The Effects of Fuel Aromatic Structure on Diesel Combustion

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ABSTRACT

A single cylinder open chamber diesel engine was used to determine the effects of fuel aromatic structure on particulate levels. A ratio-pyrometer mounted in the engine head was used to determine flame temperature. Four fuels were tested; one-ring aromatic blends of 31 and 41 cetane number and two-ring aromatic blends of 31 and 41 cetane number. The two-ring blends gave much higher particulates than one-ring blends. For each ring type, the 31 cetane number blend gave somewhat lower particulates than the 41 cetane number blend. The effect was caused by the increase in premixed burning at the lower cetane number. Evidence from the heat release and ratio-pyrometer data indicates that the major cause of the differences in exhaust particulates between the one and two rings blends was of chemical kinetic origins. Particulates produced during the last third of burning were also judged to have a significant effect on the differences noted.

THE ADDITION OF AROMATIC SPECIES to diesel fuel is known to lower the cetane number and to increase exhaust particulate levels (1,2,3). However, the effects of the aromatic structure have not been clearly identified. The objective of this paper is thus to show these effects, in particular the differences in combustion and emissions caused by the addition of one-ring and two-ring aromatics.

Changes in fuel composition, such as the addition of an aromatic species or blend, can cause many confounding changes in the diesel combustion characteristics. The chemical changes can cause significant kinetic effects that strongly influence ignition delay and particulate formation. However thermodynamic and physical properties changes that accompany the chemical changes can also influence the combustion temperature and heat release shape. The confounding nature of such changes is illustrated by the much simpler case of a laboratory diffusion flame. In such studies (4,5) naphthalene-ring containing species have been shown to be more prone to soot formation than the benzene-ring containing species. However, studies (6,7) have also shown that the ranking of sooting tendency is strongly influenced by flame temperature so that differences often attributed to chemical structure may actually be the result of flame temperature. For these reasons, such confounding effects have been minimized as far as possible in the present work by careful selection of the fuels. The differences in flame temperature have been measured using a ratio-pyrometer. Unavoidable differences in cetane number have been dealt with by making the cetane number a controlled parameter in the fuel selection process.

FUEL PROPERTIES

Two types of aromatic solvents, namely benzene-ring containing and naphthalene-ring containing, were chosen because of their markedly different behavior in soot formation in flames. Various amounts of solvents were then added to an aromatics-free fuel (JP-7) to produce four fuels with two cetane numbers.

Table 1 shows the fuel properties of the different fuels, the four special fuels are quite similar in their distillation characteristics, surface tension, viscosity and heat of combustion. They all have low sulfur content which is important given the large effect of sulfur on particulates (1). The sixth fuel shown is a blend of commercial diesel fuel and was used for comparison with the special fuels.

ENGINE OPERATION

A modified TACOM/Labeco single cylinder direct injection engine, with specification as given in Table 2, was used. Modifications were; use of a Mexican-hat shaped piston bowl, fabrication of a new engine head, use of a different fuel injection system, and increase of the compression ratio from 16:1 to 24:1. The tests were all conducted at the same swirl ratio (nominally 3) produced by a shrouded valve.

