materials had relatively low cetane numbers. The cetane numbers increased dramatically in the higher-boiling-range fractions, to the point where it was not possible to provide accurate ratings of the highest-boiling-point fraction because the compression ratio of the VCR engine could not be lowered sufficiently to accomplish ignition at TDC.

Figure 34 shows that the cetane numbers of all fractions of the FT1 material were higher than the corresponding fractions of the FT2 material. These differences are clearly related to differences in the composition of the two materials. However, although the total aromatic contents of both materials were very low, the FT1 material had significantly higher levels of aromatics than the FT2 material.

All of the Fischer-Tropsch materials were tested at five different speed and load conditions in the VCR engine. As described previously, Mode 2 was the rated torque condition for the test engine. The injection timing was adjusted for each fuel to give the maximum torque output of the engine. Mode 2 represents a test condition at which the NOx emissions are sensitive to the ignition quality of the fuel. The NOx data for this condition are presented in Figure 35. Although data are missing for the FT2 materials, the NOx emissions are clearly higher for the FT2 materials than for the FT1 materials. In addition, the differences are larger for the lower-boiling-point fractions, where the differences in the ignition quality are also larger. The corresponding data for the Mode 1 condition, a retarded timing and low-NOx condition, indicated no systematic differences between the two fuels.

The smoke data at all test conditions indicated a systematic difference between the two materials, with the FT1 always higher than the corresponding FT2 fractions. This difference is probably related to the differences in aromatic content of the two materials where FT1 has effectively zero aromatic content and FT2 has only 2% vol aromatics. In addition, there was a trend at all test conditions for the smoke emissions to increase with boiling point, due most likely to the physical effect of the boiling point on the evaporation rates of the fuel in the engine. These trends are demonstrated in Figure 36 for the Mode 2 test condition.

The unburned hydrocarbon (HC) emissions displayed an interesting trend that was consistent at all test conditions. The trend consisted of a dramatic, systematic decrease in the HC emissions with increasing average boiling point. These results are demonstrated in Figures 37 and 38 for the Modes 1 and 2 test conditions, respectively. These results are not consistent with the intuitive impression that the higher-boiling fractions would produce high HC emissions. The results are probably because the higher-boiling fractions are higher molecular weight components that are emitted as particulate, or that agglomerate or condense in the exhaust system.

The value of the Fischer-Tropsch materials is indicated by the fact that the emissions parameters, or EPs, averaged over all of the fractions of both materials, were well below the averages for all of the test materials. The EP values for all of the test materials are presented in Figure 39 for the Mode 2 test condition. The dashed line in Figure 39 represents the average EP of approximately 4.3, indicating that on average, the emissions were above target values. The average EP for the FT1 fuel fractions was 3.8 and that for the FT2 fractions was 2.86, both well above average and both below the target value.

