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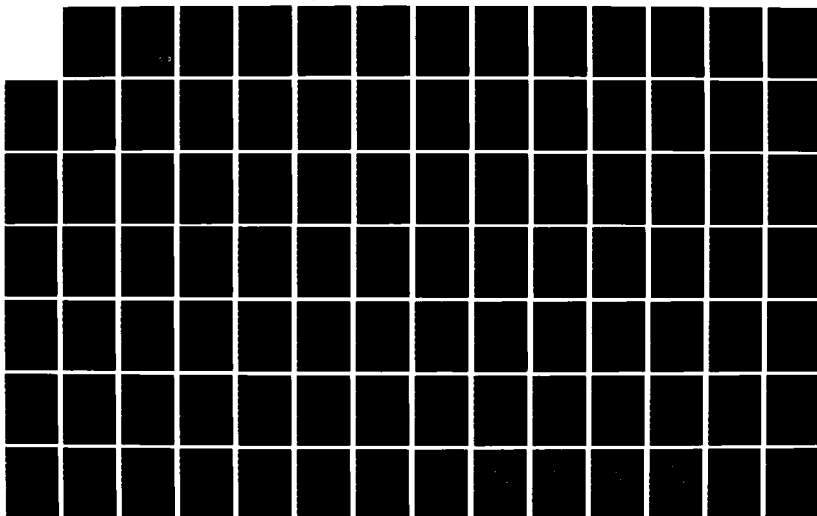
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FUEL EFFECTS ON SOOT FORMATION IN TURBOJET ENGINES

R.J. GILL AND D.B. OLSON
AEROChem RESEARCH LABORATORIES, INC.
P.O. BOX 12
PRINCETON, NEW JERSEY 08542

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NAVAL RESEARCH LABORATORY
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The results of tests on how fuel composition affects the performance of three Navy aircraft engine combustors, the TF30, T56, and T53, were analyzed. The objective of this analysis was to identify which fuel property best correlated with the smoke-related measurements: radiation flux, liner temperature rise, smoke number, and smoke emissions. The effects of fuel composition were investigated by using a series of ten Naval Air Propulsion Center jet fuels with various properties, such as hydrogen contents of 12.83 to 13.82% and total aromatic hydrocarbon contents of 15.9 to 28.5%. Several laboratory combustion characteristics of these fuels were measured and these characteristics were used in the analysis. Altogether, 15 fuel parameters were used to correlate the 45 combustor test results. The reported operating conditions of the tests, such as inlet air pressure, inlet air temperature, or fuel/air ratio, were also used as correlating parameters to determine whether variations in these variables, nearly constant for individual tests, also affected the smoke-related test results. Originator Supplied Keywords include: (over)			
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The conclusions drawn from the correlation analysis are:

(1) Overall, statistically significant correlations of fuel parameters with combustor test results were obtained in fewer than 50% of the tests. The two fuel properties that best correlated smoke-related test results were: the laboratory diffusion flame fuel consumption rate at the smoke point and the diffusion flame threshold sooting index. The average coefficient of determination, r^2 , for correlations of the best fuel parameter, the diffusion flame fuel consumption rate at the smoke point, with the 45 test results was 0.37.

(2) In about 25% of the combustor tests the operating conditions varied enough to give significant correlations between the smoke-related tests results and the values of the operating conditions.

(3) The radiation flux data were correlated with fuel properties better than the other combustor test data.

(4) The combustor liner temperature rise data correlated better with variations in the engine operating conditions than with any fuel parameter.

(5) Premixed laboratory flame measurements on the test fuels were unsuccessful in correlating the combustor results.

(6) Aromatic hydrocarbon content data, divided into mono- and polycyclic aromatic hydrocarbon classes, were unsuccessful in correlating the combustor results.

(7) Total aromatic hydrocarbon content, measured at the Naval Research Laboratory using the HPLC/DRI technique, was found to correlate the combustor test results better than the data obtained using the ASTM FIA technique. Note, however, that total aromatic content was not one of the best fuel parameters for correlating these combustor data.

(8) Based on the results of this program, no universal fuel parameter for correlating smoke-related engine test results has been identified.

Supporting Work

To support the fuel effects correlation analyses, numerous laboratory measurements were conducted on the ten test fuels and a few blending components. These measurements include: densities, molecular weights, diffusion and premixed flame soot thresholds, and diffusion and premixed flame soot yields. Some results obtained from this work are:

(1) Development of a technique and apparatus for measuring laminar diffusion flame soot yields.

(2) Development of a mixture rule for calculating diffusion flame soot yields.

(3) Testing of the diffusion flame soot threshold mixture using NMR chemical class analysis.

(4) Analysis of the significance of flame temperature in sooting premixed laminar flames.

(5) Development of an improved premixed flame mixture rule for both soot thresholds and soot yields.

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ABBREVIATIONS AND SYMBOLS

A	Fitting constant for temperature data.
a	Fitting constant for diffusion flame threshold soot index.
a'	Fitting constant for premixed flame threshold soot index.
ASTM	American Society for Testing and Materials.
AR _x (HPLC)	Volume percent of aromatic hydrocarbons determined by high pressure liquid chromatography.
AR _x (FIA)	Volume percent of aromatic hydrocarbons determined by fluorescence indicator absorption.
B	Fitting constant for temperature data.
b	Fitting constant for diffusion flame threshold soot index.
b'	Fitting constant for premixed flame threshold soot index.
c	Speed of light.
C/O	Carbon to oxygen mole ratio.
DOF	Degrees of freedom.
F/A	Total fuel to air mass ratio.
FCR	Fuel mass consumption rate.
FCR ₀	Fuel mass consumption at smoke point.
ΔFCR	Increase in fuel mass consumption rate beyond that at the smoke point necessary to produce soot at a rate of 200 μg s ⁻¹ .
FIA	Fluorescence indicator absorption.
f _v	Soot volume fraction.
f _{0v,i}	Soot volume fraction for hydrocarbon i at soot threshold.
f _{v,mix}	Soot volume fraction for hydrocarbon mixture.

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Hx	Weight percent hydrogen in fuel.
HPLC/DRI	High pressure liquid chromatography using differential refractive index detector.
h	Diffusion flame height at the smoke point.
IR	Infrared.
k	Boltzmann's constant.
LTR	Liner temperature rise.
MCAH	Weight percent monocyclic aromatic hydrocarbon content in fuel determined by HPLC.
MW	Molecular weight.
MW ₁	Molecular weight of mixture component 1.
NAPC	Naval Air Propulsion Center.
NMR	Nuclear magnetic resonance.
NRL	Naval Research Laboratory.
P _λ	Radiated power per unit wavelength at wavelength λ.
P _{in}	Combustor inlet air pressure.
PCAH	Weight percent polycyclic aromatic hydrocarbons in fuel determined by HPLC.
RF	Radiation flux.
SE	Smoke emissions.
SLTO	Sea level takeoff.
SN	Smoke number.
SP	ASTM Smoke Point.
1/SP	Reciprocal of the ASTM Smoke Point.
SPE	Soot production efficiency, defined as the slope of the soot production rate vs. fuel consumption rate curve in the 100 - 300 μg s ⁻¹ region.
SPR	Soot mass production rate from a diffusion flame.

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SPR_{mix} Soot mass production rate from a mixture.

T_0 Premixed flame temperature at soot threshold.

T_{in} Combustor inlet air temperature.

$T(f_v)$ Premixed flame temperature at 2.0 cm above the burner where the soot volume fraction is 2×10^{-7} .

TC Thermocouple.

TSI Threshold soot index.

TSI_i Threshold soot index for component i in a mixture.

TSI_{df} Diffusion flame threshold soot index.

TSI_{mix} Threshold soot index of a mixture.

TSI_{pf} Premixed flame threshold soot index.

TSI_{reg} Premixed flame threshold soot index obtained using the temperature regulated burner.

TSI_{unreg} Premixed flame threshold soot index obtained using the unregulated temperature burner.

X_1 Mole fraction of component i.

X_1 Mole fraction of paraffins from NMR analysis.

X_2 Mole fraction of MCAH from NMR analysis.

X_3 Mole fraction of PCAH from NMR analysis.

β The slope of a soot volume fraction vs. equivalence ratio plot.

β_1 The slope of a soot volume fraction vs. equivalence ratio plot for component i.

ϵ The emissivity at wavelength .

θ The slope of a soot volume fraction vs. inverse temperature plot.

θ_1 The slope of a soot volume fraction vs. inverse temperature plot for component i.

Wavelength.

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$3\lambda EP$ Three wavelength emission pyrometer.

ϕ Equivalence ratio.

ϕ_c Premixed flame soot threshold equivalence ratio.

$\phi_{c,i}$ Premixed flame soot threshold equivalence ratio for component i.

$\phi(f_v)$ Premixed flame equivalence ratio at which the soot volume fraction at 2.0 cm above the burner equals 2×10^{-7} .

$\phi_{metered}$ Combustor fuel to air equivalence ratio.

The constants, 269 and 118, were determined for the "unregulated burner" by measuring the θ_c values for 10 pure hydrocarbons for which TSIPf values had been reported by Calcote and Manos,⁴ and then performing a linear least squares fit of reported TSI values for these hydrocarbons to measured θ_c values (see Ref. 2). The "regulated burner" was not calibrated, so TSIs were calculated using the "unregulated burner" a and b values. For the purposes of correlation with the combustor results, either set of TSIs is fully self-consistent and therefore suitable.

The premixed flame TSI values for the NAPC fuels, calculated from the unregulated and regulated θ_c values, are given in Table 7. The AeroChem-A fuel mixture TSIPf values are given in Table 2.

4. Soot Volume Fraction Measurements

The soot volume fractions, f_v , the fraction of combustion gas volume occupied by the soot particles, were measured in this work by determining how the extinction of light by soot particles (due to both scattering and absorption) changed with wavelength. This variation also depends on the soot particle number density, diameter, and complex index of refraction.

Pagni and Bard²⁷ have developed a practical scheme for reducing wavelength-dependent extinction data to soot concentrations (i.e., soot volume fractions) when Mie theory applies, as it does in the present case where the soot particles are of similar size compared to the wavelength of light used in the measurements. This procedure was followed using the complex index of refraction for soot as reported by Lee and Tien.²⁸

In this work, when both the Mie theory and the simpler Rayleigh scattering theory (valid when the particles are smaller than the wavelength) f_v values were calculated (even though the Mie theory should have been used), the ratio of the soot volume fractions was approximately constant: $f_v(\text{Rayleigh})/f_v(\text{Mie}) = 2.25 \pm 0.10$. Therefore, when Mie theory values of f_v could not be calculated because of poor signal to noise ratios, then Rayleigh f_v (which could be obtained with poorer data) were obtained and divided by 2.25 as a reasonable f_v estimate.

The apparatus is shown in Fig. 4. A tunable argon ion laser (5 mW power per laser line) provided monochromatic light at 515 nm or 488 nm. A helium-neon laser provided 633 nm light. The laser beams were aligned to ensure that each laser's light beam would traverse identical paths through the flame. The pathlength of the light beams through the flame was increased by multiple

Atmospheric pressure laminar premixed flames were stabilized on a 2.1 cm i.d. stainless steel tube bundle (130 tubes, 0.1 cm i.d.), and were surrounded by an annular fuel-rich propane/air shroud flame. To control the burner temperature with or without a flame burning, both air cooling and electrical heating were used.

The jet fuels were metered using a precision bore syringe driven by a stepping motor drive. For the experiments reported here, the fuel feed rate was $0.955 \pm 0.006 \text{ cm}^3 \text{ min}^{-1}$. The liquid fuel was air-atomized into a heated vaporization chamber and mixed with additional air. Air flows were metered through calibrated, critical flow orifice systems; the air and fuel flow uncertainties were each about $\pm 0.6\%$. The soot threshold equivalence ratio could be reproduced within $\pm 2\%$.

This burner was operated in two modes. In the "unregulated burner" mode, the burner was allowed to reach thermal equilibrium with the flame, that is, the burner electrical heating coil and air cooling were turned off. In this mode, the burner surface temperature was typically $290\text{--}350^\circ\text{C}$. The "regulated burner" mode employed both air cooling and electrical heating to maintain the burner surface at $250 \pm 10^\circ\text{C}$.

Further details of the apparatus and its operation can be found in Refs. 2 and 5.

2. Soot Threshold Equivalence Ratios

The soot threshold equivalence ratio, ϕ_c , is defined as the equivalence ratio at the first appearance of visible yellow emission. Sometimes "yellow streaks" would first appear at the circumference of the flame and then, as the flame was made more fuel rich, throughout the center of the flame. In these flames, the soot threshold was taken as the first appearance of yellow streaks within the center of the flame. The soot threshold equivalence ratio for each NAPC fuel, as well as for several blending components, was determined in both the "regulated burner" and "unregulated burner" modes as shown in Table 7. The results for AeroChem-A are given in Table 2. Results for pure hydrocarbons² and other mixtures have been reported previously.⁶

3. Threshold Sooting Indices

The soot threshold equivalence ratio for any specific fuel depends on the burner apparatus employed in the measurement. For the present apparatus, the premixed flame threshold soot index, TSI_{pf} , is calculated from the relation:

$$\text{TSI}_{pf} = 269 - 118(\phi_c).$$

The data are collected in Table 5 (hydrocarbons) and Table 6 (NAPC fuels).

C. PREMIXED FLAME MEASUREMENTS

This section describes the premixed flame apparatus and measurements. The measurements were: (1) the soot threshold equivalence ratio, ϕ_c ; (2) the plateau soot volume fraction as a function of equivalence ratio; (3) flame temperatures for sooting flames using three-wavelength emission pyrometry; and (4) flame temperatures of nonsooting flames using fine wire thermocouple probes.

Most of the measurements described below were carried out over a range of equivalence ratios for each NAPC fuel. The equivalence ratio, ϕ , is defined by the equation:

$$\phi = \frac{(\text{fuel/air})_{\text{actual}}}{(\text{fuel/air})_{\text{stoichiometric}}}$$

where $(\text{fuel/air})_{\text{actual}}$ is the fuel to air mole ratio for the flame and $(\text{fuel/air})_{\text{stoichiometric}}$ is the fuel to air mole ratio for complete combustion to CO_2 and H_2O . For example, to burn a hydrocarbon of empirical formula C_xH_y in air completely to CO_2 and H_2O , the fuel to air ratio is given by (assuming 20.946% by volume O_2 in dry air,²⁵

$$(\text{fuel/air})_{\text{stoichiometric}} = \frac{1}{4.774 [x + (y/4)]}$$

For a jet fuel, the average molecular weight and the hydrogen content of the fuel are needed to calculate its average empirical formula. Using the relationship, $\text{MW}_{\text{fuel}} = x(12.01) + y(1.008)$, the following formulas are obtained:

$$x = \frac{\text{MW}_{\text{fuel}}}{12.01} \frac{100x - Hx}{100x}$$

and

$$y = \frac{\text{MW}_{\text{fuel}}}{1.008} \frac{Hx}{100x}$$

Thus for example, the empirical formula for NAPC-1 is $\text{C}_{12.91}\text{H}_{23.72}$ and $(\text{fuel/air})_{\text{stoichiometric}} = 0.0111$.

1. Premixed Flame Burner

The premixed flame burner is similar to the one used in an earlier program at AeroChem² with a few modifications.

larger than $0.3\ \mu\text{m}$ and are stable to 400°C . A small vacuum pump was used to pull smoke-laden combustion gases through the filter. The filter assembly was placed at the top of the chimney when collecting smoke samples from the diffusion flames. All of the smoke escaping from the flame was collected on the filter.

Soot production rates were measured as follows: A fresh glass fiber filter was weighed to $\pm 0.05\ \text{mg}$ and then loaded into the filter holder. A flame was established and the chimney put in place. The smoke collection probe was placed off-center of the flame axis (avoiding the smoke trail of the flame). After several minutes of burning, the burner balance was tared to zero, a timer started, and the smoke collection probe moved to the center of the smoke trail. At the end of fixed time periods (from 3 to 12 minutes, depending on the sootiness of the flame), the fuel mass consumed was recorded (= balance reading), the smoke collection probe moved out of the smoke trail, and the timer stopped. The smoke collection probe was then disassembled and the glass filter removed with forceps. The filter paper (and collected smoke sample) was then weighed to the nearest $0.1\ \text{mg}$. The soot production rate (SPR) was then calculated as the smoke mass divided by the collection time, and the fuel consumption rate (FCR) was the fuel mass consumed divided by the collection time. The procedure was repeated so that a range of flames heights (i.e., a range of FCRs), from lightly to heavily sooting was measured for each fuel.