Table 1. Properties of Cetane-Adjusted, Composition-Controlled Fuels

Property	ASTM Method	JP-7	One-Ring	Two-Rings	One-Ring	Two-Rings	Diesel #1/#2
Fuel No. Designation		1	2	3	4	5	6
Cetane Number	D 613	57.2±1	41.7±1	41.2±0.7	31.3±1	30.3±1	43.3
Density:							
Sp Gr @ 60°F	D 1298	0.7954	0.8198	0.8438	0.8383	0.8933	0.850
°API		46.4	41.1	36.2	37.3	26.9	35.6
Distillation,	D 86	°C	°C	°C	°C	°C	N.A.
IBP		198	189	202	186	199	
50		211	205	219	200	227	
FBP		259	260	287	254	287	
Viscosity, cST @ 40°C	D 455	1.57	1.36	1.55	1.22	1.59	
Lower Heat of Combustion (MJ/Kg)	D 240	43.815	43.564	44.146	43.375	43.075	42.407
Elemental Analysis, wt%	Micro-Combustion						
Carbon		85.66±0.09	86.59±0.02	87.37±0.16	87.34±0.10	89.00±0.16	86.90
Hydrogen		14.70±0.01	13.42±0.02	12.74±0.02	12.55±0.02	11.04±0.04	12.71
Sulfur	XRF	<0.01	<0.005	<0.005	<0.005	<0.005	.20
H/C Atom Ratio		2.04	1.85	1.74	1.71	1.48	1.76
Hydrocarbon Type, vol%	D 1319						
Saturates		96.9	73.9	72.9	53.0	49.9	68.4
Olefins		1.0	1.1	<0.1	1.2	<0.1	1.4
Aromatics		2.0	25.0	27.1	45.7	50.1	30.2

Table 2
Engine Specifications

TACOM/Labeco CLR
Single Cylinder
     (11.43 cm bore/11.43 cm stroke), 4-cycle
Direct Injection
Compression Ratio 24:1
Fuel Pump   American Bosch Type APE1B-80P-4843A
Injector   Holder — American Bosch AKN-90M-6425A
        Tip — American Bosch soft machined
          out by International Harvester
          4-hole
          150° included angle
          .0274 cm diameter orifice

The new engine head was designed to incorporate an instrumentation port providing access from the head to the combustion chamber. A new and smaller American Bosch injector system was chosen for this head. The instrumentation port occupies about one fourth of the flame plate. A 6.35 mm diameter window was placed in the instrumentation port as shown in Figure 1.
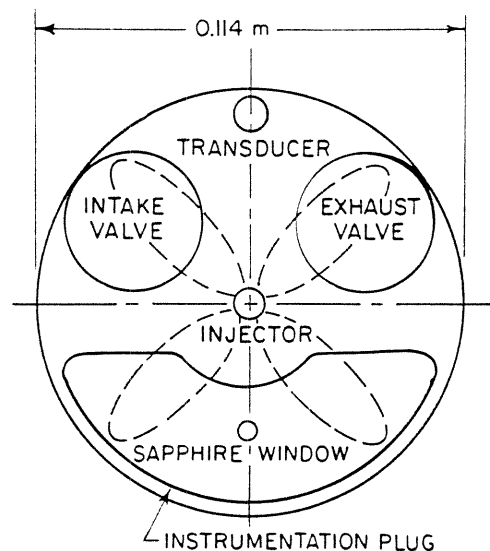

Fig. 1. View of engine head from cylinder gas side showing placement of pyrometer window relative to spray plumes.

EXHAUST PARTICULATES

A mini-dilution tunnel similar to the GMRL version (8) was used to mix the raw exhaust with filtered house air. The sampling probe in the exhaust port was modified from the GM design to allow collection of a larger raw exhaust sample thus reducing the sampling time. Teflon coated filters were chosen because of their stability, retention efficiency and compatability with solvent extractions. Filters were weighed before and after particulates collection by use of a semi-micro balance. A Soxhlet extraction method was used to extract the cyclohexane soluble fractions from the soiled filters. Drying of the filters after extraction was done by filtered, dry, hot air. A Bosch smoke meter was also used to indicate particulate levels. A good correlation was found between the mass and smoke number data (9).

HEAT RELEASE ANALYSIS

Average cylinder pressure-time data were taken with the U.W. data acquisition system. The micro-processor allows data to be taken at half crank angle intervals over a 320 crank angle cycle and to ensemble-average 44 cycles. These data were then used to compute the apparent rate of heat release. The Krieger and Borman single zone model for diesel heat release was used. This model, though greatly simplifying the combustion process, can be used to describe the pre-mixed and diffusion burning qualitatively. It also permits one to determine the ignition delay in a consistent manner.