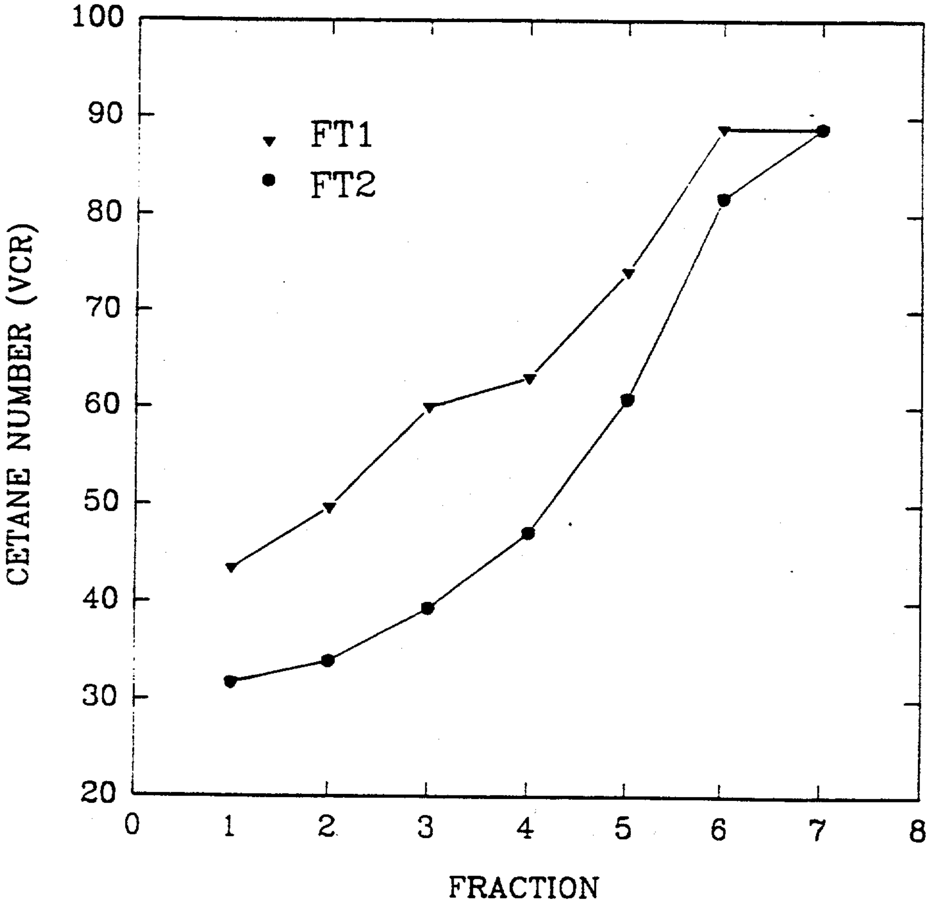

Figure 34. VCR cetane ratings of the Fischer Tropsch materials

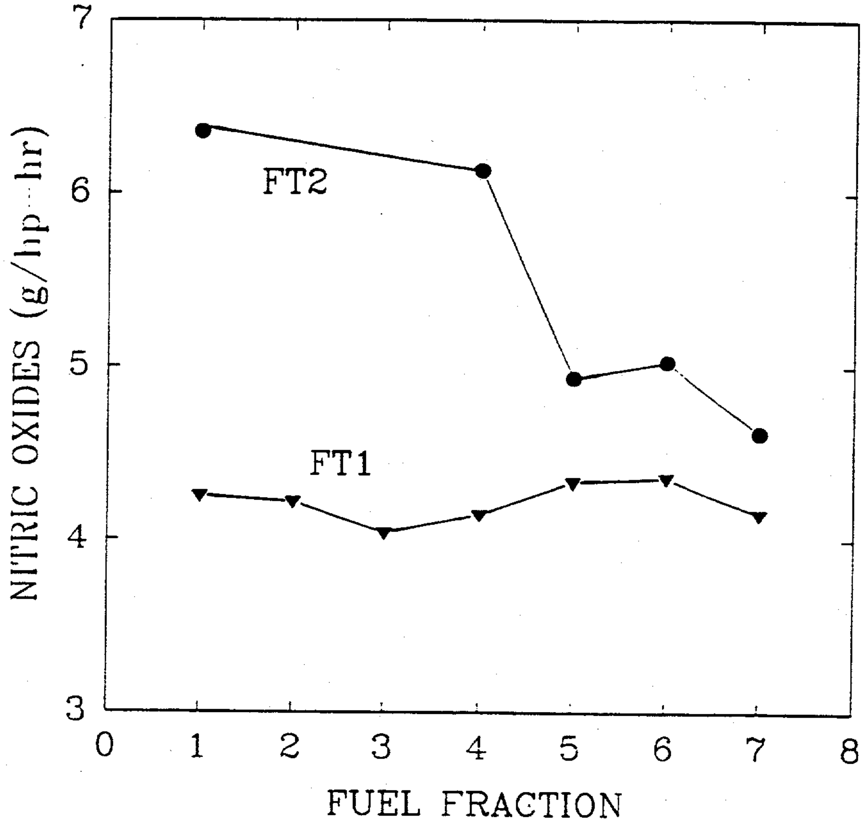

Figure 35. Nitric oxide emission data for the Mode 2 test condition

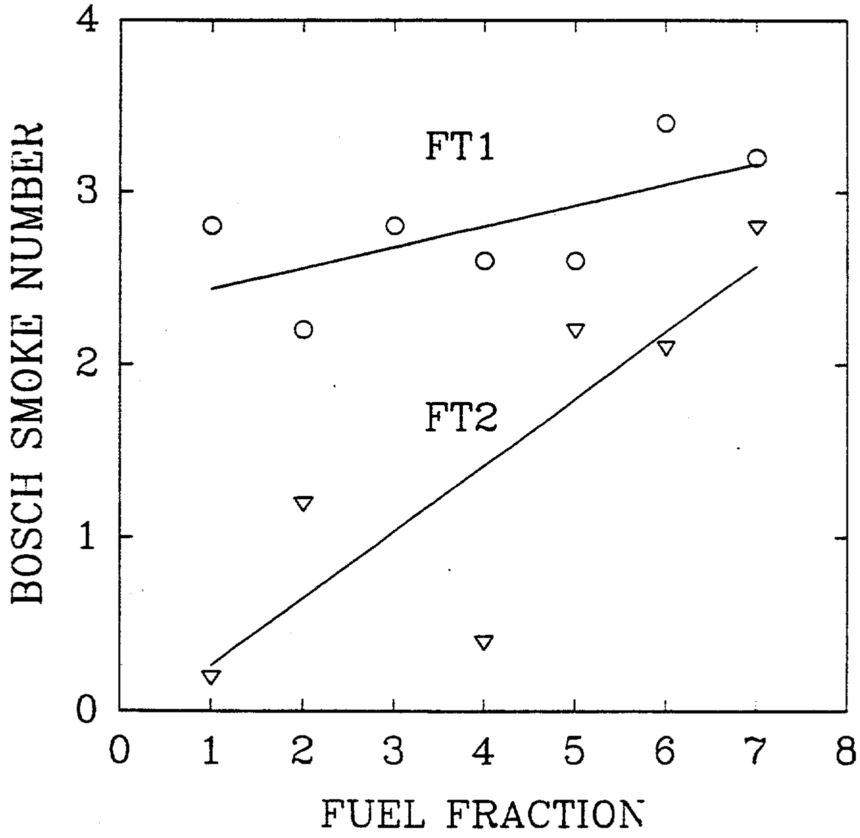

Figure 36. Bosch smoke numbers for the Mode 2 test conditions