Initially, it was thought that the soot collected on the glass filter would contain a large fraction of water or volatile organics. Therefore, the mass change of clean glass filters and smoke-laden filters which had been baked for several hours at 150°C was measured. To a precision of $0.1\ \text{mg}$, it was found that neither clean glass filters or smoke-laden filters lost or gained mass in the heat treatment. After several tests, it was determined that the heat treatment was unnecessary.

The precision of the SPR and FCR values depends primarily on the precision of the mass determinations of soot produced ($\pm 0.1\ \text{mg}$) and fuel consumed ($\pm 10\ \text{mg}$), respectively. The collection times were chosen such that 3 to 30 mg of soot was collected and 200 to 400 mg of fuel consumed, irrespective of the sootiness of the flame. Thus, the precision of a SPR value is 0.3-3% ($\pm 0.1\ \text{mg}$ out of 3-30 mg) and the precision of a FCR value is ± 2.5 -5.0% ($\pm 10\ \text{mg}$ out of 200-400 mg). The lower precision values are typical only of the data collected for the lightly sooting flames (i.e., flames near soot threshold).

These measurements of SPR and FCR are unique. Therefore, in addition to NAPC 1-10, several pure hydrocarbons, two binary mixtures of isooctane/toluene, and AeroChem-A were also measured.

2. Diffusion Flame Threshold Sooting Index - TSI

The diffusion flame Threshold Sooting Index, TSI_{df} , for each fuel was calculated from the relationship (Ref. 4):

$$TSI_{df} = a + b (MW/SP)$$

where MW is the average molecular weight of the fuel (Table 3) and SP is the AeroChem measured smoke point of the fuel. The constants, a and b, are determined for each burner system by measuring the smoke points of several previously studied pure hydrocarbons for which TSI values are known. The calibration constants for our ASTM smoke point apparatus have been previously reported⁶: $a = -1.5$ and $b = 3.32$. These TSI_{df} values are reported in Table 4. The TSI_{df} for AeroChem-A was calculated from its smoke point as 17.9 using the theoretical MW.

3. Soot Production Rates

The soot production rate is defined as the mass of smoke per second which escapes from a diffusion flame. Of course, the smoke production rate will depend on several factors including the rate at which fuel is consumed by the flame.

The apparatus used in this work is shown in Fig. 2. The burner consists of two closely fitting concentric aluminum tubes in which an ASTM specification²⁶ cotton wick was installed. The inner tube and wick were movable within the outer tube using a rack and pinion drive which provided a means of exposing more or less wick beyond the outer tube lip, and therefore, the fuel feed rate. The fuel was contained within a 13 cm³ polypropylene reservoir. This burner is lightweight and it was mounted on the weighing platform of a top loading, digital readout balance with electronic taring capability (300 g capacity, 0.01 g readability). Air was supplied to the burner through a 10.0 cm diam aluminum honeycomb, which was mounted within a brass housing. The burner tube projects through a 1.5 cm diam opening in the center of the brass housing as shown in Fig. 2. A steel washer prevents any air flow through the central hole of the brass housing. This washer did not touch the burner or affect the weight measurements. A Pyrex process pipe reducing union (10 cm i.d. at base, 5 cm i.d. at top) was mounted on the brass housing and served as a chimney.

A soot collection probe (Fig. 3) was fabricated from a metal filter holder. The filter retainer ring was machined to a flat, smooth surface on the side which contacted the glass fiber filter. This modification permitted use without the Teflon gasket and thus the filters could be removed without tearing or loss of fiber material. The binderless glass fiber filters (25 mm o.d., Type A/E, Gelman Sciences Inc.) remove 99.9% of all particles

$$MW = 1000 \frac{g}{G} \frac{K_f}{T_f} (1 - k_f T_f)$$

where g = grams of solute in solvent, G = grams of benzene, K_f = molal freezing point depression constant ($= 5.12 \text{ deg molal}^{-1}$), and k_f = correction constant ($= 0.011 \text{ deg}^{-1}$). The literature value for the freezing point of pure and dry benzene is $5.52 \pm 0.01^\circ\text{C}$ (average of values reported in Refs. 24 and 25). For jet fuels, which are mixtures of nonassociated hydrocarbons, the mole fraction weighted molecular weight is obtained.

A typical cooling curve, a temperature vs. time plot, is shown in Fig. 1 for the results obtained with a benzene/NAPC-6 mixture. For pure benzene and benzene/fuel mixtures, the liquid always supercooled; that is, the solution temperature dropped below the freezing point of the mixture, then the temperature rapidly increased within typically a 30 s time period, and finally, the temperature would remain constant to within 0.01°C over a time period of 10-20 minutes. The constant temperature region subsequent to supercooling is the true freezing point of the mixture.

The freezing point depressions, T_f , measured for all the fuels and blending components, are listed in Table 3 together with the calculated molecular weights of the fuels. The freezing point depression and calculated molecular weight of AeroChem-A are listed in Table 2.

B. DIFFUSION FLAME MEASUREMENTS

The diffusion flame measurements included the ASTM smoke point, the fuel mass consumption rate (FCR) at soot threshold (FCR₀), the increase in fuel mass consumption rate above soot threshold necessary to produce soot at a rate of $200 \mu\text{g s}^{-1}$ (ΔFCR), and the smoke production efficiency (SPE = fraction of fuel converted to smoke).

1. ASTM Smoke Point

The smoke point is the minimum flame height at which smoke just escapes from the tip of a diffusion flame. The ASTM smoke point is thoroughly described in the American Society for Testing and Materials publication ANSI/ASTM D1322-75 (Ref. 26). The ASTM smoke points for the NAPC fuels and blending components are listed in Table 4.

III. EXPERIMENTAL

This section contains a description of the laboratory procedures and apparatus utilized in this program for fuel property measurements. The fuel properties which were measured include: density, average molecular weight, ASTM smoke point, critical equivalence ratios, flame temperatures, and soot yields.

The laboratory measurements described below were carried out on NAPC-1 through 10, most of the blending agents, and AeroChem-A. The NAPC fuels available to this program are listed in Table 1. AeroChem-A was blended using six pure hydrocarbons and was used to gauge the accuracy of the test procedures against its properties, which could be calculated from its known composition. The AeroChem-A mixture was prepared by mixing weighed quantities of the pure hydrocarbons listed in Table 2. The hydrocarbons used were > 95% purity. The molecular weights, molecular formulas, and mole fractions of the hydrocarbon components, as well as the average molecular formula, mole fraction weighted MW, and weight percent hydrogen content (H%) of AeroChem-A are listed in Table 2.

A. PHYSICAL PROPERTIES

The physical properties measured for each fuel were fuel density at 20°C and the mole fraction weighted molecular weight. These properties were used in calculating the TSIs for the fuels.

1. Density

The densities of all the NAPC fuels and blending components were measured by weighing a known volume of each fuel in a calibrated volume pycnometer. The fuel mass was typically in the range of 8-10 g and was recorded to five significant figures.

The densities of all the NAPC fuels are reported in Table 3 at a temperature of $20 \pm 1^\circ\text{C}$. The density of AeroChem-A is given in Table 2. The densities are estimated to be accurate to $\pm 0.0008 \text{ g cm}^{-3}$; this uncertainty results primarily from the temperature uncertainty.

2. Molecular Weight

The molecular weights were determined by the freezing point depression technique²³ using benzene as solvent. For a highly dilute solution, the molecular weight of the solute, MW, is related to the freezing point depression of the mixture (T_f , °C) by the expression

physical properties such as viscosity, volatility, and surface tension, primarily influence combustion efficiency, extinction limits, and ignition properties. Fuel chemical properties, such as hydrogen content, smoke point, and aromatic content, affect smoke emissions, flame radiation, and wall temperature. Lefebvre did not compare the importance of these fuel chemical properties.

The most widely and recently used correlation parameter of smoke-related engine performance data is the weight percent of hydrogen (HX) in the fuel. The success of this fuel parameter, however, may result somewhat from the limited variation of fuel compositions employed in fuel effects studies of engine performance and also possibly from the fact that the HX can be precisely and reproducibly measured. Other fuel parameters which have been examined include the smoke point, total aromatic content, and aromatic content subdivided into single ring and multiple ring fractions.

Moses et al.^{20,21} found that total weight percent aromatics correlated well with measured flame radiation flux in both a T63 combustor and a Phillips 2-inch combustor. Friswell²² also noted that smoke emissions correlated well with total aromatic content in a research gas turbine.

In summarizing the results of previous studies on fuel effects on gas turbine smoke-related performance, the hydrogen weight percent is the most commonly used and possibly the best correlating parameter found to date. However, with further investigation, other laboratory fuel parameters may be found to correlate as well or better.

One limitation of almost all of these previous engine or combustor testing programs has been insufficient characterization of the chemical composition of the fuel blends. A great deal of effort has been expended on the experimental work with little characterization of the fuels beyond the most basic physical property measurements and chemical class analyses.

for 44 pure fuels including alkanes, alkenes, alkynes, and aromatics. The soot yields were found to increase nearly exponentially in every case, with increasing equivalence ratio beyond the threshold. The slopes and intercept values of semilogarithmic plots of soot yield against equivalence ratio were reported.

D. EFFECTS OF TURBULENCE ON SOOT FORMATION

All previous significant laboratory studies on fuel composition effects have been performed in laminar flames. The question naturally arises whether sooting tendencies (soot thresholds and yields) measured under laminar conditions are relevant to turbulent combustion. The possibility exists that the relative ranking of various hydrocarbons will be the same or similar to that determined in these laminar flame studies, in spite of the differences in the overall combustion processes.

Although a complete literature review has not been performed, two studies were identified^{16,17} which qualitatively show that the ordering of fuel sooting tendencies in turbulent flames is similar to the ordering in laminar flames. A total of only eight fuels was studied by these groups, so this conclusion is certainly preliminary.

E. EFFECTS OF PRESSURE ON SOOTING TENDENCIES

In a comprehensive review, Haynes and Wagner¹⁸ concluded that soot yields in both premixed and diffusion flames increase dramatically at higher pressures, whereas soot thresholds are relatively unaffected by pressure. For premixed flames, we find that the literature results are much less conclusive than Haynes and Wagner presented. They refer to only three studies of pressure effects on soot thresholds and soot yields, and in these studies the only aromatics studied were benzene and naphthalene. Furthermore, if benzene is representative of the aromatic class, the results of Macfarlane et al.¹⁴ indicate a much lower pressure dependence of the soot yield from aromatics than observed for alkanes and alkenes.

F. PREVIOUS FUEL EFFECTS CORRELATIONS

The many analyses of fuel effects that have been performed will not be discussed here. The following is only a brief overview of prior work:

Lefebvre¹⁹ for example, has recently reexamined the question of which engine performance and emission characteristics are sensitive to fuel properties. As before, Lefebvre found that fuel

threshold equivalence ratio increased as the temperature of the unburned gas in a Bunsen flame was raised. Millikan⁸ studied premixed flat ethylene/air flames on cooled porous burners and similarly found a temperature dependent soot threshold. Glassman and coworkers⁹⁻¹¹ recently discussed the importance of temperature in soot threshold measurements in diffusion and premixed flames.

Naegeli et al.¹² studied flame temperature and fuel composition effects in a turbulent research combustor simulating turbojet engine conditions. They found that higher flame temperatures, produced by increasing the inlet air temperatures, caused an increase in the quantity of soot formed (as measured by both flame emission intensity and opacity), similar to the trend observed⁹ in laboratory diffusion flames. The effects of different fuel blend compositions on soot formation, however, were found to be greater than could be explained by temperature dependence effects alone.

Olson and Madronich¹³ studied the effects of varying flame temperature and composition on soot production in atmospheric pressure, laminar premixed flames. The soot threshold equivalence ratios were found to vary with changes in the $O_2/(N_2 + O_2)$ ratios, and therefore with changes in the calculated adiabatic flame temperatures. However, it was found that the measured flame temperature at the soot threshold was not a function of the $O_2/(N_2 + O_2)$ ratio or fuel/ O_2 ratio. The soot volume fractions depended strongly on the $O_2/(N_2 + O_2)$ ratio because of the shift in the threshold equivalence ratio, but the variation in soot volume fraction with measured temperature was apparently independent of the $O_2/(N_2 + O_2)$ ratio. The soot yield was found to be dependent on the temperature in the sooting region of the flame, regardless of how that temperature was achieved.

C. SOOT YIELDS

There does not appear to be any significant comparative study of soot yields in diffusion flames. The data on soot yields in premixed flames are also minimal, but some information is available. Several very detailed studies in which the flame temperature and soot particle size and number density were measured have been performed on one or two pure hydrocarbons. This type of data is not sufficient to make conclusions about the effects of hydrocarbon structure on soot yields. Probably the most commonly referenced study is that of Macfarlane et al.¹⁴ who measured the total amount of soot produced in premixed flames of six compounds as functions of equivalence ratio and pressure. The only aromatic hydrocarbon studied, benzene, showed an unusually small amount of soot produced relative to the three alkanes studied.

Recently Olson et al.¹⁵ measured premixed flame soot yields

mental apparatuses. In diffusion flames, TSIs are defined in terms of maximum smoke-free flame height, h , (similar to the ASTM smoke point) according to the equation: $TSI_{df} = a'(MW/h) + b'$, where MW is the fuel molecular weight, and a' and b' are again scaling constants characteristic of the apparatus.

Olson and coworkers^{2,3,5} expanded the TSI data set with measurements on 56 hydrocarbons in premixed flames and 42 fuels in diffusion flames. Flame temperatures, soot concentrations, and average particle size and number density were also measured.

Formulas for calculating soot thresholds (TSIs) of hydrocarbon mixtures in both premixed flames and diffusion flames were obtained by Gill and Olson.⁶ For premixed flames the mixture rule is

$$(1.1) \quad TSI_{mix} = \sum_i X_i TSI_i$$

and for diffusion flames

$$TSI_{mix} = \sum_i X_i TSI_i$$

where TSI_{mix} is the calculated value for the mixture and X_i and TSI_i are the mole fraction and TSI values for the individual hydrocarbon components.

B. EFFECTS OF TEMPERATURE ON SOOT THRESHOLDS IN PREMIXED FLAMES

Several methods of altering flame temperatures have been used to study temperature effects on soot formation. The temperature of a flame can be increased by preheating the unburned gases, or by decreasing the diluent concentration, i.e., by reducing the N_2 fraction in a fuel/ O_2/N_2 flame. Other factors, such as changes in the fuel/air ratio or the substitution of one fuel for another, also alter the flame temperature. Typically, the flame temperatures of aromatic hydrocarbons at soot threshold are several hundred Kelvin higher than for paraffins. Because all these parameters affect flame temperatures as well as soot formation, there is confusion over the relative importance of flame temperature and fuel molecular structure upon soot thresholds and soot yields.

Several previous studies have been directed at determining the effects of changing flame temperatures on soot formation in premixed flames. Street and Thomas,⁷ for example, found that the soot

II. BACKGROUND

A. SOOT THRESHOLDS

Two types of laboratory soot threshold measurements are generally employed to rank the sooting tendencies of pure hydrocarbon fuels: premixed flame soot threshold equivalence ratios and diffusion flame smoke point flame heights.

In premixed flames the minimum fuel/air ratio (or C/O ratio) at which yellow (soot) emission is observed has been used to rank fuels as to their sooting tendencies. Generally these data show an increasing tendency to soot with increasing carbon number, and a relative ranking of hydrocarbons in the sequence²

alkynes < alkenes < n-alkanes < aromatics.

The one naphthalene-type compound studied exhibits the highest sooting tendency. The correlation of sooting tendency with hydrogen content was shown to be poor, although if consideration was restricted to only alkanes and aromatic hydrocarbons, a fairly good inverse correlation was obtained.

Data on the sooting tendencies in diffusion flames of 103 compounds have been measured or extracted from the literature by Olson et al.³ A different and more distinct relative ranking of hydrocarbon classes was obtained from that of premixed flames. That is, the ranking was:

alkanes < alkenes < alkynes < alkylbenzenes < naphthalenes.

Again the correlation of sooting tendency with hydrogen content was poor.

To quantify these types of general rankings of sooting tendencies into a more useful ranking, Calcote and Manos⁴ reviewed the literature results on threshold sooting measurements in both premixed and diffusion flames and defined a numerical index, called the threshold soot index, TSI, which can be used to compare and analyze sooting flame data. In premixed flames, TSIs are defined in terms of the minimum fuel/oxidizer equivalence ratio* at which soot is first observed, ϕ_c , according to the equation: $TSI_{pf} = a - b \phi_c$, where the constants a and b scale the index from 0 to 100 and account for systematic variations in data from various experi-

*Equivalence ratios are defined relative to stoichiometric combustion to CO₂ and H₂O, i.e., $\phi = \frac{(\text{fuel/oxygen})_{\text{actual}}}{(\text{fuel/oxygen})_{\text{stoichiometric}}}$

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performed elsewhere. The combined data from flame and fuel characterization studies were then applied to analyze the fuel performance in the combustor tests. Finally, the effects of variations in the operating conditions of the combustor tests were examined, since these variations also affect the smoke-related measurements and produce differences in the data which are not related to the fuel composition.