RATIO-PYROMETER

The ratio-pyrometer (10) was mounted in the engine head as shown in Figs. 1 and 2. A synthetic sapphire cylinder, 6.35 mm in diameter by 38 mm long, was used to gather the radiation. The rod was recessed such that its effective window diameter was 4.6 mm. A recess depth of 2.8 mm was found to give the best protection against sooting. Data at equivalence ratios up to 0.4 could be obtained at steady state engine conditions with very minimal window sooting. The radiation from the sapphire cylinder was brought out to the filters and detectors by use of a bifurcated fiber optic bundle. The radiance was measured at 847 and 644 nm using photodiode detectors. The 1000 times amplified signals were recorded at one-half crank angle intervals for 21 consecutive cycles. Temperature histories were calculated for each cycle and then the 21 histories were ensemble averaged. Portions of the data near the start of the detectable signal were clipped off by the amplifiers which had inadequate dynamic range. Toward the end of combustion (after +40°TDC) some cycles had portions with no detectable signal.

Calibration of the pyrometer was done by use of a Mole-Richardson pyrometric molarc lamp. The calibration was done with the instrument mounted in the head. Calibration with and without soot on the window gave no difference, indicating that deposits as thick as 0.1 mm were acting as gray filters.
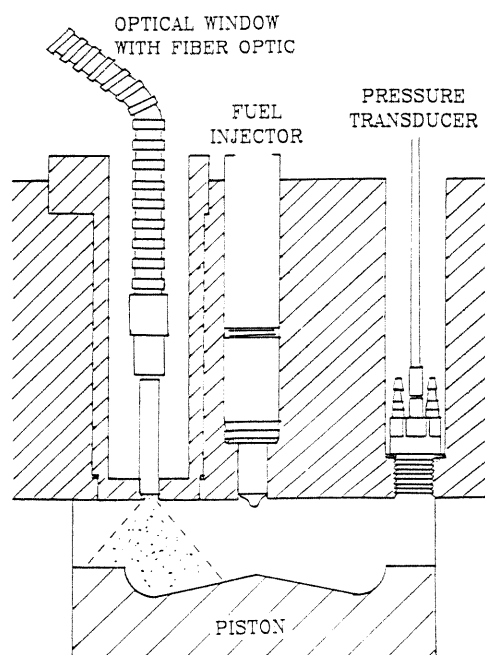

Fig. 2. View of engine from side showing pyrometer.

EXPERIMENTAL RESULTS

Ignition delay, using cylinder pressure to determine the start of burning, followed the cetane numbers in an approximately linear fashion. As shown in Figure 3, for a given cetane number the two-ring aromatics blends gave 25 to 30 percent more particulates mass than the one-ring blends. However, reduction in cetane number, by addition of aromatic solvent, reduced the exhaust particulates although the smoking tendency of the mixtures, as measured by sooting heights, increased. The reduction is attributed to an increase in the premixed burning portion as the cetane number was decreased. Such a decrease has been observed previously (11).

The data of Fig. 3 indicate that increasing the aromatic content decreases the extractables. For most of the data the extractables are proportional to the amount of aliphatics. The aromatics produced considerable more solid particulates mass, but little change in extractable mass. Chemical analysis of the extractables for aromatic content is required to draw any further conclusions.