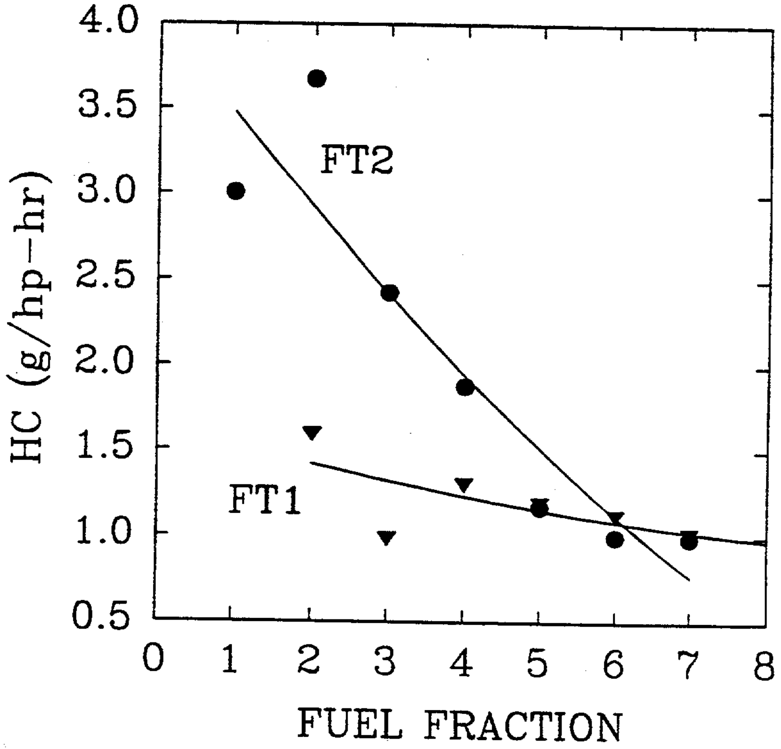

Figure 37. Hydrocarbon emissions for the Mode 1 test conditions

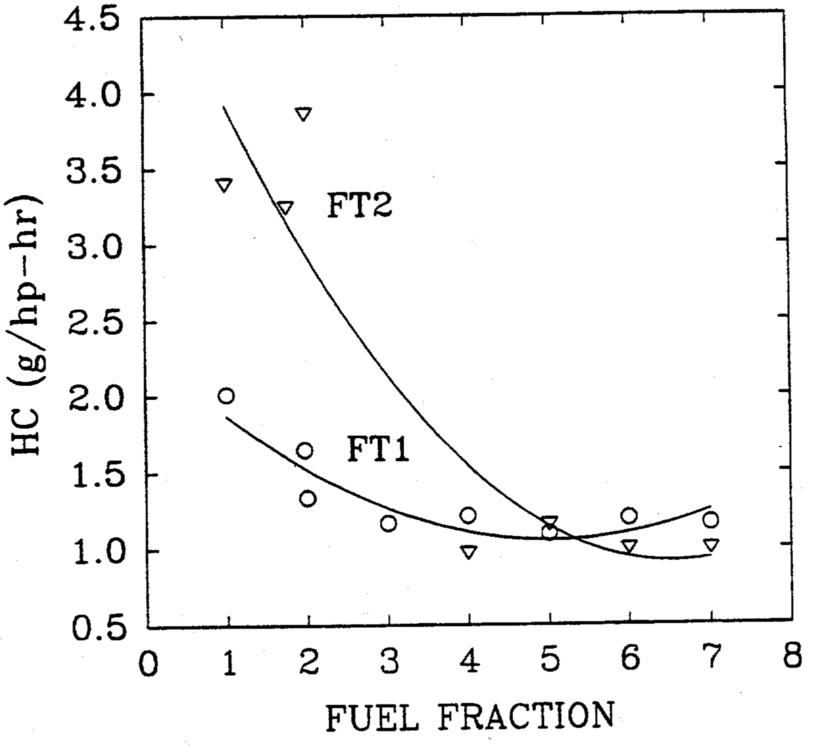

Figure 38. Hydrocarbon emissions for the Mode 2 test conditions

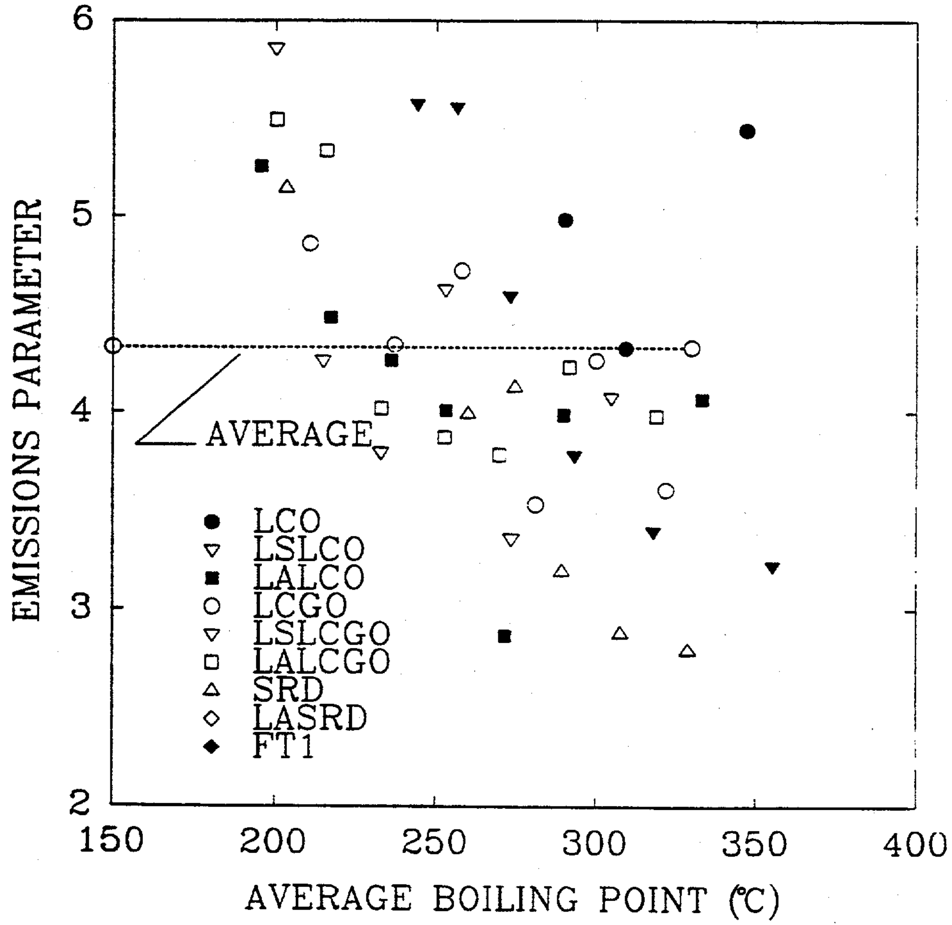

Figure 39. Emissions parameters for all test materials at the Mode 2 test conditions