I. INTRODUCTION

To insure continued future availability of aircraft jet fuel at acceptable costs, it may be necessary to modify current military specifications which could lower the quality of such fuels. In particular, with the use of heavy petroleum crudes, upgraded residual fractions, and shale or coal derived liquid fuels, the middle distillates will contain higher fractions of aromatic hydrocarbons, which will shift other fuel parameters from their current ranges. These considerations have prompted the US Navy, NASA, and the US Air Force to investigate the effects of relaxing the fuel specification for aircraft systems. A primary goal of these efforts has been to investigate the relationship between gas turbine engine performance and fuel composition and properties.

Increased aromatic hydrocarbon content is one of the fuel composition changes anticipated. A major impact of such increased aromatic content is increased soot production in the engine combustor, resulting in higher exhaust smoke emissions, accelerated turbine erosion, and more important, increased radiative heat transfer to the combustor walls. Even at moderate soot concentrations in the combustor, thermal radiation from soot particles dominates the total heat load on the combustor liner. The resulting increases in liner metal temperature greatly reduce the combustor service lifetimes, thus increasing the costs because of earlier replacements. The increased smoke production also increases plume visibility--highly undesirable from both environmental and combat mission viewpoints.

The ultimate objective of this program was to develop a laboratory method for predicting the effects on soot formation in turbojet engines caused by changes in fuel composition. Specifically, ten fuels previously evaluated in several engine combustors in a Naval Air Propulsion Center (NAPC) fuel effects program were studied in laboratory flames, and these results and other fuel properties were correlated with results of the combustor measurements. These fuels represent a fairly narrow range of chemical variation (e.g., aromatic content or hydrogen content), but even this range of variation is sufficient to greatly reduce the calculated service lifetimes of combustor liners.

This program was unique in several respects. First, the laboratory characterization of the combustion and sooting properties of the NAPC fuels was extensive. Unique procedures, apparatus, and fuel indices were developed to quantitatively specify the sooting propensity of fuel blends in terms of both soot thresholds and soot yields, and in both premixed flames and diffusion flames. Second, an effort was made to correlate the laboratory flame data with fuel composition analyses of aromatic content and structure

reflections using mirrors. The pathlength per pass was ca. 2.55 cm.

The attenuation was measured using a lock-in detection scheme. The laser beam was chopped at 140 Hz and, after passing through the flame, impinged on an optical scatter plate. The diffuse light was then detected with a large surface area photodiode. The photodiode signal was integrated for ca. 3-10 minutes to provide further signal to noise improvement.

The soot volume fraction measurements were made at a height of 2.00 ± 0.05 cm above the burner surface where the f_v is relatively constant with height above the burner. These data for NAPC 1-10, and AeroChem-A are presented in Figs. 5-10.

5. Premixed Flame Temperature Measurements

Premixed flame temperature measurements were determined by two methods. For nonsooting flames, the flame temperatures were measured using coated thermocouples. Because soot builds up on thermocouple wires, they cannot be used in sooting flames. Therefore, in sooting flames, flame temperatures were determined by multiwavelength emission pyrometry.

a. Thermocouple Measurements -- The Pt-Pt/10% Rh thermocouples TC, (S-type) were fabricated from 0.005 or 0.013 cm diam wire. The bead, formed at the junction of the dissimilar wires, was always less than 1.5 times the wire diameter. Before making flame measurements, the TC junction was coated with $\text{BeO-Y}_2\text{O}_3$ by repeatedly dipping the junction in an acid solution of BeO/YCl_3 (7%/93%, by weight) and then firing the wetted junction in a Bunsen burner flame. This thin coating (<0.001 cm) was employed to prevent catalytic heating²⁹ of the TC. The TC flame temperatures were measured with a calibrated Omega Engineering Inc., Model 199 digital readout (1 K readability, ± 2.3 K accuracy). Typically, the flame temperature was measured at 2.0 cm above the burner surface.

The recorded TC temperature is not the true flame temperature. The procedure employed for correcting the measured temperatures followed that described by Kaakan,³⁰ which relates the measured TC temperature to the true flame gas temperature and requires values for the thermal conductivity and viscosity of the flame gases and the emissivity of the TC junction. The thermal conductivity and viscosity of the flame gases were obtained by calculating the equilibrium gas mole fractions for a decalin/air flame and then calculating the properties of the mixture using Wassilijew's rule for the thermal conductivity and Wilke's rule for the viscosity.³¹ The emissivity of platinum is well known,³² (ca. 0.17) at the flame temperatures typically encountered in our

experiments. Emissivity data are not available for the platinum/rhodium alloys, so we assumed they were the same as platinum.

Typically, the corrected gas temperatures were ca. 50-150 K higher than the measured temperatures. Smaller corrections are found for thinner thermocouple wires and/or lower gas temperatures. The corrected flame gas temperatures at 2.0 cm above the burner for the NAPC fuels and AeroChem-A are given in Table 8.

b. Emission Pyrometry Measurements -- Since the submicron soot particles within a sooting flame are in good thermal contact with the flame gases, they can be assumed to be at the gas temperature. Thus their incandescent light emission can be used to measure³³ the flame gas temperature. An apparatus similar to that described by Cashdollar³⁴ was used to measure light intensity ratios for pairs of three selected wavelengths in the near IR spectral region (0.8-1.0 μm). This apparatus is referred to as a three-wavelength emission pyrometer (3 λ EP). The detector signals were corrected for the reflection/absorption losses from optical elements, differences in photodiode sensitivities, and differences in the gain of the individual amplifiers by calibrating daily against a tungsten ribbon lamp. The surface temperature of the lamp was found by measuring the 0.65 μm brightness temperature³³ of the ribbon,^{32a} using a calibrated disappearing filament optical pyrometer. The vertical resolution of the 3 λ EP was 0.18 cm.

The corrected emission intensity ratios, 0.8 μm /1.0 μm and 0.9 μm /1.0 μm , were used to calculate the flame temperatures. The basic equation is Planck's thermal emission equation.³⁵ For a radiating nonblackbody, such as incandescent soot particles, the equation is:

$$P_{\lambda} = \frac{\epsilon_{\lambda} 2\pi hc^2}{\lambda^5 [\exp(hc/kT\lambda) - 1]}$$

In this equation, P_{λ} (W m^{-3}) is the radiant intensity emitted in a unit wavelength region around λ (m) for a greybody at temperature T (K) having an emissivity of ϵ_{λ} , c is the speed of light, h is Planck's constant, and k is Boltzmann's constant. This equation can be used to calculate the theoretical intensity ratios (e.g., 0.8 μm intensity/1.0 μm intensity) for a greybody at a temperature T (K), if the emissivity of the particles is known.

The emissivity of soot particles^{33a} is generally assumed to follow an inverse power law - $\epsilon_{\lambda} = A/\lambda^n$. For ratios of intensities, the A term cancels. The dependence on wavelength, n , is often observed to be in the range 0.7 to 1.4. However, in practice, the particle temperatures derived from Planck's law are very insensitive to the value of this exponent. For example, when the value of n was varied from 0.5 to 1.5, only a 20 K change resulted in

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the derived temperature at about 1900 K. Therefore $n=1$ was selected to process all intensity ratio data. When this was done, the $0.8 \mu\text{m}/1.0 \mu\text{m}$ and the $0.9 \mu\text{m}/1.0 \mu\text{m}$ experimental intensity ratios provided two independent estimates of the flame temperature. The two temperatures were usually within 50 K of each other. The emission pyrometer temperatures listed in Table 8 are the average of the two measurements and have an estimated uncertainty of ± 30 K.

V. RESULTS AND DISCUSSION

In this section the results of the laboratory measurements on the NAPC test fuels will be discussed, the mixture rule evaluations will be explained, and the correlation analysis between fuel sooting tendencies and the smoke-related test results on the TF30, T56, and the T53 combustors will be discussed.

A. LABORATORY TEST RESULTS

1. Physical Properties

a. Fuel Densities -- The densities of the NAPC test fuels and their blending components are listed in Table 3. These data are in good agreement with API gravity data previously reported by NAPC.^{36a}

b. Fuel Molecular Weights -- The experimental procedure for measuring fuel molecular weights (MW) has been described in the experimental section. The observed freezing point depression, T_f , and calculated MW for each fuel are listed in Table 3. The accuracy of the MW values for jet fuels was estimated by investigating three pure hydrocarbons and AeroChem-A. These results are presented in Table 9. The average uncertainty in these MW is ± 4 g mol⁻¹.

2. Diffusion Flame Results

a. ASTM Smoke Points -- The ASTM smoke points (SP) have been measured by AeroChem, NRL, and NAPC for NAPC 1-10. In several cases there is disagreement in the reported SP (see Fig. 11 and Table 4). The NRL data agree better with the AeroChem data ($r^2 = 0.92$, 8 points) than do the NAPC data ($r^2 = 0.75$, 10 points), and both the NRL and NAPC data sets show a systematic shift to smaller SP at high values compared with the AeroChem SP measurements. The AeroChem SP data were used in the correlation study.

b. Diffusion Flame Threshold Sooting Index - TSI_{df} -- The TSI_{df} values for the NAPC fuels, listed in Table 4, were calculated according to the formula given in Section II.A using the mole fraction weighted MW and the AeroChem measured ASTM SP for each fuel. The TSI_{df} values increase with increasing total aromatic content (Fig.12) and decreasing fuel hydrogen content (Fig.13). These trends are in accord with the laboratory results of pure compound TSI_{df}'s.^{3,4} However, it should also be noted that several fuels do not follow the trends set by the other fuels. For example in Fig. 12, two blending components (xylene tower bottoms and HCGO) and NAPC-16 (JP-7) appear out of line with the others fuels. In

Fig. 13, 60 Golden and xylene tower bottoms are out of line with the remaining fuels.

These out of line cases should be given their proper perspective. That is, these particular fuels/blending components will probably never be used as jet fuels, but they do serve a role in testing jet engines because they are unusual. In testing these types of fuels, a better understanding of why particular fuel properties (such as hydrogen content, TSI or total aromatics) correlate the engine test results has been one of the major goals of the present work.

c. Soot Production Rates -- The soot production rates of hydrocarbons have not been previously characterized for diffusion flames. The present work provides the only detailed measurements on a set of liquid fuels. The measurement consists of determining the total mass of soot which escapes from the tip of a diffusion flame. As an example, the mass of soot produced per unit time (soot production rate, SPR), is plotted in Fig. 14 against the fuel consumption rate (FCR) for a diffusion flame of NAPC-9. This curve is typical of the data obtained for the NAPC fuels and several pure hydrocarbons (see Fig 15). Specifically, the SPR increases most rapidly just above soot threshold and then increases more slowly as the FCR increases well beyond soot threshold (except for n-heptane). Thus in diffusion flames the conversion of additional fuel to soot is most efficient near soot threshold and becomes less efficient for increasingly smoky flames (probably due to decreased flame temperatures).

The SPR curves were characterized using three parameters: the fuel mass consumption rate at soot threshold (FCR_0), the efficiency of fuel to soot conversion (soot production efficiency, $SPE = \Delta SPR / \Delta FCR$ determined using linear least squares analysis of the data in the 100 to 300 $\mu g\ s^{-1}$ SPR region), and the difference in FCR measured at soot threshold and at a SPR of 200 $\mu g\ s^{-1}$ (ΔFCR). These three parameters are illustrated in Fig. 14 by the leftmost arrow on the FCR axis (FCR_0), the solid line segment (SPF), and the "distance" between the two FCR axis arrows (ΔFCR).

These three parameters were measured for NAPC 1-10 and are given in Table 4.

3. Premixed Flame Results

The premixed flame measurements made in this program included soot threshold equivalence ratios, premixed flame threshold sooting indices, soot volume fractions, and flame temperatures. Most of the experiments were performed using both temperature regulated and unregulated burners.

a. Soot Threshold Equivalence Ratio, ϕ_c -- The soot threshold equivalence ratio data are shown in Table 7. For eight of the ten NAPC fuels, the regulated burner ϕ_c 's are larger than with the unregulated burner. The regulated burner temperatures were always lower than those of the unregulated burner, burning the same fuel, so that the final flame temperatures on the regulated burner were always slightly lower. This apparently decreases the sooting tendencies, resulting in larger values of ϕ_c . The premixed ϕ_c 's do not follow a systematic trend with either the hydrogen or total aromatic content of the NAPC fuels (1-10).

b. Premixed Flame Threshold Soot Indices, TSIPf -- The two soot threshold equivalence ratio measurements, on regulated and unregulated burners, were used to calculate the regulated and unregulated TSIPf sets given in Table 7. As discussed by Calcote and Manos,⁴ there are large quantitative differences between the sooting tendencies of a set of fuels burned in a diffusion flame (TSIDf values) and the sooting tendencies of the same fuels when burned as premixed flames (TSIPf values).

c. Soot Volume Fractions, (f_v) -- There was no systematic difference in the soot volume fractions measured on the temperature regulated and unregulated burners, as verified by measuring the soot volume fractions of AeroChem-A. This is illustrated in Fig. 5.

The f_v measured for the NAPC fuels, Figs. 6-10, increased for equivalence ratios beyond the soot threshold and generally tended to level off as the flames were made fuel richer. Therefore, the increase in f_v was usually a strongly nonlinear function of the equivalence ratio of the flame. These data were parametrized by measuring the equivalence ratio at which the flame reached a $f_v = 2 \times 10^{-7}$. This parameter, $\phi(f_v)$, would be expected to follow the ordering of the ϕ_c 's for the NAPC fuels, if in premixed flames soot yields and soot threshold data correlate in the same manner as in diffusion flames. When this parameter was plotted, Fig. 16, against regulated burner ϕ_c data for the NAPC fuels, a fair linear correlation was observed. However, $\phi(f_v)$ plotted against the unregulated burner ϕ_c data showed no significant variation.

d. Premixed Flame Temperatures -- The premixed flame temperatures were measured at the same position, 2.0 cm above the burner as the f_v were measured. As described in the experimental section, thermocouple temperatures were obtained in nonsooting flames, whereas three-wavelength emission pyrometer temperatures were determined in the sooting flames. The two sets of data were found to agree to about ± 50 K, as shown in Fig. 17 for NAPC-4. The results of linear least squares analysis of the temperature measurements for each fuel are presented in Table 10. Here, both

the intercept and slope, as well as the coefficient of determination (r^2) for each analysis are presented. The linear least squares fits were used to calculate the flame temperatures at θ_c and at $\theta(f_v)$ (see Table 7). No trend between premixed flame temperatures and either fuel hydrogen (Fig. 18) or aromatic content can be seen. However, note that the temperatures at $f_v = 2 \times 10^{-7}$ are significantly lower (by ≥ 100 K) than at soot threshold.

B. MIXTURE RULES

At the start of this program, it was proposed that detailed chemical analyses (such as GC/MS identification of all components present in significant quantities) of the ten NAPC jet fuels be performed by the Navy. This, however, was determined to be too costly. The basis for this proposal was that a large number of pure hydrocarbons have been quantitatively characterized in laboratory tests which rank their sooting tendencies, and that mixture rules for calculating the properties of blends from the properties of the pure components have been developed. Thus it was suggested that measuring the composition of the test fuels would allow their sooting tendencies to be calculated. Possibly this can be done in future work.

The soot threshold mixture rules for premixed and diffusion flames were developed at AeroChem in an earlier Air Force funded program and the results of this work published.⁶ An analysis of the mixture rule for premixed flames was performed by Madronich during this program and it has also been published.³⁷

1. Diffusion Flame Mixture Rules

There are two mixture rules for diffusion flames. The soot threshold, or TSI mixture rule, can be used to estimate the soot threshold of a blend based on its composition and the soot thresholds of the components. The soot yield mixture rule is similar and can be used to calculate the soot yield of a blend.

a. Soot Threshold Mixture Rule -- The soot threshold mixture rule was evaluated by estimating the TSIs for AeroChem-A and several of the NAPC fuels. The calculation for AeroChem-A is presented in Table 11 (using data from Table 2 and Ref. 3).

The calculated mixture rule TSI_{df} value can be compared with the measured value given in Table 2, which shows that the mixture rule TSI for AeroChem-A is about 2.5 TSI units higher than observed. Employing the ASTM lamp TSI calibration formula given in the experimental section, the mixture rule TSI can also be used to calculate the ASTM smoke point, which gives a value of 21.0. The observed ASTM smoke point is 23.5, a difference of 2.5

units. The stated interlaboratory accuracy of the ASTM smoke point method is 3 smoke point units (see Ref. 21), so the mixture rule predicts the ASTM smoke point within this tolerance. In previous work,⁶ better agreement between observed and mixture rule calculated TSI values was routinely obtained. The difficulty in calculating an accurate TSI for AeroChem-A probably lies in the value used for the TSI_{df} of toluene. The Ref. 3 suggested value is 44, although the measured value in that work was 38. Using the ASTM apparatus, TSI_{df} 's for toluene were measured in the range 35-39. If $TSI = 36$ (instead of 44) is used for toluene in the AeroChem-A calculation, the calculated result is $SP = 22.1$, still slightly smaller than the measured value (23.5).