Measurements of exhaust NO_x and CO showed no significant change with fuel type. Typically an increased amount of premixed burning increases the amount of NO produced, however this effect was offset by the longer ignition delay which retarded the combustion event for the fixed injection timing used here.
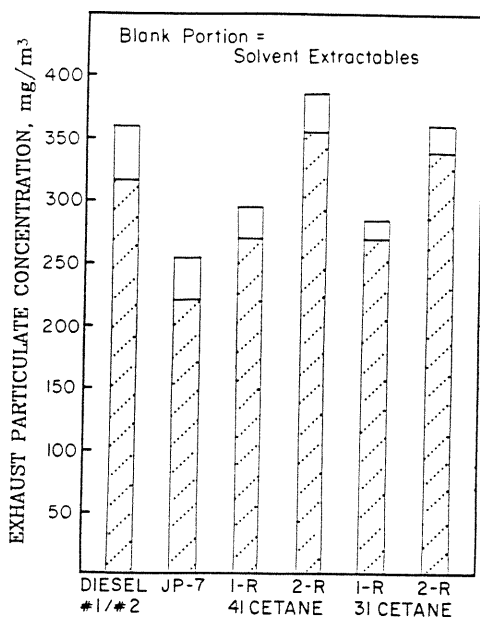
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Fig. 3. Exhaust particulate concentration for the different fuels of Table 1. Engine conditions: 1000 rpm, N.A., 22° btdc injection and 0.5 equivalence ratio.
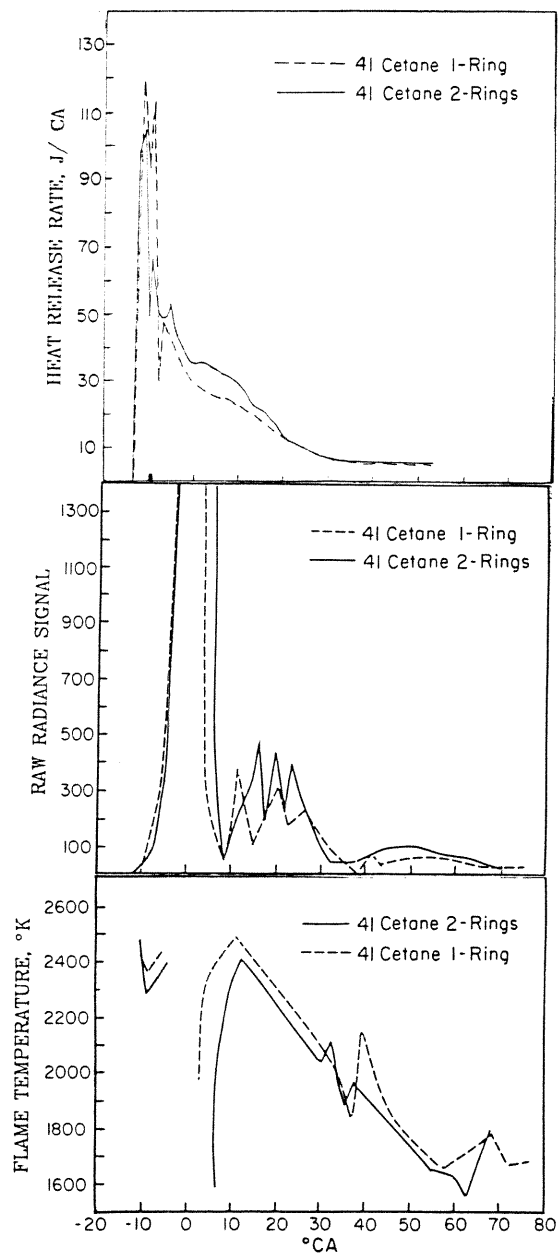

Fig. 4. Heat release, radiance and flame temperature for the 41 cetane number fuels. Engine conditions; 1000 rpm, N.A., 22° btdc injection and 0.4 equivalence ratio.

In general, differences in the exhaust particulate levels between one and two ring blends could be caused by differences in flame temperatures, however such differences should be small because the blends used here had very similar heating values (see Table 1). Figure 4 shows the heat release, radiance and temperature histories for the 41 cetane one and two ring blends. The one ring fuel gave a slightly higher temperature (75°C), had about 5 percent more premixed burning and showed a more rapid drop in radiance following the off-scale radiance spike which peaked at about TDC. Note that the radiance spike, in the region of -10 to +10 crankdegrees, starts at what is commonly defined as the start of premixed burning (12). The two ring blend had a larger amount of burning in this region and up to 20° ATDC.