Table 11. Task 3 Correlation Inputs

	FUEL IDENTIFICATION									
Name of Variables	Blend #1	Blend #2	Blend #3	Blend #4	Blend #5	Blend #6	Blend #7	Blend #8	Blend #9	Blend #10
Acnaphthe	0.268	0.335	0.055	4.723	2.396	1.359	2.389	1.878	1.064	0.299
Acnaphthy	0.171	0.205	0.039	2.789	1.469	1.034	1.414	1.252	0.767	0.120
Alkbenz	3.972	4.840	1.463	6.424	3.617	5.624	3.943	4.621	3.346	5.821
Alk_naph	0.545	0.503	0.050	4.129	2.094	0.719	2.090	1.407	2.101	0.627
Arotricy	0.027	0.039	0.006	0.401	0.203	0.597	0.203	0.400	0.287	0.023
Aro_tot	10.571	12.196	2.654	23.066	12.200	14.105	12.860	13.152	11.348	14.641
Indans	3.500	4.206	0.777	2.645	1.384	3.516	1.711	2.450	2.062	4.771
Indenes	2.076	2.053	0.259	1.801	0.959	1.187	1.030	1.073	1.604	2.954
Naphth	0.019	0.000	0.000	0.134	0.068	0.021	0.067	0.044	0.086	0.067
nmrAlp	3.344	3.983	0.866	10.875	5.688	5.335	5.870	5.512	2.611	4.534
nmrAro	1.625	1.783	1.240	6.657	3.654	2.911	3.948	3.283	2.012	1.878
nmrCh	8.373	16.487	6.966	6.134	4.619	24.352	6.550	14.486	9.062	13.969
nmrCh2	50.453	42.695	52.487	49.918	56.218	30.721	51.202	43.469	53.369	45.039
nmrCh3	31.243	35.024	38.451	26.404	29.804	36.700	32.427	33.252	32.320	33.252
Para	59.149	39.331	80.838	64.239	75.041	15.979	72.539	45.510	60.577	45.412
Para_di	6.116	14.319	3.963	1.899	1.626	22.946	2.931	12.286	6.892	10.548
Para_tri	2.083	7.464	2.314	0.077	0.039	9.738	1.196	4.888	3.007	4.409
Par_mono	17.073	26.668	10.245	10.648	11.007	37.250	10.447	24.128	17.472	23.657
Sat_tot	84.395	87.744	97.352	76.877	87.713	85.895	87.114	86.804	87.966	83.995
SpGr	0.774	0.842	0.781	0.843	0.816	0.872	0.812	0.844	0.816	0.824
Total UV	3.417	4.080	0.838	13.524	6.917	6.122	7.181	6.520	4.329	4.444
UVdi	0.686	0.730	0.075	6.722	3.409	1.568	3.399	2.489	1.790	0.765
UVmono	2.725	3.351	0.763	5.880	3.041	3.797	3.322	3.419	2.178	3.672
UVtri	0.000	0.000	0.000	0.938	0.476	0.761	0.469	0.619	0.360	0.000
Vis40	3.031	3.142	2.040	3.708	3.688	2.904	2.874	3.296	3.321	3.159
Vis100	1.169	1.220	0.894	1.336	1.352	1.147	1.115	1.250	1.278	1.220
VParom	14.721	14.440	10.264	35.700	23.434	15.996	22.982	19.715	15.239	13.782
VPolef	4.043	2.586	4.891	4.255	5.221	0.845	4.573	3.033	3.721	1.624
VPsat	76.268	82.940	84.886	60.054	71.349	83.127	72.470	77.238	80.226	83.229
WtPC	81.488	86.257	85.043	86.725	85.887	86.937	85.884	86.412	85.392	85.062
WtPH	13.663	13.670	14.951	13.475	14.254	12.924	14.213	13.589	14.033	13.711
WtPS	0.012	0.009	0.001	0.005	0.004	0.004	0.003	0.004	0.017	0.009

Low-Emissions Fuels

As discussed above, ten low-emissions fuels were formulated using linear programming techniques. The constraints on the properties and the compositions used in the calculations had to be relaxed in several cases to meet the emissions requirements. The aromatic content and the cetane number data, presented in Table 10, are plotted in Figures 40 and 41, respectively, for the ten low-emissions fuels. The target cetane number for fuels 3, 4, and 7 was 55 CN, while the aromatic content was to vary over a range from less than 10%–30%. The actual cetane numbers for these fuels were in the range 42 to 43 CN and the aromatics ranged from 1%–30%. The target aromatic content for fuels 5, 6 and 8 was 15%, with cetane number varying from 63 to 75 CN. The actual cetane numbers of these fuels ranged from 30 to 60 CN and the aromatic content varied from 8%–15%, with variation due to limits imposed by the available blending materials. It should be pointed out that several of the fuel components had to be recreated from the feedstocks for Task 3, making some variation of originally measured properties and the ones prevalent in Task 3. Further these materials were available in short supply making it impractical to perform the number of CN replicates necessary to reduce variability of results.

These results reiterate that the cetane number does not always blend linearly. The resulting fuels, although lower in cetane number than originally planned, do offer the opportunity to study the effects of variation in aromatic content at nearly constant cetane number (Fuels 3, 7 and 4 in order of aromatic content) and the effects of variation in cetane number at modest variation in aromatic content (Fuels 5, 8, and 6 in order of cetane number).

We believe that the Mode 2 test conditions provide a more-sensitive measurement of the fuel effects on the NOx emissions than the other modes because the injection timing was adjusted for maximum torque on each fuel. The Mode 2 NOx data for the 10 low-emissions fuels are presented in Figure 42. The corresponding data for HC, CO, and smoke emissions are presented in Figures 43 through 45, respectively. The results in Figure 42 indicate a trend towards increased NOx emissions as the aromatic content is increased from 1%–30%. In addition, HC emissions appear to decrease and CO and smoke emissions increase with the increase in aromatic content.

Increasing the cetane number from 30 to 60, while holding aromatic content in the range from 8 to 15, results in a significant reduction in NOx emissions. This variation in the cetane number results in a corresponding increase in HC, CO, and smoke emissions.

Fuel 1 was designed to be the lowest-emissions fuel that could be produced from the large number of potential blending materials that were available in this study. Although the NOx emissions of this fuel were clearly the lowest, other fuels had lower levels of the other emissions. This demonstrates the utility of using the emissions parameter for the fuel-to-fuel comparisons.

The EPs computed from the linear programming model and the actual values based on the measured emissions are presented in Figure 46 for the Mode 2 test conditions, and several points can be made. First, the predicted EP values are all very close to the target level of 4. This is indicative of the results of the linear programming model, in which the EP was set as one of the constraints. The second point is that the actual EPs follow the same trends as the predicted, indicating that the basis of the modeling work is correct in a linear sense. The same conclusion was also arrived at in the detailed statistical analysis, where the relationships between the emissions and the fuel properties and composition are linear. The third observation is that the actual EP values are significantly below the predicted and the targets in 8 out of the 10 cases, with EPs in the range of 3.5.

