Summary and Conclusions

Five different diesel-fuel feed and blendstocks were hydrotreated to at least two levels of sulfur and aromatic content. These materials were then distilled to seven or eight fractions by boiling point. The raw materials, as well as all of the fractions making 80 samples overall, were then subjected to a series of combustion-bomb and engine tests to determine the ignition, combustion, and emissions characteristics of each material. In addition, all materials were characterized extensively in terms of physical and chemical properties and chemical composition.

The resulting data base was statistically analyzed to develop preliminary relationships between the emissions characteristics and the fuel properties and composition. The results of these analyses indicated linear relationships. Linear programming techniques were then used to formulate 10 different low-emissions fuels based on blending to meet specific emissions targets designed to be indicative of future emissions standards. The predicted emissions performance and the actual emissions were trendwise similar over the speed/load range of the test engine. The actual emissions characteristics were, in fact, much better than targets and the corresponding baseline data for most of the fuels.

The following specific conclusions can be drawn from the results of this project:

1. Ignition quality and emissions characteristics are related to boiling point as indicated by the strong functional relationships between these parameters and the average boiling point of each fraction.

2. The proposed new specifications for reformulated diesel fuel limiting the end point and the aromatics content may not be compatible with each other and may lead to increased particulate emissions. Reducing the end point will reduce the cetane number in some feedstocks and can also reduce the effectiveness of hydrogenation in reducing the aromatics content. This overall cetane number reduction could have an adverse effect on NOx also.

3. Ignition and emissions characteristics are directly related to aromatic content and type of fuel, where:

$$CN = A_1+A_2\times(\text{Alkylbenzenes})+A_3\times(T50\%) +A_4\times(\text{Indenes})+A_5\times(\text{Paraffins}) +A_6\times(\text{Specific Gravity})+A_7\times(\text{Viscosity@40°C})$$

where the concentrations are in wt%, specific gravity is in gM/mL, viscosity is in centistokes (cSt), and where:

$A_1 = 277.1 \qquad R^2 = 0.94$

$A_2 = 0.54$

$A_3 = 0.31$

$A_4 = -1.83$

$A_5 = -0.13$

$A_6 = -437.3$

$A_7 = -1.98$

4. Because of the relationship between ignition quality and aromatics, the variation of the emissions characteristic is accounted for in the aromatic description of the fuel.

5. The aromatic content of the fuel is not always uniformly distributed across the boiling range of the fuel. In some cases, such as for the light-coker gas oil, the aromatics are concentrated in the heavier fractions.

6. Within the range of variation possible in the project, the relationships between emissions and fuel composition are linear, so that linear programming techniques can be used to design low-emissions diesel fuels.

7. Low-emissions diesel fuels can be formulated using raw materials that can, on the average, have relatively high-emissions characteristics. This is accomplished by processing and blending to achieve the emissions and cost goals.

8. The F-T diesels showed superior performance by two measures of cetane number determination. FT-1 blended linearly with petroleum stocks having a wide range of cetane numbers. The results did not show whether the contributions of aromatics dilution versus paraffin structure provide this good cetane number behavior.

9. The aromatics are distributed over the boiling range of the straight-run diesel fuel, similar to the light-cycle oils. Unlike the light-cycle oils, however, hydrotreatment appears to be much more effective in reducing the aromatics content of the heavier fractions of this fuel. In fact, cetane number was decreased by hydrogenation in mid boiling range.

10. The power output of the engine was not strongly affected by large variations in the fuel properties as long as the air-fuel ratio set point is held constant. Ignition depends on the cetane number, but the power is related mainly to the apparent combustion efficiency.

11. The emissions characteristics of the materials tested in this program are dominated by composition of the materials. The compositional data always provided more information in the regression models than the physical properties.

12. The nitric oxide emissions are modeled as:

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

where concentrations are in wt% and the coefficients are:

$A_1 = -96.34 \qquad R^2 = 0.82$

$A_2 = 0.22$

$A_3 = 0.24$

$A_4 = 1.17$

where the aromatic structure dominates the relationship.

13. The smoke emissions are related to the fuel properties in the following relationship where:

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

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

$A_1 = 2.24 \qquad R^2 = 0.61$

$A_2 = -0.065$

$A_3 = -0.029$

$A_4 = 0.08$

$A^5 = 0.027$

$A^6 = -0.013$

And where a significant portion of the variation in smoke could not be accounted for in the fuel variables. Experimental error or physical processes may account for the remainder of the variations.

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