Six of the NAPC 1-10 group of test fuels and NAPC-19 and 20 were blended from other components (e.g., kerosene, DFM, or XTB). The TSI_{df} mixture rule was used to calculate the TSIs of these eight fuels from the measured TSIs of their blending components. Table 12 gives the reported volumetric composition of NAPC 1-4, 7, 8, 19, and 20, as well as weight and mole fractional compositions derived using the measured densities and average molecular weights. Several of these fuels contain blend stocks which were not available to this program, so their exact properties were not known. Thus the furnace oil (139-81) used in NAPC-2 and 3, the HCGO (148-81) used in NAPC-7, and the DFM (118-81) used in NAPC-8 were estimated to be similar to other blending components which were tested experimentally. The TSIs calculated using mole weighting are also shown in Table 12. The calculated TSIs compare favorably with the measured values, with the largest differences for NAPC-19 and 20 (about 7 and 4 TSI units, respectively). This agreement shows that the mixture rule can be applied to calculating the TSIs and thus the smoke points of blends.

Another approach evaluated for calculating the TSIs of fuels was to use analytical information from NMR experiments³⁸ on these fuels. Additional detailed data were available from this analytical work, but only the composition and average molecular weight information was used on three classes of the fuels: (1) paraffins, (2) monocyclic aromatic hydrocarbons, and (3) polycyclic aromatic hydrocarbons. Estimated TSIs for the fractions in the three different classes for NAPC 1-9, 16, kerosene, XTB, FO, 40G, and 60G are plotted in Fig. 19 against the measured molecular weights from the NMR analysis.³⁸ A regression analysis of calculated TSIs, obtained from the equation $TSI(calc) = X_1 (2.7 + 0.083 MW_1) + X_2 (50.9) + X_3 (103)$, where X_1 , X_2 , and X_3 are the mole fractions of the three component classes and MW_1 is the molecular weight of the paraffin class, against the observed TSIs (Fig. 20) was performed. The results are good for NAPC 1-9, 16, XTB, kerosene, and FO, but the calculated TSIs are low for 40G and 60G. It is clearly an oversimplification to use a constant TSI for the various monocyclic and polycyclic aromatic fractions of these

fuels where the molecular weight of these fractions varies over such a large range, e.g., 119 to 250 g mol⁻¹ for the monocyclic aromatics.

Two additional calculations were performed where the estimated TSIs of the monocyclic and polycyclic aromatics were varied with molecular weight. In these fits, the discrepancy for 40G and 60G was eliminated although the accuracy for the subset of NAPC 1-9 was slightly degraded.

b. Soot Yield Mixture Rule in Diffusion Flames -- Diffusion flame soot yield data obtained in this work on pure hydrocarbons are plotted in Fig. 15 and tabulated in Table 5. Only those hydrocarbons which are components of AeroChem-A were tested. The data were least squares fit to parabolic equations of the form: $SPR = a + b (FCR) + c (FCR)^2$ or $SPR = a' + b' (\Delta FCR) + c' (\Delta FCR)^2$. The fitting parameters (a,b,c) and (a',b',c') are collected in Table 13. The quantity ΔFCR is the difference between the measured fuel mass consumption rate, FCR, and the mass consumption rate at soot threshold for the fuel (FCR_0).

To develop a mixture rule, two binary mixtures of toluene/isooctane were prepared and their SPR curves measured. The binary mixture measurements are compared in Fig. 21 with the values calculated from the SPR mixture rule. This rule, empirically determined, is:

$$SPR_{mix}(\Delta FCR_{mix}) = \sum_i X_i SPR_i(\Delta FCR_i).$$

In this equation, X_i is the mole fraction of component i, $SPR_i(\Delta FCR_i)$ = soot production rate for fuel component i from the ΔFCR_i fitting equations, and $SPR_{mix}(\Delta FCR_{mix})$ is the calculated SPR for the binary mixture. For these calculations, the mixture rule gives a SPR for each ΔFCR_{mix} value. The ΔFCR_{mix} values are converted to FCR_{mix} values by adding the experimentally observed FCR_0 for the mixture (from Table 13).** As can be seen in Fig. 21, the SPR mixture rule fits the mixture data well at low fuel consumption rates and somewhat underpredicts SPRs at higher FCRs.

To test the accuracy of the mixture rule with a more complex fuel mixture, SPRs were calculated for the AeroChem-A fuel mixture. The results are presented in Fig. 22. The fit is good at low SPR but is again poorer at high SPRs.

** The FCR_0 values for the mixtures can be calculated using the soot threshold mixture rule; they were found to be in agreement with the experimental values.

In summary, the SPR mixture rule, evaluated with a limited set of experimental data, appears reliable for predicting SPRs for simple mixtures, but it is not as satisfactory for complex fuel blends, especially at high SPRs.

2. Premixed Flame Mixture Rules

The premixed flame mixture rule for calculating the soot threshold of fuel blends was developed⁶ in an earlier program. Mixture rules for calculating soot yields of blends were developed under this work.

a. Soot Threshold Mixture Rule in Premixed Flames --

The premixed flame mixture rule has been found⁶ to reproduce experimental data on binary and ternary mixtures to within ± 4 TSI units. When this rule was applied to AeroChem-A (see Table 11), the result was TSI = 82.5 compared with the measured TSI of 70 for the unregulated burner (with which the mixture rule was developed). The breakdown of the calculation is most likely due to inaccurate TSI values for the hydrocarbon components which comprise AeroChem-A. The dominant terms in the mixture rule summation are for tetralin and toluene. Next in importance are the terms associated with 1-methylnaphthalene and decalin.

The compounds which have the largest uncertainty in their reported² TSIs are toluene and 1-methylnaphthalene. The reported TSIs for toluene cover the range 74 to 93 and for 1-methylnaphthalene, 86 to 110. If the mixture rule and the smallest reported TSI values for each and every fuel component were used, the calculated TSI for AeroChem-A would be estimated as 75, still larger than measured.

An improved mixture rule was proposed by Madronich³⁷ and extended in this program by Olson and Madronich.¹³ More effort is needed to improve this work (which also includes soot yield calculations), but a preliminary calculation for AeroChem-A using unpublished data from this laboratory¹⁵ on the component hydrocarbons yields a calculated TSI = 73. This result is within the experimental uncertainty of the measured value of 70 (unregulated burner).

b. Soot Yield Mixture Rule in Premixed Flames -- A soot yield mixture rule for premixed flames was also proposed in this program. The basic rule is

$$f_{v,mix}(\phi_{mix}) = \sum_i X_i f_{v,i}(\phi_{mix})$$

where the fuel/air equivalence ratios of the components are taken as equal to that of the entire mixture (ϕ_{mix}). Thus, this formula proposes that each component contributes soot independent of the

other components, except for the competition for the available oxidizer. Using previous work from this laboratory on pure hydrocarbons, the individual $f_{v,i}$ may be evaluated from the relationship

$$f_{v,i}(\theta) = f_{v,i} \exp(\beta_i (\theta - \theta_{c,i}))$$

yielding a proposed mixture rule

$$f_{v,mix}(\theta_{mix}) = \sum_i X_i f_{v,i} \exp(\beta_i (\theta_{mix} - \theta_{c,i}))$$

This mixture rule, evaluated at soot threshold, reduces to the improved TSI mixture rule discussed above. However, when soot volume fractions at $\theta > \theta_c$ are calculated for AeroChem-A, they are much larger than experimentally observed, as shown by the dashed line in Fig. 5. A general hypothesis for this failure of the mixing rule can be obtained by comparing the flame temperatures of AeroChem-A and those of the components. At the observed soot threshold ($\theta_c \approx 1.7$), the AeroChem-A flame temperature is about 1720 K, whereas that of pure n-tetradecane would be about 1630 K and that of tetralin would be 1805 K. Thus soot volume fractions for the components calculated on the basis of the normal flame temperatures would not be expected to correspond to data from flames with quite different temperatures.

The analysis of temperature effects on soot thresholds and soot yields performed in this work led to the development of a further refinement in the soot yield mixture rule (and corresponding soot threshold mixture rule). In that work it was established that the soot volume fraction of a pure hydrocarbon could be fitted by the expression

$$f_v(T) = f_v(T_0) \exp [\theta(1/T) - (1/T_0)]$$

where T_0 is the flame temperature at soot threshold and θ is the slope of a plot of $\ln f_v$ vs. $1/T$.

Evaluation of this soot yield mixture rule,

$$f_{v,mix}(T_{mix}) = \sum_i X_i f_{v,i}(T_{0,i}) \exp [\theta_i(1/T_{mix}) - (1/T_{0,i})]$$

is hindered by two difficulties: First the experimental AeroChem-A flame temperature measurements are fairly uncertain. In Table 10, an unsatisfactory r^2 of 0.86 was found as was an unusually small B of -235 K/ θ for AeroChem-A. It would be anticipated that $B \approx -450$ K/ θ for this type of fuel and the emission pyrometer temperatures, in fact, give a larger slope than the TC temperatures. Second, the θ_i values and flame temperatures for the pure hydrocarbons (from a previous program⁵) are uncertain and scattered. Nonetheless, Fig. 23 shows the experimental f_v data for AeroChem-A plotted against

flame temperature (estimated using $B = -450 \text{ K/}^\circ$). The data are fit by the equation (which disregards the curvature):

$$f_{v,mix} = 1.5 \times 10^{-8} \exp [38,800 (1/T) - (1/T_0)]$$

where $T_0 = 1710 \text{ K}$. Using the parameters listed in Table 14 for the components of AeroChem-A, the mixture rule calculation yields the results shown in Fig. 23 as a dashed line, and described by the equation:

$$f_{v,mix}(\text{calc}) = 2.3 \times 10^{-8} \exp [36,300 (1/T) - (1/T_0)]$$

The agreement between the observed and calculated f_v values is good, but it should be noted that there are large uncertainties in the temperatures for the experimental data and the parameters for the pure hydrocarbons used in the calculation. The results are, however, encouraging and indicate that our analysis of soot yields in premixed flames, emphasizing the importance of the flame temperature, is basically correct.

C. CORRELATIONS OF COMBUSTOR TEST RESULTS

The objective of this program was to develop laboratory measurements and procedures with which to better judge the influence of various fuels on smoke-related engine and combustor performance tests. To determine which fuel properties provide the most reliable predictions, correlations were made between several laboratory measurements on the structure-related properties of the test fuels NAPC 1-10 with the results of combustor tests. This section discusses the fuel properties used in the correlations, the sources of the combustor performance tests, functional relations between performance tests and fuel properties, goodness-of-fit criteria, and the interpretation of the correlation analysis results.

1. Correlation Parameters

The fuel parameters which were tested for correlations with the combustor test results include both chemical composition and laboratory flame measurements. The chemical properties, measured at NRL and NAPC, included the hydrogen content, total aromatic hydrocarbon content, and monocyclic and polycyclic aromatic hydrocarbon contents. The laboratory scale flame measurements, performed in this program, included premixed flame and diffusion flame threshold sooting indices, several soot yield parameters, premixed flame soot volume fractions, and premixed flame temperatures.

The chemical composition analyses of total aromatic hydrocarbon content by high performance liquid chromatography (HPLC) methods were performed at NRL.³⁹⁻⁴¹ The other chemical compositions

and hydrogen contents of the fuels were determined by ASTM analyses at NAPC and the results have been incorporated into several combustor test reports (see below), but have not been published separately.

In addition to the fuel properties, several combustor operating conditions were correlated against the smoke-related engine test results. These operating condition parameters include the inlet air pressure (P_{in} , kPa), inlet air temperature (T_{in} , K), total fuel to total air ratio (F/A , g fuel/kg air), fuel carbon to total oxygen ratio (C/O , mole ratio), and the metered fuel/air equivalence ratio ($\phi_{metered}$). The last two quantities were derived from the reported F/A ratios and the fuel hydrogen content ($H\%$), and the AeroChem measured average molecular weight.

The NAPC fuels tested in this program are listed in Table 1. The properties of the fuels are reported in Tables 3, 4, and 7.

2. Sources of Combustor Test Data

The smoke-related engine performance data from tests on the TF30, T56, and T53 combustors included the Smoke Number (SN, no units), the maximum liner temperature rise (LTR, K), the smoke emissions (SE, soot mass per unit volume combustor exhaust gas, $mg\ m^{-3}$), and radiation flux (RF, $kW\ m^{-2}$). These measurements were carried out for NAPC 1-10 at several power levels in the following combustor testing programs: T53 combustor tests reported by Rutter,³⁶ T56 combustor tests reported by Reider et al.,¹ and the TF30 combustor tests reported by Beal⁴² and Herrin.⁴³ The original data have been converted to a consistent set of metric units in Tables 15 to 17.

The performance tests are generally independent measurements. However, for the T56 combustor, the smoke emissions were calculated from the measured Smoke Numbers. A discrepancy in the smoke emission data for NAPC-7 was discovered in the T56 report, so these data were recalculated using the reported relationship and Smoke Numbers.¹ These recalculated values are shown in Table 16.

3. Functional Form of Correlations

The correlations between the smoke-related combustor data and the fuel or operating condition parameters were of the linear form: $y = a + bx$. For a single power level (idle, cruise, dash, etc.), the combustor smoke-related test values (y = Smoke Number, smoke emissions, liner temperature rise, or radiation flux) measured for the fuel set were correlated to either the fuel parameters (x = hydrogen content, total aromatics, smoke point, TSI, SPE, etc.),

or the operating conditions used in testing each individual fuel ($x = F/A$, C/O, inlet pressure, inlet temperature or $\dot{Q}_{\text{metered}}$). The latter five independent variables were correlated to determine if the operating conditions were held sufficiently constant during fuel tests at a single power level. This was necessary because the combustor data are quite sensitive to changes in the operating conditions. Thus, apparently minor variations in the nominal combustor operating conditions can mask the effects of the fuel variations.

Only linear correlations were performed because the data were observed to be either roughly linearly related to a fuel or operating condition parameter, or data looked random.

4. Regression Criteria

Several goodness-of-fit criteria exist for least squares analysis. Commonly employed tests are the correlation coefficient (r), the square of the correlation coefficient or coefficient of determination (r^2), the chi-square test, the Fisher or F-test, and "student's t-test." A complete discussion of the various goodness-of-fit criteria, including the coefficient of determination, can be found in Edwards⁴⁴ or Bevington.⁴⁵ For linear least square analyses (i.e., fits of the form $y = a + bx$), the coefficient of determination, r^2 , is a reliable criterion for judging a correlation between x and y variables. This parameter ranges from 0 to +1. A value of $r^2 = 0$ indicates no correlation between y and x , and $r^2 = 1$ indicates a perfect correlation.