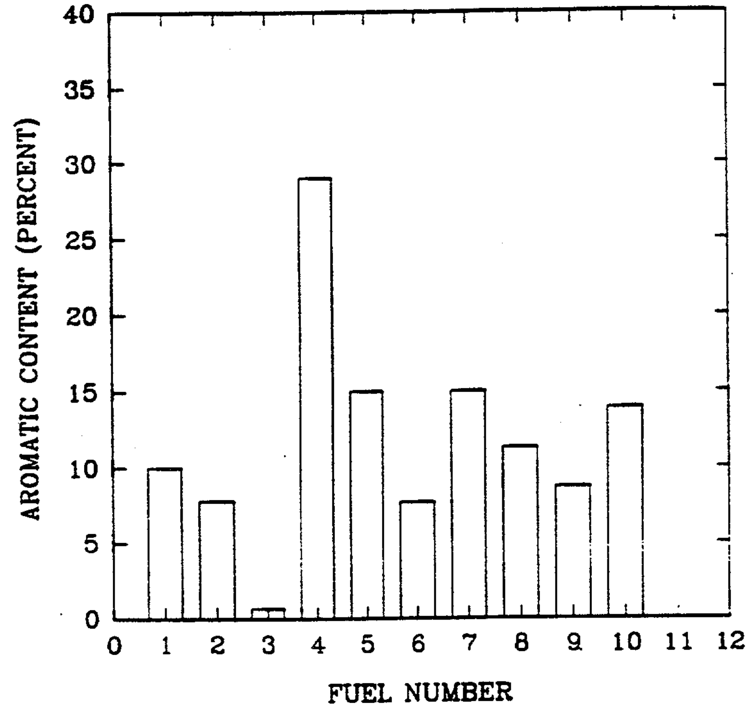

Figure 40. Aromatic content of the low-emissions fuels

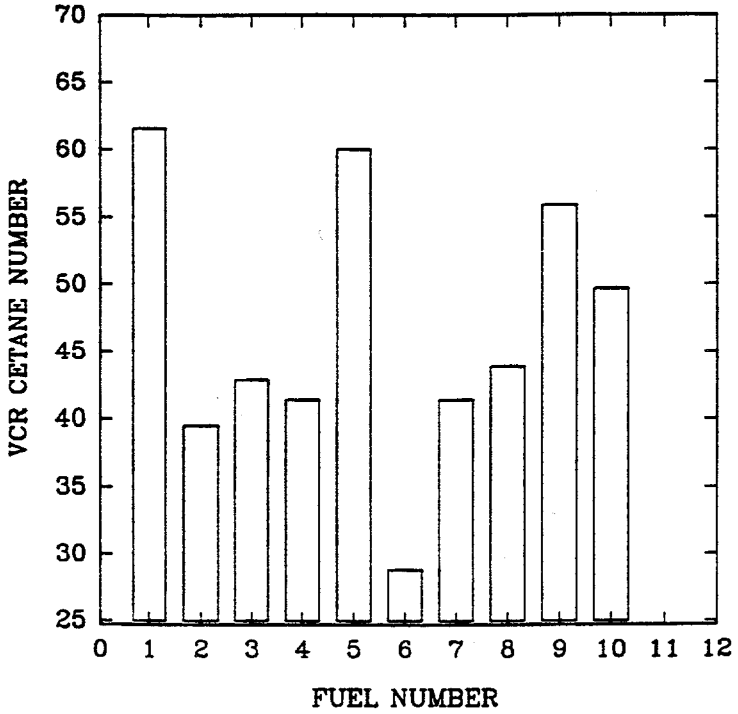

Figure 41. VCR cetane numbers of the low-emissions fuels

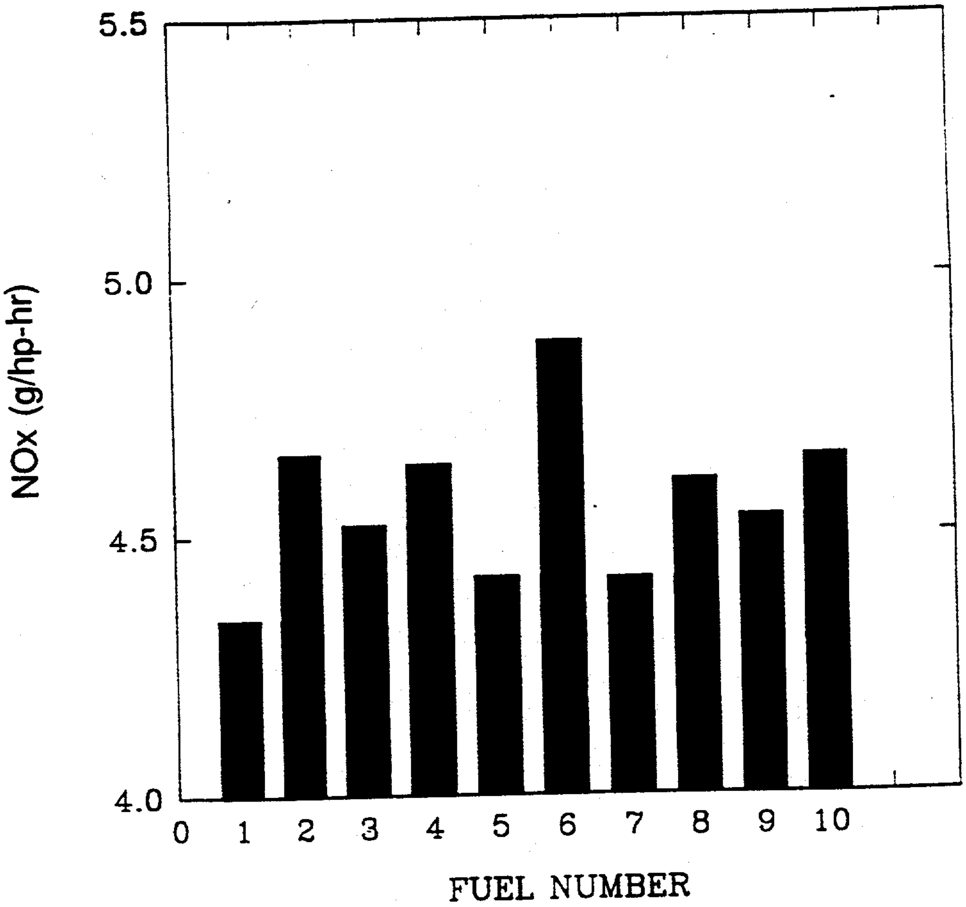

Figure 42. NOx emissions for the low-emissions fuel at Mode 2

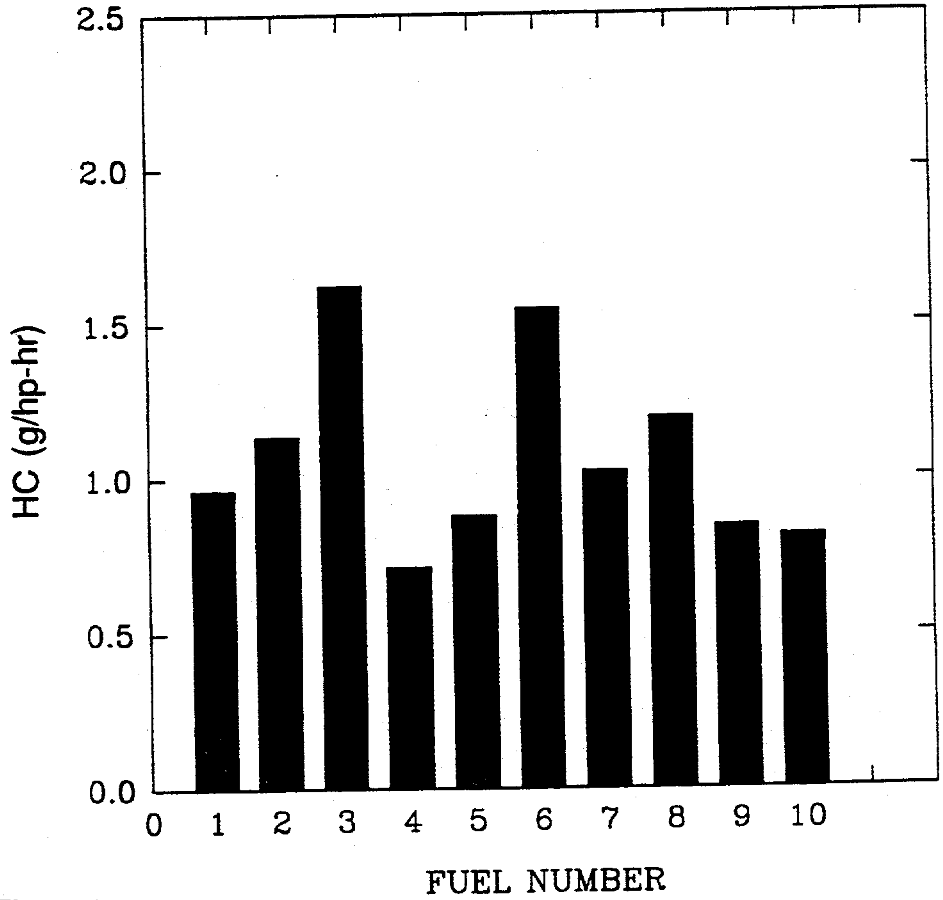

Figure 43. Hydrocarbon emissions for the low-emissions fuels at Mode 2

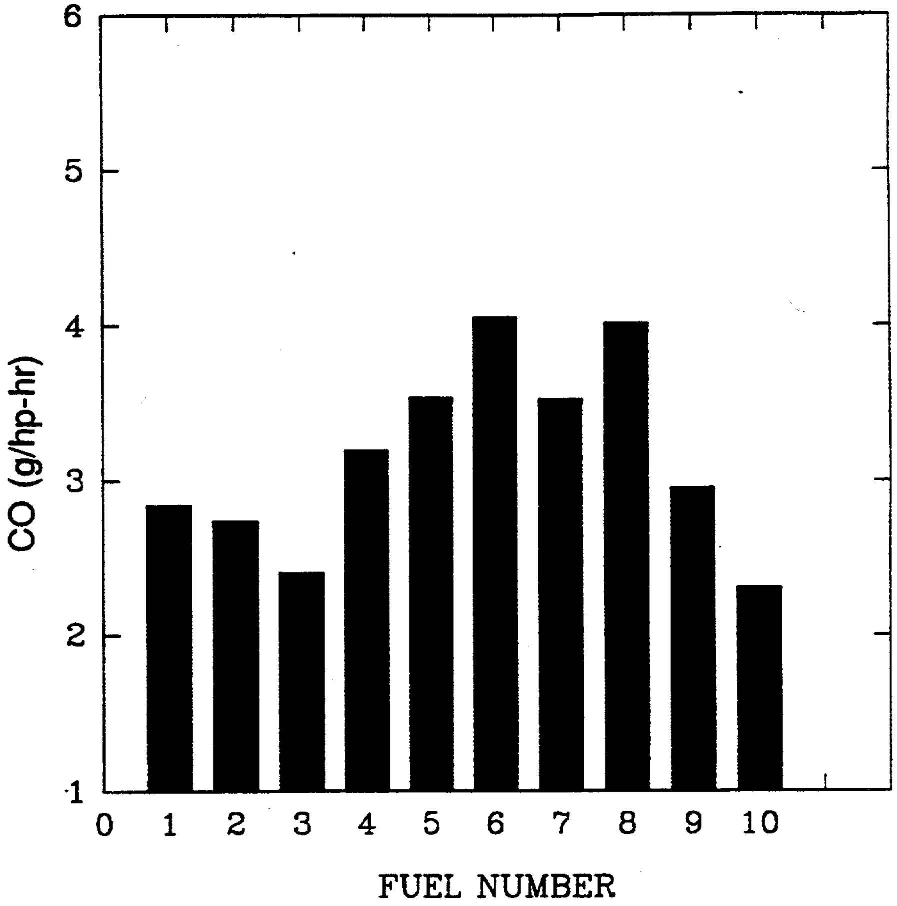

Figure 44. CO emissions for the low-emissions fuel at Mode 2

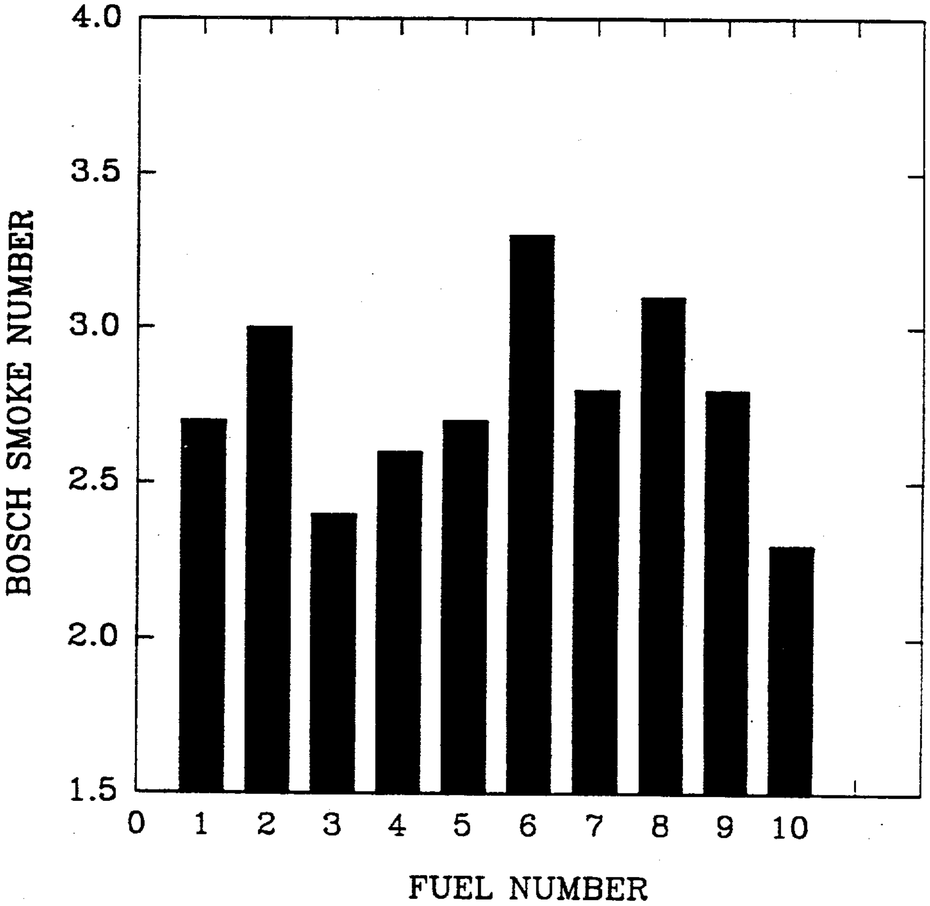

Figure 45. Bosch smoke number for the low-emissions fuels at Mode 2

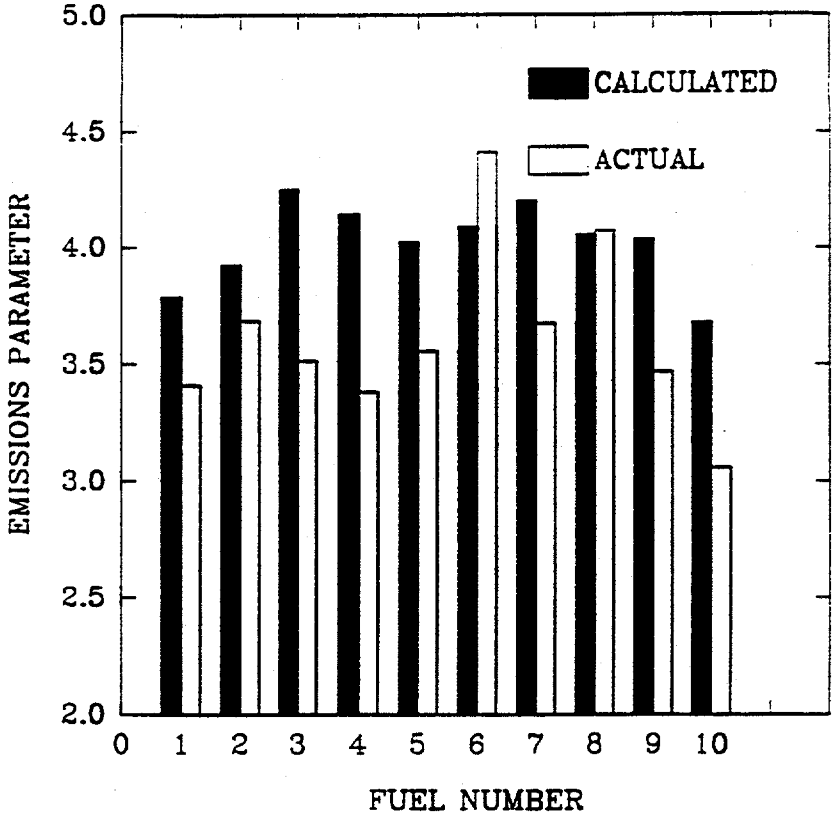