Interpretation of these data must take into account that the standard deviation in temperature was about 100°K up to about 30° ATDC; after that the data were more erratic with some cycles giving no recordable signal in that region. The spike in the radiance curve is interesting in terms of its rapid decrease. It is unlikely that this decrease could be caused by the geometrical view of the flame plume, because the swirl ratio was only three. It is thought that rapid mixing and oxidation due to the high temperature caused this drop. The rise in radiance from 10 to 30° ATDC may be attributed to continued production of soot, but with lower temperatures and agglomeration of soot contributing to a lower oxidation rate. After 30° the burning and oxidation are both low giving an approximately constant radiance.

The slightly higher volatility of the one ring blend may have contributed to its larger premixed burning and thus to the smaller amount of mixing controlled burning compared to the two ring blend. The 300°C difference in temperature during the period from 5° to 10° ATDC must be attributed to fuel-air-ratio differences and could account for the more rapid drop off of the radiance signal for the one ring blend. It appears that the net result of production and oxidation in the region of 10° to 30° ATDC governed the difference in particulates observed

in the exhaust stream. In this case the oxidation rate should have favored the destruction of one ring particulates because of the higher temperature. However, the larger burning rate of the two ring fuel in this region coupled with its greater potential for sooting due to its chemical structure predominated, resulting in its higher particulate level in the exhaust.

The trends between the one and two ring blends at 31 cetane were similar to those at 41 cetane, but much less obvious. All of the differences previously noted were greatly reduced. The reduction in particulates for the two ring blend in going from 41 to 31 cetane can be attributed to the five percent increase in premixed burning. The smaller reduction in particulates for the one ring blend can similarly be explained by its smaller (two percent) increase in premixed burning. However, this smaller increase was unexpected because the ignition delay increase in going from 41 to 31 cetane was the same for both the one and two ring blends. Volatility differences were in the wrong direction to produce this effect so some other factors such as atomization or enthalpy of vaporization may have been the cause.

Because of the design of the research head and ratio-pyrometer it was felt that only small changes in inlet pressure could be allowed. Thus data were taken for the JP-7 fuel with a boost pressure of only 23.6 KPa above the naturally aspirated case. Two cases were considered, constant equivalence ratio (0.3) and constant fuel flow. Constant fuel flow gave an equivalence ratio of 0.4 at the naturally aspirated condition. The boosted condition gave 1.6 Bosch smoke number compared to the values of 1.8 at the same equivalence ratio and N.A., and 2.1 at the higher (0.4) equivalence ratio and N.A. Thus boosting the pressure at constant fuel rate lowered the exhaust particulate as expected. However, boosting at constant equivalence ratio also lowered the particulates. This last result, shown in Fig. 5, is interesting in that the amount of premixed burning was about the same, but the amount of burning in the 10° to 30° ATDC portion as well as the temperature in that region favored more net soot formation for the boosted case. The radiance signal was smaller for the boosted case however, and showed a larger difference in the range of 30 to 40° ATDC. At this point little burning or oxidation should have been taking place for either case. This may indicate that the boosted pressure with its higher partial pressure of oxygen extended the oxidation period and thus reduced the net particulate output.