However, in comparing the magnitude of r^2 from several fits, the number of data points (x, y pairs) being correlated must also be considered. Tables 18 through 33 list the coefficients of determination for the linear least squares analyses of the fuel and operating parameters against the combustor test results. The 95% and 99% confidence level r^2 values (95% CL r^2 and 99% CL r^2) are given at the bottom of each column in the tables. The meaning of the 95% CL r^2 value (and similarly the 99% CL r^2) is as follows: If a set of random variates is selected (e.g., 15 x and 15 y values drawn independently) a linear correlation performed, and the r^2 determined, and then this process of drawing random variates and performing correlations repeated many more times, the r^2 values for these correlations of random variates will fall below the "95% CL r^2 " in 95% of all the correlations. Only in 5% of the correlations of these random data will the r^2 be above the "95% CL r^2 " value. Note, however, that the 95% CL r^2 value depends on the number of degrees of freedom (DOF). The DOF is defined as the number of (x, y) pairs being correlated minus the number of fitting parameters (2 for linear fits). For the correlations performed in this work, DOF = number of fuels correlated at the power level

TABLE 4. DIFFUSION FLAME PROPERTIES OF NAPC FUELS

NAPC no.	Description	Smoke Point			TSI _{df}	FCR _o	ΔFCR _o	SPE
		NRL	NAPC	AeroChem				
1	SUNTECH-1	18.6	17	17.0	33.5	0.52	0.85	0.204
2	SUNTECH-2	18.1	18	18.7	32.1	0.56	0.86	0.198
3	SUNTECH-3	20.0	20	20.8	25.2	0.63	0.88	0.202
4	SUNTECH-4	20.8	21	22.2	24.9	0.67	0.90	0.190
5	Low Aromatic JP-5	21.3	21	23.3	22.9	0.74	0.87	0.185
6	Fuel Oil #2	---	17	17.0	35.4	0.51	0.85	0.210
7	20/80 HCGO/NAPC-9	15.0	14	13.0	42.2	0.40	0.86	0.223
8	50/50 DFM/NAPC-5	17.5	16	18.6	30.1	0.61	0.85	0.201
9	HiAromatic JP-5	18.4	21	18.6	27.3	0.63	0.83	0.194
10	Oil Shale JP-5	---	21	20.6	24.2	0.75	0.87	0.195
16	JP-7			36.0	14.3			
17	DFM			18.5	33.7			
18	Fuel Oil #2			17.1	36.4			
19	SUNTECH-A			10.4	51.5			
20	SUNTECH-B			14.1	38.1			
22	JP-5			20.8	24.5			
--	SUNTECH Kerosene	19.7		22.9	21.9			
--	SUNTECH XTB	10.3		7.7	49.4			
--	SUNTECH FO	17.4		23.2	25.4			
--	SUNTECH 40G	15.3		12.5	49.8			
--	SUNTECH 60G	12.1		10.7	70.8			
--	SUNTECH Kerosene			23.3	21.1			
--	SUNTECH #2 dist.			19.7	31.1			
--	SUNTECH HCGO			6.6	87.6			

TABLE 3. NAPC FUI PROPERTIES

NAPC no.	Description	Density (g cm ⁻³)	H%	T _f	MW (g mol ⁻¹)	Aromatic content, %			
						Total (vol.%)		MCAH (wt%)	PCAH
						FIA	HPLC	HPLC	HPLC
1	SUNTECH-1	0.8293	13.36	1.11	179	32.1	28.5	27.5	5.1
2	SUNTECH-2	0.8338	13.48	1.06	189	25.0	19.8	18.6	3.5
3	SUNTECH-3	0.8173	13.66	1.17	167	23.6	22.8	22.0	4.0
4	SUNTECH-4	0.8160	13.82	1.11	176	20.5	18.6	18.5	2.0
5	Low Aromatic JP-5	0.8143	13.79	1.14	171	15.0	15.9	14.5	3.0
6	Fuel Oil #2	0.8379	13.22	1.06	189	18.6	25.0	11.2	18.3
7	20/80 HCGO/ NAPC-9	0.8435	12.83	1.18	171	32.6	26.4	20.9	9.7
8	50/50 DFM/ NAPC-5	0.8280	13.54	1.12	177	21.0	18.6	14.4	6.4
9	HiAromatic JP-5	0.8203	13.49	1.22	161	22.7	22.7	24.6	1.5
10	Oil Shale JP-5	0.8047	13.70	1.21	159	24.0	21.8	22.5	1.1
16	JP-7	0.7980	14.5	1.12	171		2.2 ^a	2.4	---
17	DFM	0.8318	13.20	1.02	196		17.6 ^a	14.9	5.2
18	Fuel Oil #2	0.8373	13.4	1.03	195		21.0 ^a	20.2	3.5
19	SUNTECH-A	0.8600	12.2	1.24	166		27.9 ^a	16.0	16.8
20	SUNTECH-B	0.8416	12.9	1.20	168		23.2 ^a	15.2	11.9
22	JP-5	0.8184	13.7	1.20	163		15.6 ^a	15.4	2.2
--	SUNTECH Kerosene	0.8056	14.01	1.20	161		17.3 ^{a,b}	17.9 ^b	1.5 ^b
--	SUNTECH XTB	0.8760	9.95	1.77	118		99.9 ^{a,b}	99.0 ^b	0.9 ^b
--	SUNTECH FO	0.8138	13.96	1.04	188		16.0 ^{a,b}	12.4 ^b	6.0 ^b
--	SUNTECH 40G	0.8873	12.74	1.10	193		23.2 ^{a,b}	20.2 ^b	6.2 ^b
--	SUNTECH 60G	0.9028	12.48	0.93	233		39.1 ^c	---	---
--	SUNTECH Kerosene	0.8025	13.86	1.21	159		17.4 ^a	16.3	3.4
--	SUNTECH #2 dist.	0.8308	13.52	1.03	193		16.5 ^a	13.5	5.4
--	SUNTECH HCGO	0.9427	9.95	1.27	177		52.1 ^a	13.4	50.0

^a Calculated from HPLC wt%;

$$\text{HPLC vol.\% Total Aromatics} = \frac{\text{HPLC wt\% MCAH}}{1.11} + \frac{\text{HPLC wt\% PCAH}}{1.25}$$

^b LC/GC data.^c Weight percent.

TABLE 2. COMPOSITION AND MEASURED AND CALCULATED PROPERTIES OF AEROCHEM-A

Hydrocarbon	Formula	Composition		Moles	Mole fraction
		MW	Mass (g)		
n-tetradecane	C ₁₄ H ₃₀	198.40	248.22	1.2511	0.2693
n-heptane	C ₇ H ₁₆	100.21	124.36	1.2410	0.2672
decalin	C ₁₀ H ₁₈	138.25	120.18	0.8693	0.1872
toluene	C ₇ H ₈	92.14	60.08	0.6521	0.1404
tetralin	C ₁₀ H ₁₂	132.21	66.61	0.5038	0.1085
1-methylnaphthalene	C ₁₁ H ₁₀	142.20	18.08	0.1271	0.0274
"Totals"			637.53	4.6444	1.0000

Measured Properties

Density at 20°C	0.7996 g cm ⁻³
Freezing point depression	1.42°C
Estimated molecular weight	134 g mol ⁻¹
ASTM Smoke Point	23.5
φ _c , unregulated burner	1.69
φ _c , regulated burner	1.73

Calculated Properties

Average formula	C _{7.2} H _{13.5}
Mole fraction weighted MW	137.3 g mol ⁻¹
Hydrogen content, wt%	13.53
TSI _{df}	17.9
TSI _{pf} , unregulated burner	70
TSI _{pf} , regulated burner	65

Premixed Flame Soot Volume Fraction Measurements

Equivalence ratio (φ)	Soot volume fraction (10 ⁻⁷)	Burner type
1.83	0.30	unregulated
1.86	0.52	regulated
1.90	0.52	unregulated
2.00	1.50	unregulated
2.04	1.69	regulated
2.08	2.25	unregulated
2.21	3.94	unregulated

Diffusion Flame Smoke Production Measurements

Fuel consumption rate (μg s ⁻¹)	Soot production rate (μg s ⁻¹)
810	12
830	29
930	40
1070	78
1290	125
1610	187
1920	232
2390	307

TABLE 1. LIST OF NAPC FUELS

NAPC no.	Description	NAPC PE no.	NRL no.	Notes
1	SUNTECH-1	140-81	81-13	
2	SUNTECH-2	146-81	81-14	
3	SUNTECH-3	147-81	81-15	
4	SUNTECH-4	123-81	81-16	
5	Low Aromatic JP-5	101-81	81-9	
6	Fuel Oil #2	113-81	81-10	Home Heating Oil
7	20/80/HCGO/NAPC-9	152-81	81-17	Hydro Catalytic Gas Oil
8	50/50 DFM/NAPC-5	119-81	81-12	Diesel Fuel, Marine
9	HiAromatic JP-5	131-81	81-19	
10	Oil Shale JP-5	106-81	J-22	
16	JP-7	31-83	83-41	
17	DFM	30-83	83-42	
18	Fuel Oil #2	32-83	84-3	
19	SUNTECH-A	49-83	83-43	
20	SUNTECH-B	54-83	83-44	
22	JP-5	44-83	83-45	
--	SUNTECH Kerosene	128-81	81-20	
--	SUNTECH XTB	125-81	81-21	Xylene Tower Bottoms
--	SUNTECH FO	127-81	81-22	Furnace Oil
--	SUNTECH 40G	129-81	81-24	40 Golden
--	SUNTECH 60G	130-81	81-25	60 Golden
--	SUNTECH Kerosene	39-83	84-8	
--	SUNTECH #2 dist.	40-83	84-9	
--	SUNTECH HCGO	41-83	84-10	

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(5) A quantitative evaluation of the effectiveness of soot-reducing additives should be performed in well-characterized laboratory flames.

- (b) Use test fuels with a wider range of properties, e.g., H%, Ar%, SP.
- (c) Perform a more extensive chemical characterization of the test fuels.
- (d) Measure the flame temperature in the primary and secondary combustion zones. Optical measurements are probably best for this and should include a measurement of the flame emissivity.
- (e) Consider alternative liner temperature measurement techniques.
- (f) Use fuels with properties that are not highly correlated. For example, H% should not be strictly correlated with the SP or aromatic content of the series of fuels.
- (g) An effort should be made to identify why in some tests neither fuel properties nor operating condition variations correlate the test data. Some process that perturbs the combustor data is occurring, but has not been identified in previous work. It is impossible to identify this process from only the reported results of the investigation. A specific investigation of this problem is needed during the combustor/engine testing program.
- (h) Further correlation analyses should be performed, with particular efforts to simultaneously consider operating condition variations and fuel property differences.

(2) Further laboratory investigations are necessary to understand the chemical and physical processes that are occurring in soot formation, and to identify which are relevant to turbojet engine combustion and fuel effects combustion.

(3) The effects of fuel composition on soot formation should be studied under more realistic conditions. In particular, experiments should be performed at higher pressures: 100-2000 kPa (1 to 20 atm).

(4) Fuel effects on soot formation should be studied in turbulent flames for comparison with the data available from laminar flames.

V. CONCLUSIONS AND RECOMMENDATIONS

A. CONCLUSIONS

(1) Overall, statistically significant correlations of fuel parameters with combustor test results were obtained in fewer than 50% of the tests. The two fuel parameters that best correlated smoke-related test results were the laboratory diffusion flame fuel consumption rate at the smoke point (FCR_0) and the diffusion flame threshold soot index (TSI_{df}). The average coefficient of determination, r^2 , for correlations of the best fuel parameter, the diffusion flame fuel consumption rate at the smoke point, with the 45 test results was 0.37.

(2) In about 25% of the combustor tests the operating conditions varied enough to give significant correlations between the smoke-related test results and the values of the operating conditions.

(3) The radiation flux data, RF, were correlated with fuel properties better than the other combustor test data.

(4) The combustor liner temperature rise data, LTR, correlated better with the engine operating conditions than with any fuel parameter.

(5) Premixed laboratory flame measurements on the test fuels were not useful for correlating the combustor results.

(6) Aromatic hydrocarbon content data, divided into mono- and polycyclic aromatic hydrocarbon classes, were not useful for correlating the combustor results.

(7) Total aromatic hydrocarbon content, measured at the Naval Research Laboratory using the HPLC/DRI technique, was found to correlate the combustor test results better than the data obtained using the ASTM FIA technique. Note, however, that total aromatic content was not one of the best fuel parameters for correlating these combustor data.

(8) Based on the results of this program, no universal fuel parameter for correlating smoke-related engine test results has been identified.

B. Recommendations

(1) In future fuel effects testing programs:

(a) Better control the F/A, C/O, T_{in} , and P_{in} .

were correlated with SPE, Hx , SP, $1/SP$, $TSIdf$, and FCR_o . The very high r^2 values for the T56 results are particularly noteworthy. The fuel parameter and operating condition correlations at the 99% CL were all unsuccessful for the TF30. The T53 fuel parameter correlations were moderately successful. When one of the fuel parameters of the group Hx , SP, $1/SP$, $TSIdf$, FCR_o or SPE was successful (95% CL) for these combustors, all of the parameters were successful. This suggests that these fuel parameters are equally good parameters for predicting SE levels in these combustors. For the T53 and T56 combustors, there were no successful correlations with any of the operating conditions. Two power levels in the TF30 combustor tests correlated with the operating conditions. In all three combustors, when a fuel parameter was successful, the operating conditions were not, and vice versa.

d. SAE Smoke Number (SN) - The SN correlations are tabulated in Tables 30, 31, and 32 and the summary in Table 33. The results of these correlations provided similar information to the results obtained with the SE tests. At the 99% CL, the best fuel correlating parameter was SPE, although no fuel parameter correlated any of the TF30 test results for SN.

e. Correlations By Engine Type - Radiation flux correlated with fuel properties much better than SN or SE, and LTR correlated much poorer than SN or SE for these three combustors together. Table 34 shows the same coefficient of determination data analyzed by engine type. The best fuel correlating parameter at the 95% CL, FCR_o , was successful in 20 out of 45 total tests, and the T56 and T53 data sets were definitely correlated better than the TF30 data. At the 99% CL, the best overall correlating parameter was SPE followed by $TSIdf$. In Table 34, the operating conditions are not individually listed. "All" is used to indicate the number of times any operating condition was successful. The operating conditions correlated the TF30 data much better than the other combustor data. This reemphasized the contention that unless the operating conditions are held rigidly constant (or the effects of the operating condition variations accurately accounted for in the analysis), fuel effects can be hidden by the usually random operating condition variations.

b. Maximum Liner Temperature Rise (LTR) - The LTR correlations are given in Tables 22, 23, and 24. The LTR summary, Table 25, shows clearly that the fuel parameters do not accurately correlate the LTR results. The best correlating parameter was an operating condition parameter, the C/O ratio, which was successful (at the 95% CL) in 50% of the correlations (12). Specifically, the TF30 data were correlated better by the C/O parameter than the T53 and T56 results. However at two power levels where the C/O parameter was successful for the TF30, fuel parameters were also successful (SPE was the best). Overall, fuel parameters were generally unsuccessful in correlating the LTR results for these combustors. Particularly note that at the 99% CL, no parameter, fuel or operating condition successfully correlated any of the 8 T56 or T53 tests. Although the high dependence of the TF30 test results on operating conditions generally invalidates those engine tests as meaningful in attempting to correlate LTR with fuel properties, the situation is less clear for the other data. A fuel effects correlation may exist but these data are simply inadequate to show it. Clearly more work and better data are needed in this area, since LTR is probably the most practically important variable being studied because of its direct influence on the combustor service lifetimes.

The reports of the TF-30 and T53 studies state that the liner temperature data are correlated with H_x . In the TF30 report,⁴² before correlations were performed with H_x , the liner temperature data were corrected for (1) variations in the inlet temperatures, (2) variations in the actual fuel-air ratios, and (3) differences in the heating values of the fuels. To perform these corrections, it was assumed that the variations of liner temperatures with inlet temperature and with fuel-air ratio were identical for all fuels. The measured variations for NAPC-5 were used to correct data sets obtained using other fuels. No validation of these assumptions was made. In this work, the ten NAPC fuels were found to exhibit a wide variation in the change of laboratory premixed flame temperature with fuel-air ratio (-226 to -499 K/θ, see Table 10) as would be expected for flames with various amounts of radiative heat losses. This method of "correcting" test data results needs further study to determine its validity.

c. Smoke Emission (SE) - Individual smoke emission correlations are presented in Tables 16, 17 and 18, and are summarized in Table 19. Fuel parameters were successful in fewer than 50% of the total number of tests carried out with the three combustors. Overall, at the 95% CL, SPE, H_x , $1/SP$, TSI_{df} , AR_x (HPLC), and FCR_o correlated 5 out of 12 cases and in that order of decreasing r^2 . At the 99% CL, however, the best correlating parameters were AR_x (HPLC) and SPE, which successfully correlated 4 and 3 cases. For the T56 combustor, shown in Table 27, all power level tests were successfully correlated by AR_x (HPLC) and three out of four tests

minus 2. Further examples and use of the coefficient of determination and confidence levels can be found in Ref. 44.

In this work, the success of a fuel (or operating condition) parameter in correlating the combustor test results was judged by a simple criterion. If the coefficient of determination, r^2 , was equal to or greater than the 95% CL r^2 or the 99% CL r^2 value, then the fuel or operating condition parameter being correlated was deemed "successful" at that confidence level.