Figure 46. Emissions parameter, calculated and measured at Mode 2

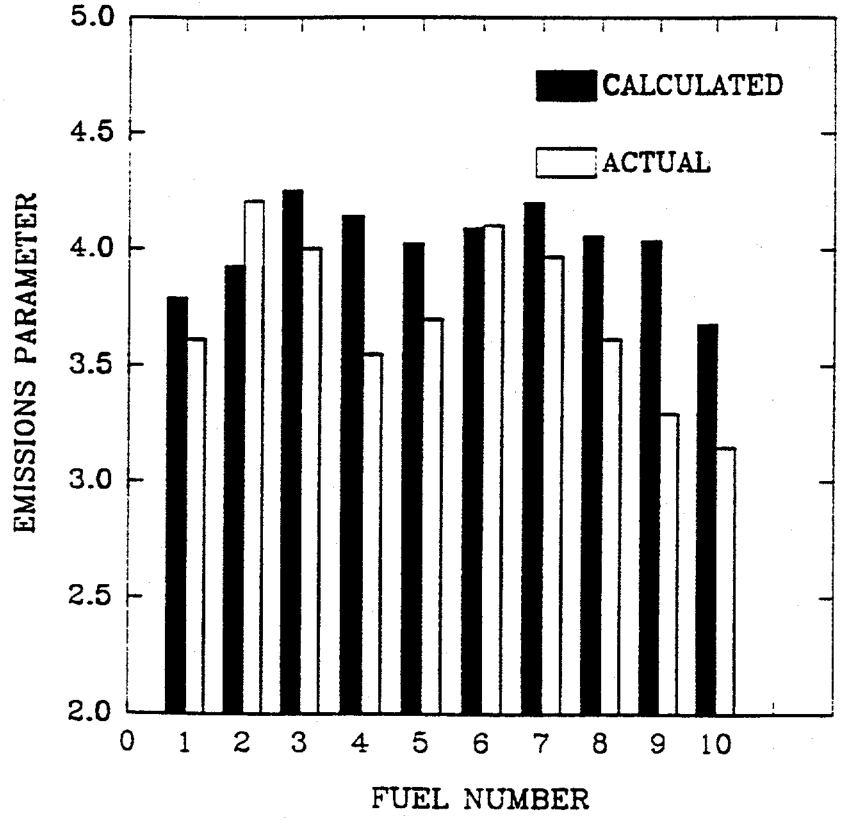

Figure 47. Emissions parameter, calculated and measured at Mode 1

As shown in Figure 39, the average EP for the 80 fuels examined in this project was 4.3 at the Mode 2 test condition. The reduction from 4.3 to 3.5 indicates that full-boiling-range low-emissions fuels can be designed and produced using actual blendstocks. Similar conclusions can be drawn from the data at the other test conditions, as can be verified by examining the Mode 1 EP values for the low-emissions fuels and all test materials, in Figures 47 and 