Both the one and two ring 41 cetane fuels showed similar reductions in exhaust smoke when the intake pressure was increased at constant fuel flow rate. However, the differences in late burning just discussed for the JP-7 fuel were not observed. The only large difference between the N.A. and boosted data for these two fuels was that the boosted condition gave a much smaller radiance spike.
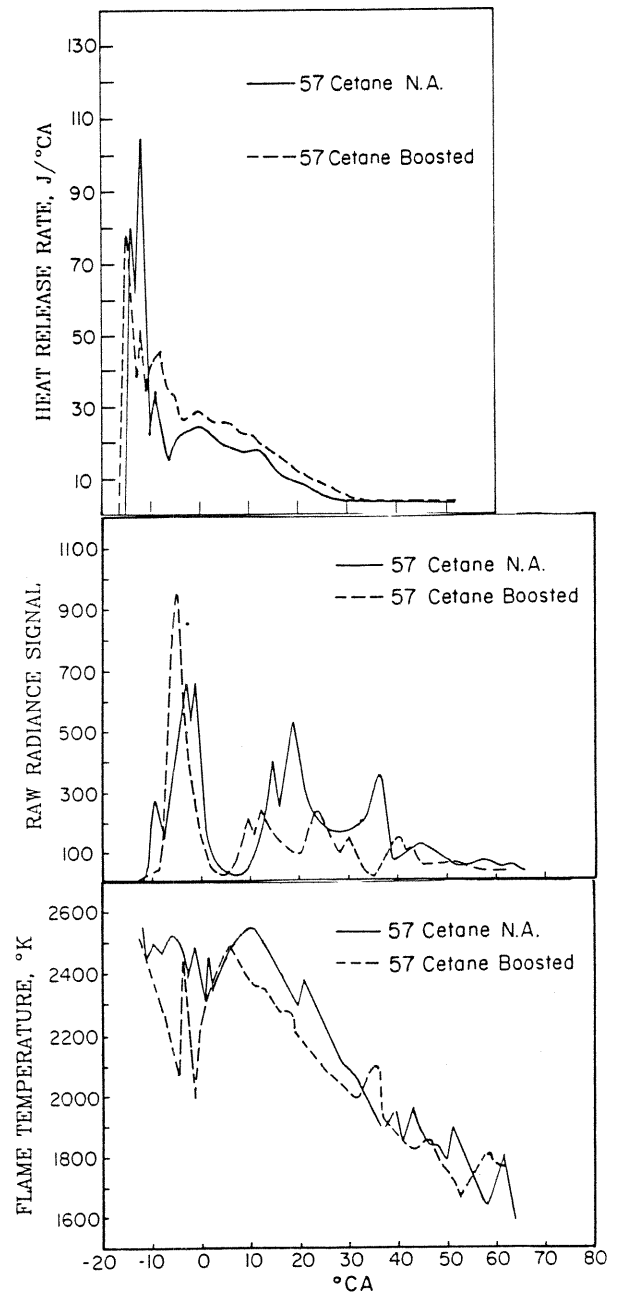

Fig. 5. Heat release, radiance and flame temperature for JP7 fuel. Engine conditions; 1000 rpm, 22° btdc injection and equivalence ratio 0.3 for N.A. and inlet pressure increased by 23.6 kPa.
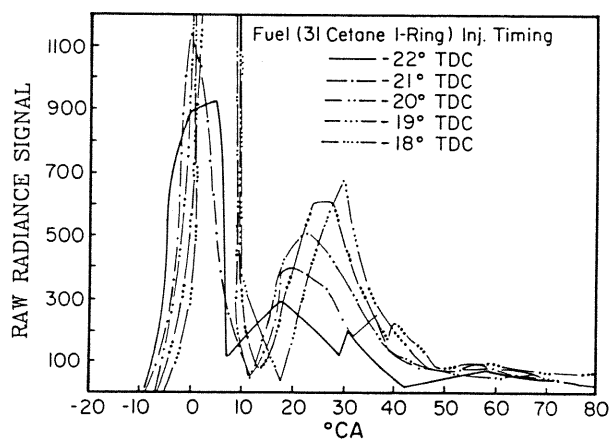
Fig. 6. Radiance data for 31 cetane number one-ring blend fuel. Engine conditions; 1000 rpm, N.A., 0.4 equivalence ratio and various injection timings.
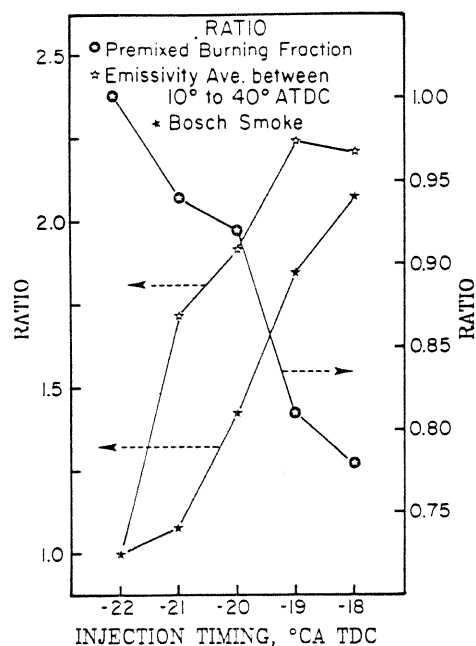