5. Results of the Correlation Analyses

A large number of linear correlations were performed. These correlation results are presented in Tables 18 through 33. Each table contains the coefficients of determination for a single engine and one of the smoke-related performance tests. In these tables, the fuel (fitting) parameters being correlated are listed in the left-hand column and the other columns are headed by the power level for which the correlation was performed. The last items in each power level column are the specific fuels employed in the tests (not all ten fuels were used in some tests) and the 95% CL and 99% CL r^2 values.

a. Radiation Flux (RF) - Radiation flux is a performance test which measures the visible and infrared radiation emitted from the combustion zone of the engine. From Tables 18, 19, 20 or the RF summary Table 21, it was found that FCR_0 and hydrogen content (H%) successfully correlated RF in 8 out of 11 possible tests (i.e., three or four power levels for three combustors = eleven tests) at the 95% CL and that TSI_{df} , SPE, and $1/SP$ successfully correlated the RF data in 4, 3, and 3 out of 11 tests at the 99% CL. Based on the overall average r^2 , TSI_{df} is a slightly better correlating parameter than the other fuel parameters. Each of FCR_0 , H%, TSI_{df} , SP, $1/SP$, and SPE were successful correlating parameters (at the 95% CL) in more than 50% of the RF tests, and in that order of decreasing success. Particularly noteworthy is the fact that H% and FCR_0 correlate all the results for the T53 combustor (at the 95% CL). The fuel composition parameters (AR%, MCAH, PCAH), premixed flame parameters, and all of the operating condition parameters, all poorly correlate the RF test results. These results show that laboratory scale diffusion flame tests (FCR_0 , SP, TSI_{df} , etc.), and H%, could be used as RF correlation parameters. They are successful irrespective of combustor type and for most power levels. Furthermore (see Tables 18, 19, and 20), in greater than 90% of the cases where one fuel parameter was successful at the 95% CL (i.e., one of H%, FCR_0 , TSI_{df} , SP or $1/SP$), the others in this group were also successful. In this sense, they are not completely independent fuel parameters. In fact, when H% was correlated against SP, an $r^2 = 0.95$ was obtained; FCR_0 vs. SP gave $r^2 = 0.85$.

TABLE 5. DIFFUSION FLAME SOOT PRODUCTION FOR PURE HYDROCARBONS, BINARY MIXTURES, AND AEROCHEM-A

Component	FCR (mg s ⁻¹)	SPR (μg s ⁻¹)	Component	FCR (mg s ⁻¹)	SPR (μg s ⁻¹)
n-tetradecane	3.67	16	n-heptane	5.17	0.7
	3.71	24		6.67	41
	3.78	38		7.22	87
	4.06	124		8.67	235
	4.25	151		9.33	310
	4.56	173			
	4.92	213			
	5.00	217			
	5.33	248			
Isooctane (2,2,4-trimethylpentane)	1.73	9.3	Decalin	0.83	18
	1.78	28		0.93	42
	1.83	55		1.13	82
	1.87	48		1.62	198
	1.89	55		1.79	218
	2.00	88		2.21	297
	2.29	137		2.46	338
	2.44	183			
	3.06	268	Tetralin	0.32	4.3
	3.50	337		0.44	39
	4.22	427		0.56	55
				0.73	114
Toluene	0.33	17.8		0.96	180
	0.56	89.4		1.50	310
	0.94	179			
	1.08	218	AeroChem-A	0.81	12
	1.50	292		0.83	29
				0.93	40
1-methyl-naphthalene	0.17	3.6		1.07	78
	0.26	34.8		1.29	125
	0.39	85.6		1.61	187
	0.58	152		1.92	232
	0.83	218		2.39	307
	1.06	270			
			Toluene/isooctane	0.95	9.0
Toluene/isooctane (40/60, v/v)	0.53	11	(15/85, v/v)	0.97	31
	0.64	27		1.25	95
	0.70	67		1.38	120
	0.88	112		1.75	196
	1.29	204		2.17	263
	1.88	317		3.22	420

TABLE 6. DIFFUSION FLAME SOOT PRODUCTION FOR NAPC FUELS

Fuel	FCR (mg s ⁻¹)	SPR (μg s ⁻¹)	Fuel	FCR (mg s ⁻¹)	SPR (μg s ⁻¹)
NAPC-1	0.56	4.7	NAPC-2	0.60	14
	0.61	19		0.61	11
	0.64	34.2		0.69	35.6
	0.78	71.4		0.83	75.3
	1.00	119		1.17	144
	1.04	138		1.56	228
	1.33	182		2.06	317
	1.44	210			
	1.72	273			
	2.00	327			
NAPC-3	0.71	18	NAPC-4	0.74	8.6
	0.73	32.7		0.79	34
	0.83	53.3		0.87	57.3
	1.22	139		1.08	99.2
	1.61	218		1.72	222
	1.83	262		2.56	371
	2.11	312			
	2.33	343			
NAPC-5	0.79	14	NAPC-6	0.56	11
	0.86	35.0		0.67	43.1
	1.03	74.3		0.90	96.0
	1.12	100		1.29	189
	1.39	157		1.50	226
	1.89	249		1.78	282
	2.17	295		2.00	331
NAPC-7	0.46	13.7	NAPC-8	0.69	15.6
	0.52	29.8		0.72	30.8
	0.75	86.4		0.93	86.0
	1.07	155		1.12	134
	1.25	195		1.50	200
	1.67	291		1.78	260
	1.89	333		2.11	327
NAPC-9	0.67	7.6	NAPC-10	0.77	3.1
	0.72	35.3		0.83	22
	0.93	84.0		1.00	69.3
	1.21	145		1.38	152
	1.44	195		1.67	210
	1.67	240		1.89	249
	2.17	324		2.11	296

TABLE 7. PREMIXED FLAME PROPERTIES OF NAPC FUELS

NAPC no.	Description	Unregulated burner		Regulated burner				
		ϕ_c	TSI_{pf}	ϕ_c	TSI_{pf}	T_{ϕ_c}	$\phi(f_v)$	$T(f_v)$
1	SUNTECH-1	1.67	72	1.71	67	1690	2.00	1565
2	SUNTECH-2	1.66	73	1.63	77	1720	2.02	1555
3	SUNTECH-3	1.66	73	1.72	66	1685	2.05	1560
4	SUNTECH-4	1.70	68	1.77	60	1685	2.03	1580
5	Low Aromatic JP-5	1.67	72	1.71	67	1705	2.07	1580
6	Fuel Oil #2	1.69	70	1.65	74	1720	1.94	1585
7	20/80 HCGO/NAPC-9	1.58	83	1.69	70	1695	1.90	1590
8	50/50 DFM/NAPC-5	1.69	70	1.86	50	1695	2.19	1580
9	HiAromatic JP-5	1.68	71	1.80	57	1715	2.14	1615
10	Oil Shale JP-5	1.67	72	1.81	55	1685	2.12	1620
16	JP-7	---	--					
17	DFM	1.66	73					
18	Fuel Oil #2	---	--					
19	SUNTECH-A	1.65	74					
20	SUNTECH-B	1.63	77					
22	JP-5	---	--					
--	SUNTECH Kerosene	1.70	68					
--	SUNTECH XTB	1.57	84					
--	SUNTECH FO	1.70	68					
--	SUNTECH 40G	1.66	73					
--	SUNTECH 60G	---	--					
--	SUNTECH Kerosene	1.65	74					
--	SUNTECH #2 dist.	---	--					
--	SUNTECH HCGO	1.53	88					

TABLE 8. PREMIXED FLAME TEMPERATURES (K) FOR NAPC FUELS AND AEROCHEM-A
 Temperatures measured at 2.0 cm above burner surface.

Fuel	ϕ	T(K)	Method ^a	Fuel	ϕ	T(K)	Method ^a
NAPC-1	1.49	1783	TC	NAPC-2	1.50	1770	TC
	1.53	1770	TC		1.54	1757	TC
	1.58	1751	TC		1.59	1747	TC
	1.62	1727	TC		1.63	1738	TC
	1.81	1724 ^b	EP		1.75	1637	EP
	1.85	1618	EP		1.83	1631	EP
	1.90	1588	EP		1.91	1582	EP
	1.99	1564	EP		2.01	1553	EP
	2.11	1508	EP		2.13	1527	EP
	2.24	1494	EP				
NAPC-3	1.47	1786	TC	NAPC-4	1.52	1773	TC
	1.51	1775	TC		1.56	1767	TC
	1.55	1761	TC		1.61	1744	TC
	1.60	1741	TC		1.66	1721	TC
	1.82	1613	EP		1.88	1670	EP
	1.91	1594	EP		1.88	1730	EP
	2.05	1557	EP		1.98	1594	EP
	2.18	1535	EP		1.98	1593	EP
					2.07	1562	EP
					2.09	1550	EP
					2.18	1528	EP
NAPC-5	1.52	1765	TC	NAPC-6	1.19	1935	TC
	1.56	1756	TC		1.30	1884	TC
	1.61	1744	TC		1.43	1827	TC
	1.66	1727	TC		1.59	1775	TC
	1.82	1655	EP		1.80	1613	EP
	1.94	1611	EP		1.92	1559	EP
	2.09	1588	EP		2.05	1515	EP
	2.26	1514	EP		2.22	1515	EP
NAPC-7	1.14	1978	TC	NAPC-8	1.18	1945	TC
	1.24	1923	TC		1.28	1891	TC
	1.36	1850	TC		1.41	1818	TC
	1.50	1800	TC		1.57	1777	TC
	1.86	1594	EP		1.97	1672	EP
	1.95	1551	EP		2.02	1662	EP
	2.05	1513	EP		2.03	1652	EP
	2.18	1475	EP		2.07	1584	EP
					2.12	1615	EP
					2.13	1628	EP
					2.17	1525	EP
					2.24	1589	EP
					2.27	1529	EP
					2.33	1578	EP

^a TC = thermocouple measurement; EP = three-wavelength emission pyrometer measurement.

TABLE 8. (continued)

Fuel	ϕ	T(K)	Method ^a	Fuel	ϕ	T(K)	Method ^a
NAPC-9	1.19	1921	TC	NAPC-10	1.51	1769	TC
	1.30	1863	TC		1.55	1737	TC
	1.44	1810	TC		1.59	1735	TC
	1.61	1767	TC		1.64	1709	TC
	2.00	1666	EP		1.97	1762 ^b	EP
	2.10	1629	EP		2.06	1651	EP
	2.20	1590	EP		2.17	1602	EP
	2.30	1558	EP		2.26	1578	EP
	2.39	1554	EP		2.36	1559	EP
NAPC-17	1.25	1900	TC	NAPC-19	1.22	1965	TC
	1.34	1847	TC		1.30	1923	TC
	1.44	1803	TC		1.40	1886	TC
	1.57	1769	TC		1.51	1844	TC
NAPC-20	1.21	1976	TC	SUNTECH XTB PE no. 125-81	1.47	1831	TC
	1.29	1931	TC		1.49	1829	TC
	1.38	1880	TC		1.51	1824	TC
	1.49	1846	TC	SUNTECH FO PE no. 127-81	1.45	1781	TC
SUNTECH kerosene PE no. 39-83	1.47	1780	TC		1.51	1767	TC
	1.51	1764	TC		1.58	1741	TC
	1.55	1747	TC		1.65	1705	TC
	1.60	1724	TC	SUNTECH HCGO PE no. 41-83	1.15	2020	TC
SUNTECH 40G PE no. 129-81	1.22	1928	TC		1.21	1973	TC
	1.33	1882	TC		1.29	1925	TC
	1.45	1820	TC		1.38	1884	TC
	1.61	1765	TC	SUNTECH kerosene PE no. 128-81	1.50	1769	TC
AEROCHEM-A	1.44	1794	TC		1.54	1759	TC
	1.52	1770	TC		1.59	1742	TC
	1.57	1757	TC		1.63	1715	TC
	1.61	1715	TC				
	1.84	1824	EP				
	1.86	1715	EP				
	1.93	1681	EP				
	2.04	1692	EP				
	2.04	1620	EP				
	2.16	1625	EP				
	2.17	1581	EP				

TABLE 9. MOLECULAR WEIGHT DETERMINATION OF HYDROCARBONS
BY FREEZING POINT DEPRESSION MEASUREMENTS IN BENZENE

Hydrocarbon	Freezing point depression (°C)	Experimental MW (g mol ⁻¹)	Theoretical MW (g mol ⁻¹)	MW Error ^a
1-methylnaphthalene	1.76	138	142	-4
n-tridecane	0.96	189	184	+5
n-butylbenzene	1.53	134	134	0
AeroChem-A	1.42	134	137	-3

^a MW error $\equiv$ (experimental MW) - (theoretical MW).

TABLE 10. LINEAR LEAST SQUARES ANALYSES
OF PREMIXED FLAME TEMPERATURES
PRESENTED IN TABLE 8

Fitting function: Temperature, K = A + B ϕ ;
r² = coefficient of determination.

Fuel	A, K	B, K ϕ^{-1}	r ²
NAPC-1	2404	-419	0.984
NAPC-2	2407	-423	0.969
NAPC-3	2352	-387	0.968
NAPC-4	2370	-388	0.985
NAPC-5	2288	-342	0.990
NAPC-6	2474	-457	0.965
NAPC-7	2539	-499	0.995
NAPC-8	2314	-333	0.948
NAPC-9	2263	-304	0.994
NAPC-10	2095	-226	0.977
NAPC-17	2398	-406	0.967
NAPC-19	2461	-410	0.994
NAPC-20	2539	-470	0.980
SUNTECH XTB (PE# 125-81)	2089	-175	0.942
SUNTECH Kerosene (PE# 39-83)	2414	-431	0.999
SUNTECH Kerosene (PE# 128-81)	2381	-406	0.953
SUNTECH FO (PE# 127-81)	2338	-381	0.975
SUNTECH 40G (PE# 129-81)	2444	-425	0.993
SUNTECH HCGO (PE# 41-83)	2688	-586	0.987
AEROCHEM-A	2126	-235	0.865

TABLE 1L MIXTURE RULE CALCULATIONS OF PREMIXED FLAME
AND DIFFUSION FLAME THRESHOLD SOOTING INDICES
FOR AEROCHEM-A

Hydrocarbon	Mole fraction, X_i	Diffusion flame		Premixed flame	
		TSI_i	$X_i TSI_i$	TSI_i	$X_i (1.1)^{TSI_i}$
n-tetradecane	0.2693	5.4	1.5	63	120
n-heptane	0.2672	2.6	0.7	62	98
decalin	0.1872	15	2.8	81	422
toluene	0.1404	44	6.2	85	463
tetralin	0.1085	61	6.6	97	1123
1-methylnaphthalene	0.0274	91	2.5	100	378
		Sum1 = 20.3		Sum2 = 2604	

$$\text{Diffusion Flame TSI} = \text{Sum1} = 20.3$$

$$\text{Premixed Flame TSI} = \frac{\log (\text{Sum2})}{\log (1.1)} = 82.5$$

TABLE 12. CALCULATED DIFFUSION FLAME TSIs FOR NAPC FUELS

NAPC no.	Composition					TSI _i	TSI _{df} (mixture)	
	V _i	W _i	X _i	PE no.			Calculated	Observed
1	0.735	0.725	0.659	127-81	FO	25.4	31.8	33.5
	0.082	0.080	0.085	128-81	Kerosene	21.9		
	0.150	0.159	0.230	125-81	XTB	49.4		
	0.033	0.036	0.026	130-81	60G	70.8		
2	0.930	0.925	0.912	139-81 ^a	FO	30?	31.7	32.1
	0.030	0.033	0.047	125-81	XTB	49.4		
	0.040	0.043	0.041	129-81	40G	49.8		
3	0.450	0.445	0.465	128-81	Kerosene	21.9	26.9	25.2
	0.070	0.075	0.107	125-81	XTB	49.4		
	0.480	0.488	0.429	{ 127-81 139-81 ^a	FO	26.6		
4	0.475	0.471	0.501	128-81	Kerosene	21.9	25.2	24.9
	0.475	0.474	0.433	127-81	FO	25.4		
	0.030	0.032	0.047	125-81	XTB	49.4		
	0.020	0.022	0.019	129-81	40G	49.8		
7	0.200	0.227	0.211	148-81 ^a	HCGO	87.6?	40.0	42.2
	0.800	0.773	0.789	131-81	NAPC-9	27.3		
8	0.500	0.505	0.459	118-81 ^a	DFM	33.7?	28.3	30.1
	0.500	0.495	0.541	101-81	NAPC-5	22.9		
19	0.528	0.489	0.523	39-83	Kerosene	21.1	44.2	51.5
	0.161	0.173	0.152	40-83	#2 dist.	31.1		
	0.311	0.338	0.325	41-83	HCGO	87.6		
20	0.240	0.227	0.258	39-83	Kerosene	21.1	42.0	38.1
	0.550	0.539	0.504	40-83	#2 dist.	31.1		
	0.210	0.234	0.239	41-83	HCGO	87.6		

^a Fuels not tested in this work.