48, respectively. The corresponding data for the other test conditions are presented in Appendix C.

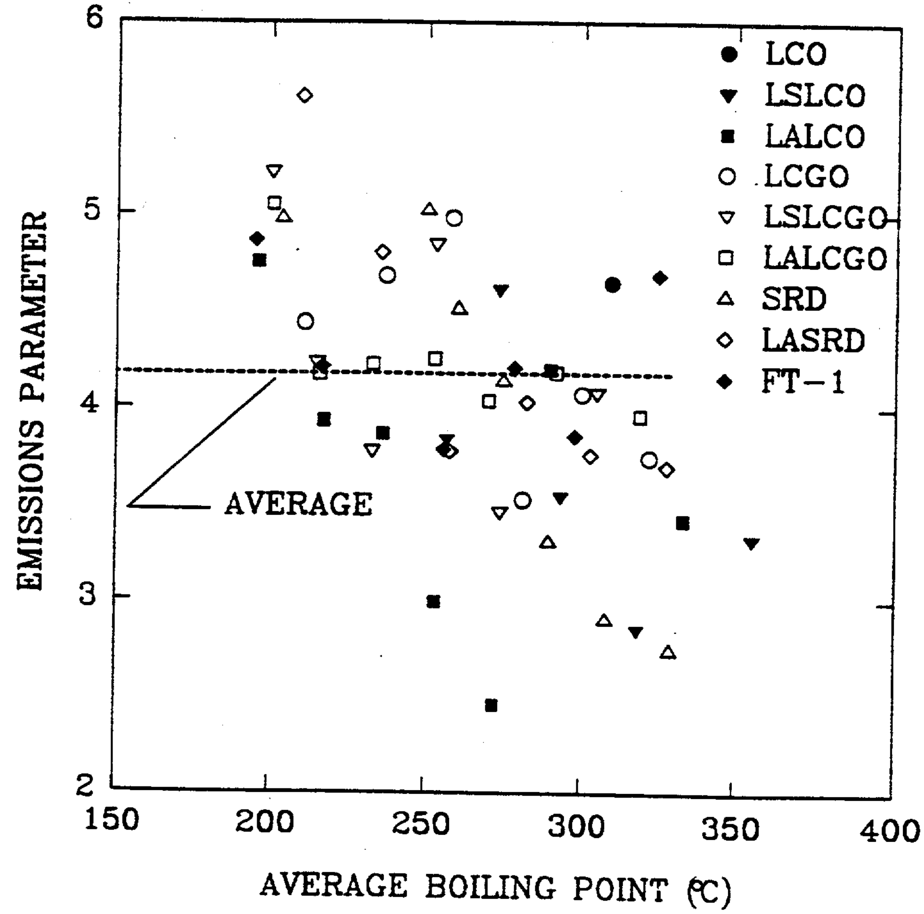

Figure 48. Emissions parameters for all test materials at the Mode 1 test conditions

Clean-Fuel Discussion

The results of the experiments indicated that aromatic content, aromatic type, cetane number, distillation, and density are all important in affecting the engine performance and emissions. These results agree with recent findings reported in the literature. The results, however, also indicate that the overall chemical structure is important in controlling the emissions and cetane number. It is simply not enough, for instance, to reduce the total aromatic content; the reduction of the tricyclic aromatic content also appears to be very important for NOx and smoke control. This may be most efficiently accomplished by hydrotreating the heavier fractions of the diesel fuel. Also, the cetane number relationship to the emissions is simply a manifestation of chemical structure that inheritently produces lower emissions. The data base from these experiments is extensive and could be the subject of much additional analysis. The following section is a brief summary of the most important conclusions drawn from analyses that have been completed to date.