Fig. 7. Ratio of premixed burned fraction, average emissivity and smoke number at various injection timings to the values at 22° btdc. Same engine conditions and fuel as in Figure 6.

Boosting the inlet pressure at constant inlet temperature and fuel rate has little effect on exhaust NO_x, but decreases particulates. Reduction of NO_x by injection retard however increases particulates. Figure 6 shows the radiance signal for various injection timings for the N.A. case and the 31 cetane, one ring blend. The large spikes between 20° and 40° ATDC increased with injection retard. The temperatures for all cases were the same in this region, all varying from 2200°K to 1900°K with increasing crankangle. Figure 7 shows the effect of the retarded timing relative to the -22° case. The Bosch smoke increase and premixed fraction decrease are to be expected. The emissivity ratio is the average value from 10.5° to 40° ATDC. The emissivity is approximately proportional to the in-cylinder particulate concentration and thus increases in the expected manner.

CONCLUSIONS

The major objective of this work was to determine how fuel aromatic content and aromatic structure affect diesel combustion and exhaust particulates. The results show, as expected, that aromatic content causes both an increase in ignition delay and an increase in exhaust particulates. Increasing the ignition delay increases the amount of premixed burning which

tends to reduce particulate production. Thus an increasing addition of aromatics, while producing harsh combustion, does not monotonically increase the amount of exhaust particulates.

The addition of aromatics did not significantly increase the amount of soluble fraction of the particulates. Thus the relative amount of soluble fraction decreased. It thus seems important that the effect of aromatic content on soluble fraction composition be established in future work.

As anticipated, the two ring aromatic blends gave higher exhaust particulates than the one ring blends. The two ring blends had a slightly lower temperature during the mixing controlled combustion period and less premixed burning than the one ring blends. The two ring aromatic solvent used was less volatile than the one ring aromatic solvent even though the volatility of each final blend was similar to that of the base fuel. The data may thus indicate that the droplet vaporization process distilled off some of the one ring solvent during the ignition delay, thus increasing the amount of that fuel that burned as premixed fraction. The fact that the ignition delay was affected about the same way by both the one and two ring blends indicates that in the region of ignition the mixture was typical of total fuel content rather than only the more volatile component. This is possible

since small droplets which completely vaporize would give a mixture typical of the entire fuel composition. The slight depression of flame temperature may have also been due to vaporization differences. The richer mixture being the cooler and being formed from the less volatile two ring blend. Note that the lower temperatures throughout the late portion of the combustion period also would reduce the rate of oxidation of particulates. While these combustion differences may be important they do not seem large enough to explain the substantial differences in exhaust particulate levels between the one ring and two ring blends. We thus believe that the chemical rate of soot production is the major cause of these differences.

While it is interesting that a very large peak in soot appears right after the end of premixed burning and that the heat release curve prediction of the end of premixed burning agrees very well with the prediction from the radiance data, the rapid decrease in radiance from this peak value is even more significant. It is unlikely that this rapid decrease was caused by geometrical view factors or dilution because of the very short time involved. We conclude that the reduction was caused by rapid oxidation of the soot at the high product temperatures. As a consequence, the mixing controlled burning taking place later, during the last third of the combustion period, can control the exhaust particulate level even though the rate of particulate production is much lower during that period than during the early portion of mixing controlled burning.

ACKNOWLEDGEMENTS

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