TABLE 13. LEAST SQUARES ANALYSES OF SOOT PRODUCTION RATES (SPR)
FOR PURE HYDROCARBONS, BINARY MIXTURES, AND AEROCHEM-A

Fuel	Function no. 1 ^a			Function no. 2 ^b			FCR ₀ ^c (mg s ⁻¹)	Goodness of fit ^d	
	a	b	c	a'	b'	c'		r ²	σ
n-heptane	386.7	-158.8	16.2	1.5	16.1	16.2	5.40	0.998	8.5
n-tetradecane	-1851.3	769.3	-70.8	25.9	245.4	-70.8	3.70	0.985	12.4
toluene	-90.7	353.5	-65.5	3.2	316.8	-65.5	0.28	0.999	4.6
tetralin	-89.0	286.8	-13.3	1.4	278.3	-13.3	0.32	0.997	8.6
decalin	-200.9	285.0	-26.9	2.5	243.6	-26.9	0.77	0.999	5.3
isooctane	-455.4	322.8	-27.2	10.2	231.5	-27.2	1.68	0.996	9.3
1-methyl- naphthalene	-72.0	453.8	-124.0	1.6	411.7	-124.0	0.17	1.000	2.6
AeroChem-A	-196.7	291.6	-34.1	2.9	240.4	-34.1	0.75	0.998	5.5
15/85 toluene/ isooctane (v/v)	-244.3	295.8	-27.8	11.6	243.0	-27.8	0.95	0.986	19.9
40/60 toluene/ isooctane (v/v)	-170.0	365.7	-56.9	4.8	306.5	-56.9	0.52	0.996	10.1

^a $\text{SPR}, \mu\text{g s}^{-1} = a + b \text{ FCR} + c (\text{FCR})^2$ where $\text{FCR} \approx$ fuel consumption rate, mg s^{-1} .

^b $\text{SPR}, \mu\text{g s}^{-1} = a' + b'(\Delta\text{FCR}) + c' (\Delta\text{FCR})^2$ where $\Delta\text{FCR} (\text{mg s}^{-1}) = \text{FCR} - \text{FCR}_0$

^c FCR_0 = Fuel consumption rate at $\text{SPR} \approx 0$.

^d r^2 = coefficient of determination; σ = standard deviation of fit = $[(\text{SPR}_{\text{obs}} - \text{SPR}_{\text{calc}})^2 / (N-3)]^{1/2}$, where $N \equiv$ number of data points used in fit.

TABLE 14. SOOT YIELD PARAMETERS FOR AEROCHEM-A COMPONENTS

Component	X_i	$f_{v,i}^o$ (10^{-8})	θ_i (K)	T_o (K)
n-heptane	0.267	~ 1.0	49,900	1540
n-tetradecane	0.270	1.3	31,500	1630
decalin	0.187	1.7	40,900	1670
toluene	0.140	2.3	42,300	1730
tetralin	0.109	3.6	34,200	1805
1-methylnaphthalene	0.027	5.0	29,100	1845

TABLE 15. TEST DATA FOR TF30 COMBUSTOR

NAPC no.	Operating conditions			Engine tests			
	F/A (g kg ⁻¹)	Inlet tempera- ture (K)	Inlet pres- sure (kPa)	Smoke emis- sions (mg m ⁻³)	Smoke number (SAE)	LTR (K)	RF (kW m ⁻²)
Idle							
1	9.7	447.8	379.9	2.93	---	91.7	---
2	9.9	447.2	380.6	3.59	---	93.9	---
3	9.3	449.4	375.8	2.62	---	107.8	---
4	9.0	447.2	424.0	---	---	132.8	---
5	8.9	441.1	397.1	2.10	---	120.6	---
6	10.3	445.0	397.1	6.80	---	141.1	---
7	10.2	443.3	398.5	2.54	---	130.0	---
8	15.9	450.6	377.1	4.16	---	133.3	---
9	8.6	449.4	368.9	---	1.5	128.3	---
10	8.9	446.7	370.9	---	1.4	125.6	---
Cruise							
1	12.3	625.0	759.8	3.01	---	206.7	397.3
2	12.5	624.4	777.0	3.31	---	208.9	---
3	13.4	626.7	754.3	7.66	---	213.9	431.3
4	12.8	619.4	761.9	4.93	---	205.0	408.6
5	11.8	623.3	770.1	2.79	---	198.3	351.9
6	12.3	622.2	749.5	7.58	---	199.4	454.0
7	12.7	621.7	742.6	7.91	---	209.4	510.8
8	13.4	628.3	768.1	7.21	---	220.0	465.4
9	11.6	625.6	877.0	---	25.0	214.4	---
10	11.7	621.7	882.5	---	23.8	233.9	---
SLTO							
1	19.3	746.7	757.0	3.20	15.9	268.3	567.5
2	19.3	745.0	727.4	2.41	13.2	262.2	567.5
3	19.0	752.8	1785.7	5.36	---	325.6	692.4
4	19.3	744.4	745.3	2.88	10.8	263.9	624.3
5	19.0	746.1	761.9	2.23	12.1	257.8	544.8
6	19.8	746.7	750.1	---	12.2	281.7	658.3
7	19.9	745.6	746.7	0.57	14.6	294.4	692.4
8	19.7	749.4	735.0	2.11	---	273.3	590.2
9	17.9	753.3	1792.6	---	17.0	318.9	---
10	17.0	753.3	1789.2	---	17.3	321.7	---
Dash							
1	20.1	777.8	746.0	---	11.2	292.2	624.3
2	20.6	780.0	743.9	---	13.1	291.7	590.2
3	19.0	782.2	1530.6	2.82	---	339.4	692.4
4	19.9	780.6	751.5	1.77	8.2	280.0	635.6
5	19.9	785.0	779.8	1.13	6.5	279.4	556.2
6	20.8	780.0	743.3	2.40	---	305.6	669.7
7	20.8	783.3	743.9	2.98	11.4	307.8	737.8
8	21.2	777.2	749.5	3.20	11.7	311.7	624.3
9	18.9	781.7	1578.9	---	8.6	351.7	---
10	17.6	778.9	1558.9	---	9.9	350.0	---

TABLE 16. TEST DATA FOR T56 COMBUSTOR

NAPC no.	Operating conditions			Engine tests			
	F/A (g kg ⁻¹)	Inlet tempera- ture (K)	Inlet pres- sure (kPa)	Smoke emis- sions (mg m ⁻³)	Smoke number (SAE)	LTR (K)	RF (kW m ⁻²)
Idle							
1	9.6	435.9	368.9	24.90	47.9	243.9	111.8
2	10.5	456.5	369.6	21.40	44.5	256.1	109.7
3	10.7	450.4	369.6	23.40	46.5	264.4	115.2
4	10.1	443.2	383.3	21.40	44.5	230.6	108.4
5	9.4	441.5	368.2	21.40	44.5	212.8	96.7
6	11.3	447.6	374.4	25.30	48.3	255.6	122.3
7	10.1	442.0	368.9	31.00 ^a	52.8	246.7	132.5
8	10.6	442.0	372.9	23.60	46.7	225.6	106.1
9	10.5	442.0	369.6	24.30	47.4	228.3	110.8
10	10.2	447.0	371.6	21.90	45.0	241.7	---
Cruise							
1	21.7	533.7	480.6	19.30	42.2	469.4	137.4
2	22.2	550.9	480.6	13.50	34.2	462.2	150.3
3	22.3	553.7	486.1	17.70	40.3	458.3	127.7
4	22.1	549.3	484.0	16.50	38.8	460.6	134.9
5	22.3	550.9	475.0	14.20	35.4	443.9	131.2
6	22.2	550.9	479.9	19.80	42.8	438.3	142.5
7	22.4	550.9	479.9	20.50	44.7	436.1	158.0
8	22.3	549.8	478.5	16.40	38.6	441.7	142.8
9	21.9	546.5	484.7	17.10	39.5	437.8	130.2
10	21.9	532.0	473.7	16.70	39.0	474.4	---
Climb-out							
1	18.2	596.5	963.9	25.20	48.2	436.7	142.4
2	18.1	594.8	966.0	19.80	42.8	437.8	158.5
3	18.5	594.8	947.3	20.70	43.8	445.0	136.8
4	18.4	594.8	961.1	20.30	43.4	428.3	155.7
5	18.4	595.4	952.2	19.60	42.6	405.6	155.2
6	18.4	594.8	946.6	27.50	50.1	393.9	148.4
7	18.5	594.3	963.9	27.40 ^a	50.0	398.3	156.2
8	18.3	591.5	947.3	22.40	45.6	405.6	149.0
9	18.4	594.3	966.6	20.30	43.4	406.1	142.5
10	18.1	571.5	957.7	22.90	46.0	441.7	---
SLTO							
1	22.1	599.8	999.0	27.40	50.0	542.2	158.4
2	22.0	602.6	999.7	15.60	37.5	534.4	159.4
3	22.3	603.2	993.5	19.50	42.5	546.1	153.7
4	22.4	602.6	996.3	18.80	41.7	506.1	161.6
5	22.3	602.6	994.9	18.10	40.8	498.9	170.0
6	22.0	602.0	1008.7	22.10	45.3	475.0	152.5
7	22.3	603.7	1014.9	20.70 ^a	43.8	496.1	168.5
8	22.1	600.4	1012.8	17.50	40.1	492.8	151.3
9	22.3	603.2	1001.8	23.00	46.1	501.1	157.4
10	21.9	583.7	1008.7	20.90	44.0	540.0	---

^a Recalculated value.

TABLE 17. TEST DATA FOR T53 COMBUSTOR

Operating conditions				Engine tests			
NAPC no.	F/A (g kg ⁻¹)	Inlet tempera- ture (K)	Inlet pres- sure (kPa)	Smoke emis- sions (mg m ⁻³)	Smoke number (SAE)	LTR (K)	RF (kW m ⁻²)
Idle							
1	13.3	440.9	271.7	1.90	7.4	330.6	35.8
2	13.6	440.9	270.5	1.61	8.3	318.3	32.9
3	13.1	439.8	272.3	1.19	8.0	346.7	27.3
4	13.0	440.4	270.4	---	5.8	411.1	22.2
5	12.7	439.8	272.3	1.88	8.0	351.7	29.5
6	13.6	440.9	272.4	5.52	8.2	316.7	27.3
7	13.3	441.5	272.8	4.42	16.0	441.1	34.6
8	13.1	443.7	271.9	2.50	5.3	331.1	26.7
9	13.1	443.2	272.5	1.35	5.9	398.9	27.3
10	13.2	439.8	272.6	0.86	4.0	325.0	23.9
Cruise							
1	15.9	540.4	588.1	3.68	15.9	490.0	111.9
2	15.7	539.8	590.5	4.21	16.5	493.3	128.4
3	15.7	538.2	586.4	1.84	6.9	461.7	96.4
4	15.6	540.9	588.8	1.68	4.5	488.3	91.4
5	15.5	541.5	590.9	---	---	474.4	---
6	16.1	538.7	592.3	2.53	16.1	559.4	126.1
7	16.2	543.7	588.3	2.19	14.6	511.1	135.2
8	16.3	538.2	589.3	2.53	7.1	518.3	105.6
9	15.8	540.4	589.3	1.87	17.9	518.9	105.6
10	15.6	539.8	586.9	1.93	5.1	500.6	107.9
"Normal"							
1	18.6	570.9	690.2	---	19.4	577.8	202.2
2	18.5	569.8	688.8	3.01	17.9	572.2	209.0
3	18.7	569.3	689.1	2.83	10.9	560.0	174.9
4	18.5	569.3	690.2	1.40	5.8	590.6	142.0
5	18.2	570.9	689.0	---	---	536.1	---
6	18.5	569.8	688.5	2.53	16.9	650.0	187.4
7	18.6	569.8	687.7	3.84	13.2	607.2	207.9
8	18.6	671.5	687.5	1.30	6.9	506.1	193.1
9	18.2	569.8	688.0	2.15	20.7	605.6	205.6
10	17.9	570.4	688.0	1.93	6.9	546.1	147.7
"Military"							
1	19.5	576.5	726.0	3.91	19.6	591.7	236.3
2	19.4	575.4	725.3	1.36	14.3	621.7	238.0
3	19.4	575.4	726.0	2.69	12.2	601.1	197.7
4	19.4	576.5	725.3	1.09	9.4	615.0	226.1
5	19.3	580.9	725.3	---	12.0	566.1	197.7
6	19.9	578.2	730.2	3.06	16.9	680.6	239.7
7	19.6	576.5	725.9	3.65	13.0	639.4	248.8
8	20.1	528.7	726.5	1.20	11.6	699.4	244.2
9	19.5	577.6	725.7	2.07	14.2	658.3	228.3
10	18.8	576.5	726.8	3.55	10.2	601.7	179.5

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TABLE 31. SMOKE NUMBER (SAE) LINEAR LEAST SQUARES COEFFICIENTS
OF DETERMINATION, r^2 , FOR T56 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Climb-out	Sea-level Takeoff
1. Fuel composition parameters				
Hx	0.86	0.50	0.65	0.11
ARx (HPLC)	0.54	0.69	0.59	0.62
ARx (FIA)	0.38	0.29	0.24	0.19
MCAH	0.02	0.05	0.00	0.30
PCAH	0.32	0.33	0.60	0.04
2. Diffusion flame parameters				
SP	0.81	0.50	0.63	0.14
1/SP	0.88	0.52	0.62	0.11
TSI	0.71	0.40	0.62	0.06
FCR ₀	0.70	0.42	0.51	0.07
ΔFCR	0.17	0.04	0.09	0.15
SPE	0.82	0.63	0.71	0.08
3. Premixed flame parameters				
TSI _{reg}	0.04	0.00	0.05	0.00
TSI _{unreg}	0.55	0.19	0.19	0.00
θ(f _v)	0.31	0.28	0.35	0.05
T(f _v)	0.02	0.04	0.02	0.09
4. Operating condition parameters				
T _{in}	0.11	0.02	0.00	0.02
P _{in}	0.08	0.04	0.01	0.00
F/A	0.02	0.01	0.01	0.00
C/O	0.04	0.02	0.15	0.01
θ _{metered}	0.00	0.15	0.11	0.04
NAPC fuels used in correlations				
	1-10	1-10	1-10	1-10
35% CL r^2	0.40	0.40	0.40	0.40
99% CL r^2	0.58	0.58	0.58	0.58

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TABLE 30 SMOKE NUMBER (SAE), LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR TF30 COMBUSTOR

<u>Fitting parameter</u>	<u>Combustor power level</u>	
	<u>Sea-level</u>	<u>Takeoff</u>
<u>Dash</u>		
1. Fuel composition parameters		
Hx	0.39	0.35
ARx (HPLC)	0.60	0.24
ARx (FIA)	0.74	0.44
MCAH	0.58	0.11
PCAH	0.00	0.24
2. Diffusion flame parameters		
SP	0.48	0.51
1/SP	0.43	0.34
TSI	0.41	0.50
FCR ₀	0.43	0.52
Δ FCR	0.49	0.40
SPE	0.33	0.39
3. Premixed flame parameters		
TSI _{reg}	0.07	0.04
TSI _{unreg}	0.32	0.10
$\phi(f_v)$	0.16	0.01
T(f _v)	0.07	0.21
4. Operating condition parameters		
T _{in}	0.22	0.36
P _{in}	0.01	0.73
F/A	0.05	0.50
C/O	0.10	0.56
$\phi_{metered}$	0.00	0.44
NAPC func's used in the correlations	1,2,4-7	1,2,4,5,7,8
95% CL r^2	0.66	0.66
99% CL r^2	0.84	0.84

TABLE 29. SUCCESSFUL CORRELATIONS OF SMOKE EMISSIONS DATA

<u>Fitting parameter</u>	<u>Number of successful correlations</u>				<u>Average r² for successes</u>	<u>Average r² for all tests</u>
	<u>TF30</u>	<u>T56</u>	<u>T53</u>	<u>Total</u>	<u>95%/99%</u>	<u></u>
1. Fuel composition parameters						
Hx	0/0	3/2	2/0	5/2	0.66/0.76	0.41
ARx (HPLC)	0/0	4/3	1/1	5/4	0.64/0.67	0.36
ARx (FIA)	0/0	0/0	1/0	1/0	0.58/...	0.23
MCAH	0/0	0/0	0/0	0/0	/...	0.11
PCAH	1/0	1/1	1/1	3/2	0.74/0.77	0.36
2. Diffusion flame parameters						
SP	0/0	3/2	1/0	4/2	0.65/0.72	0.40
1/SP	0/0	3/2	2/0	5/2	0.62/0.76	0.40
TSI _{df}	0/0	3/2	2/0	5/2	0.60/0.68	0.38
FCR _o	0/0	3/1	2/0	5/1	0.56/0.69	0.35
ΔFCR	0/0	0/0	0/0	0/0	/....	0.13
SPE	0/0	3/3	2/0	5/3	0.68/0.72	0.45
3. Premixed flame parameters						
TSI _{reg}	0/0	0/0	0/0	0/0	/...	0.10
TSI _{unreg}	1/0	1/1	1/1	3/2	0.70/0.68	0.27
θ(f _v)	0/0	0/0	1/0	1/0	0.45/...	0.19
T(f _v)	0/0	0/0	0/0	0/0	/...	0.13
4. Operating condition parameters						
T _{in}	0/0	0/0	0/0	0/0	/...	0.05
P _{in}	1/0	0/0	0/0	1/0	0.50/...	0.16
F/A	1/0	0/0	0/0	1/0	0.87/...	0.20
C/O	1/0	0/0	0/0	1/0	0.88/...	0.24
θ _{metered}	1/0	0/0	0/0	1/0	0.80/...	0.18
Total number of						
correlations	4	4	4	12		

TABLE 28. SMOKE EMISSIONS LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR T53 COMBUSTOR

<u>Fitting parameter</u>	<u>Combustor power level</u>			
	<u>Idle</u>	<u>Cruise</u>	<u>Normal</u>	<u>Military</u>
1. Fuel composition parameters				
Hx	0.58	0.05	0.67	0.27
ARx (HPLC)	0.14	0.03	0.44	0.73
ARx (FIA)	0.00	0.13	0.58	0.32
MCAH	0.31	0.00	0.00	0.08
PCAH	0.91	0.01	0.17	0.12
2. Diffusion flame parameters				
SP	0.42	0.09	0.67	0.31
1/SP	0.44	0.04	0.66	0.29
TSI	0.58	0.15	0.64	0.18
FCR ₀	0.49	0.16	0.68	0.11
Δ FCR	0.05	0.10	0.10	0.11
SPE	0.51	0.01	0.72	0.38
3. Premixed flame parameters				
TSI _{reg}	0.18	0.30	0.44	0.00
TSI _{unreg}	0.09	0.00	0.76	0.22
$\theta(f_v)$	0.45	0.05	0.40	0.08
T(f _v)	0.00	0.35	0.12	0.05
4. Operating condition parameters				
T _{in}	0.02	0.00	0.00	0.04
P _{in}	0.07	0.14	0.26	0.13
F/A	0.20	0.01	0.26	0.00
C/O	0.27	0.02	0.42	0.01
θ_{metered}	0.10	0.00	0.05	0.05
NAPC fuels used in correlations	1-3, 5-10	1-4, 6-10	2-4,6, 7,9,10	1-4,6, 7,9,10
95% CL r^2	0.44	0.44	0.57	0.50
99% CL r^2	0.64	0.64	0.76	0.70

TABLE 27 SMOKE EMISSIONS LINEAR LEAST SQUARES COEFFICIENTS
OF DETERMINATION, r^2 , FOR T56 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Climb-out	Sea-level Takeoff
1. Fuel composition parameters				
Hx	0.86	0.50	0.67	0.11
ARx (HPLC)	0.50	0.73	0.59	0.64
ARx (FIA)	0.39	0.28	0.23	0.22
MCAH	0.02	0.05	0.00	0.33
PCAH	0.30	0.37	0.63	0.03
2. Diffusion flame parameters				
SP	0.80	0.50	0.63	0.14
1/SP	0.89	0.50	0.63	0.11
TSI	0.72	0.41	0.64	0.06
FCR ₀	0.69	0.43	0.52	0.08
Δ FCR	0.14	0.05	0.09	0.17
SPE	0.82	0.62	0.72	0.08
3. Premixed flame parameters				
TSI _{reg}	0.04	0.01	0.07	0.00
TSI _{unreg}	0.61	0.16	0.20	0.00
$\phi(f_v)$	0.33	0.29	0.39	0.05
T(f _v)	0.02	0.03	0.02	0.06
4. Operating condition parameters				
T _{in}	0.11	0.02	0.00	0.02
P _{in}	0.08	0.05	0.01	0.00
F/A	0.01	0.01	0.02	0.00
C/O	0.03	0.01	0.17	0.01
$\phi_{metered}$	0.00	0.18	0.10	0.04
NAPC fuels used in correlations	1-10	1-10	1-10	1-10
95% CL r^2	0.40	0.40	0.40	0.40
99% CL r^2	0.58	0.58	0.58	0.58

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TABLE 26. SMOKE EMISSIONS, LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR TF30 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Sea-level Takeoff	Dash
1. Fuel composition parameters				
Hx	0.05	0.20	0.51	0.45
ARx (HPLC)	0.03	0.08	0.02	0.35
ARx (FIA)	0.10	0.01	0.06	0.44
MCAH	0.35	0.06	0.06	0.02
PCAH	0.69	0.33	0.62	0.19
2. Diffusion flame parameters				
SP	0.06	0.19	0.36	0.64
1/SP	0.01	0.20	0.50	0.52
TSI	0.09	0.15	0.40	0.55
FCR ₀	0.07	0.18	0.29	0.54
Δ FCR	0.35	0.01	0.04	0.36
SPE	0.06	0.43	0.47	0.59
3. Premixed flame parameters				
TSI _{reg}	0.02	0.04	0.02	0.08
TSI _{unreg}	0.21	0.08	0.74	0.14
$\theta(f_v)$	0.02	0.02	0.15	0.00
T(f _v)	0.06	0.18	0.38	0.23
4. Operating condition parameters				
T _{in}	0.02	0.01	0.00	0.38
P _{in}	0.02	0.50	0.01	0.63
F/A	0.09	0.42	0.50	0.87
C/O	0.09	0.47	0.54	0.88
ϕ_{metered}	0.09	0.35	0.36	0.80
NAPC fuels used in the correlations				
	1-3,5-8	1-8	1,2,4,5,7,8	4-8
95% CL r^2	0.57	0.50	0.66	0.77
99% CL r^2	0.76	0.70	0.84	0.92

TABLE 25. SUCCESSFUL CORRELATIONS OF LINER TEMPERATURE RISE DATA

<u>Fitting parameter</u>	<u>Number of successful correlations</u>				<u>Average r² for successes</u> <u>95%/99%</u>	<u>Average r² for all tests</u>
	TF30	T56 (95% CL/99% CL)	T53	Total		
1. Fuel composition parameters						
Hx	1/1	0/0	0/0	1/1	0.83/0.83	0.26
ARx (HPLC)	0/0	0/0	0/0	0/0	/...	0.13
ARx (FIA)	0/0	0/0	1/0	0/0	/...	0.11
MCAH	0/0	1/0	0/0	1/0	0.48/...	0.15
PCAH	0/0	0/0	2/0	2/0	0.56/...	0.32
2. Diffusion flame parameters						
SP	2/1	0/0	0/0	2/1	0.69/0.77	0.25
1/SP	1/1	0/0	0/0	1/1	0.83/0.83	0.24
TSIdf	1/1	0/0	0/0	1/1	0.78/0.78	0.24
FCR _o	1/0	0/0	1/0	2/0	0.59/....	0.23
ΔFCR	0/0	0/0	0/0	0/0	/....	0.16
SPE	2/1	0/0	0/0	2/1	0.77/0.90	0.25
3. Premixed flame parameters						
TSI _{reg}	0/0	0/0	0/0	0/0	/...	0.08
TSI _{unreg}	0/0	0/0	0/0	0/0	/...	0.08
θ(f _v)	0/0	0/0	0/0	0/0	/...	0.12
T(f _v)	0/0	0/0	0/0	0/0	/...	0.13
4. Operating condition parameters						
T _{in}	0/0	1/0	0/0	1/0	0.42/...	0.17
P _{in}	0/0	0/0	0/0	0/0	/...	0.13
F/A	3/3	0/0	1/0	4/3	0.74/0.85	0.38
C/O	3/3	1/0	2/0	6/3	0.66/0.88	0.42
θ _{metered}	3/2	0/0	0/0	3/2	0.74/0.76	0.30
Total number of correlations	4	4	4	12		

TABLE 24. LINER TEMPERATURE RISE (MAX) LINEAR LEAST SQUARES
COEFFICIENTS OF DETERMINATION, r^2 , FOR T53 COMBUSTOR

<u>Fitting parameter</u>	<u>Combustor power level</u>			
	<u>Idle</u>	<u>Cruise</u>	<u>Normal</u>	<u>Military</u>
1. Fuel composition parameters				
H*	0.08	0.28	0.41	0.32
AR* (HPLC)	0.01	0.09	0.26	0.16
AR* (FIA)	0.07	0.01	0.01	0.00
MCAH	0.06	0.16	0.07	0.06
PCAH	0.02	0.53	0.58	0.39
2. Diffusion flame parameters				
SP	0.06	0.29	0.39	0.33
1/SP	0.14	0.21	0.33	0.25
TSI	0.04	0.27	0.42	0.28
FCR ₀	0.06	0.18	0.45	0.28
Δ FCR	0.03	0.34	0.17	0.24
SPE	0.05	0.19	0.34	0.25
3. Premixed flame parameters				
TSI _{reg}	0.01	0.00	0.09	0.03
TSI _{unreg}	0.22	0.00	0.00	0.00
$\theta(f_v)$	0.06	0.02	0.31	0.11
T(f_v)	0.08	0.16	0.01	0.09
4. Operating condition parameters				
T _{in}	0.03	0.01	0.16	0.02
P _{in}	0.01	0.32	0.03	0.37
F/A	0.10	0.42	0.14	0.40
C/O	0.06	0.43	0.22	0.44
$\phi_{metered}$	0.19	0.38	0.02	0.27
NAPC fuels used in correlations				
	1-10	1-10	1-7, 9,10	1-7, 9,10
95% CL r^2	0.40	0.40	0.44	0.44
99% CL r^2	0.58	0.58	0.64	0.64

TABLE 23. LINER TEMPERATURE RISE (MAX) LINEAR LEAST SQUARES
COEFFICIENTS OF DETERMINATION, r^2 , FOR T56 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Climb-out	Sea-level Takeoff
1. Fuel composition parameters				
Hx	0.15	0.21	0.23	0.10
AR% (HPLC)	0.33	0.00	0.00	0.03
AR% (FIA)	0.20	0.07	0.07	0.19
MCAH	0.03	0.24	0.31	0.48
PCAH	0.14	0.26	0.36	0.35
2. Diffusion flame parameters				
SP	0.16	0.12	0.14	0.05
1/SP	0.12	0.16	0.18	0.07
TSI	0.16	0.14	0.18	0.09
FCR ₀	0.24	0.13	0.12	0.05
Δ FCR	0.00	0.20	0.21	0.07
SPE	0.33	0.10	0.09	0.03
3. Premixed flame parameters				
TSI _{reg}	0.30	0.00	0.00	0.00
TSI _{unreg}	0.07	0.06	0.04	0.00
$\theta(f_v)$	0.27	0.01	0.03	0.01
T(f_v)	0.14	0.03	0.09	0.08
4. Operating condition parameters				
T _{in}	0.36	0.42	0.10	0.15
P _{in}	0.02	0.01	0.04	0.21
F/A	0.31	0.31	0.26	0.04
C/O	0.32	0.41	0.37	0.11
$\theta_{metered}$	0.28	0.12	0.05	0.00
NAPC fuels used in correlations	1-10	1-10	1-10	1-10
95% CL r^2	0.40	0.40	0.40	0.40
99% CL r^2	0.58	0.58	0.58	0.58

TABLE 22. LINER TEMPERATURE RISE (MAX), LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR TF30 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Sea-level Takeoff	Dash
1. Fuel composition parameters				
Hx	0.01	0.00	0.83	0.52
ARx (HPLC)	0.04	0.00	0.42	0.20
ARx (FIA)	0.20	0.12	0.24	0.10
MCAH	0.29	0.06	0.00	0.03
PCAH	0.14	0.06	0.50	0.45
2. Diffusion flame parameters				
SP	0.00	0.04	0.77	0.60
1/SP	0.01	0.02	0.83	0.51
TSI	0.00	0.01	0.78	0.55
FCR ₀	0.01	0.02	0.72	0.48
Δ FCR	0.00	0.01	0.15	0.51
SPE	0.01	0.06	0.90	0.63
3. Premixed flame parameters				
TSI _{reg}	0.16	0.32	0.01	0.02
TSI _{unreg}	0.01	0.02	0.44	0.13
$\theta(f_v)$	0.01	0.27	0.30	0.00
T(f _v)	0.38	0.06	0.37	0.11
4. Operating condition parameters				
T _{in}	0.02	0.48	0.08	0.15
P _{in}	0.13	0.01	0.00	0.36
F/A	0.05	0.79	0.87	0.89
C/O	0.05	0.80	0.92	0.93
$\theta_{metered}$	0.05	0.76	0.68	0.77
NAPC fuels used in the correlations	1-10	1-8	1,2,4-8	1,2,4-8
95% CL r^2	0.40	0.50	0.57	0.57
99% CL r^2	0.58	0.70	0.76	0.76

TABLE 21. SUCCESSFUL CORRELATIONS OF RADIATION FLUX DATA

<u>Fitting parameter</u>	<u>Number of successful correlations</u>				<u>Average r² for successes</u>	<u>Average r² for all tests</u>
	<u>TF30</u>	<u>T56</u>	<u>T53</u>	<u>Total</u>	<u>95%/99%</u>	
	<u>(95% CL/99% CL)</u>					
1. Fuel composition parameters						
Hx	2/0	2/1	4/1	8/2	0.60/0.74	0.48
ARx (HPLC)	0/0	1/0	0/0	1/0	0.56/...	0.25
ARx (FIA)	0/0	0/0	1/0	1/0	0.43/...	0.04
NCAH	0/0	0/0	0/0	0/0	/...	0.23
PCAH	0/0	0/0	0/0	0/0	/...	0.23
2. Diffusion flame parameters						
SP	2/0	2/1	3/1	7/2	0.62/0.70	0.47
1/SP	2/1	2/1	3/1	7/3	0.61/0.71	0.47
TSIdf	2/0	2/2	3/2	7/4	0.65/0.71	0.51
FCRo	2/0	2/1	4/1	8/2	0.63/0.76	0.50
ΔFCR	0/0	0/0	1/0	1/0	0.59/...	0.13
SPE	3/2	2/1	1/0	6/3	0.67/0.80	0.45
3. Premixed flame parameters						
TSIreg	0/0	0/0	1/0	1/0	0.44/...	0.18
TSIunreg	0/0	0/0	2/0	1/0	0.40/...	0.29
θ(fv)	0/0	1/0	1/0	2/0	0.50/...	0.29
T(fv)	0/0	0/0	0/0	0/0	/...	0.12
4. Operating condition parameters						
Tin	0/0	0/0	0/0	0/0	/...	0.05
Pin	0/0	0/0	0/0	0/0	/...	0.13
F/A	1/0	0/0	1/1	2/1	0.67/0.64	0.26
C/O	1/0	0/0	1/1	2/1	0.71/0.71	0.33
θmetered	1/0	0/0	1/0	2/0	0.53/...	0.16
Total number of correlations	3	4	4	11		

TABLE 20. RADIATION FLUX LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR T53 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Normal	Military
1. Fuel composition parameters				
Hx	0.42	0.72	0.50	0.52
ARx (HPLC)	0.27	0.20	0.28	0.23
ARx (FIA)	0.43	0.18	0.25	0.18
MCAH	0.09	0.05	0.02	0.00
PCAH	0.04	0.34	0.08	0.27
2. Diffusion flame parameters				
SP	0.39	0.69	0.56	0.53
1/SP	0.40	0.64	0.43	0.49
TSI	0.45	0.75	0.48	0.66
FCR ₀	0.47	0.59	0.56	0.74
Δ FCR	0.17	0.19	0.59	0.15
SPE	0.26	0.54	0.27	0.34
3. Premixed flame parameters				
TSI _{reg}	0.35	0.44	0.34	0.32
TSI _{unreg}	0.40	0.42	0.24	0.09
$\theta(f_v)$	0.26	0.38	0.12	0.48
T(f_v)	0.19	0.00	0.07	0.08
4. Operating condition parameters				
T _{in}	0.01	0.17	0.07	0.03
P _{in}	0.00	0.24	0.07	0.02
F/A	0.12	0.23	0.13	0.64
C/O	0.17	0.33	0.24	0.71
θ_{metered}	0.05	0.09	0.02	0.44
NAPC fuels used in correlations	1-10	1-4, 6-10	1-4,6, 7,9,10	1-7, 9,10
95% CL r^2	0.40	0.44	0.50	0.44
99% CL r^2	0.50	0.64	0.70	0.64

TABLE 19. RADIATION FLUX, LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR T56 COMBUSTOR

Fitting parameter	Combustor power level			
	Idle	Cruise	Climb-out	Sea-level Takeoff
1. Fuel composition parameters				
Hx	0.76	0.58	0.01	0.01
ARx (HPLC)	0.56	0.08	0.19	0.03
ARx (FIA)	0.36	0.25	0.02	0.01
MCAH	0.02	0.03	0.21	0.01
PCAH	0.40	0.21	0.00	0.07
2. Diffusion flame parameters				
SP	0.70	0.57	0.00	0.00
1/SP	0.74	0.61	0.01	0.02
TSI	0.69	0.74	0.04	0.00
FCR ₀	0.79	0.62	0.01	0.00
Δ FCR	0.02	0.03	0.08	0.08
SPE	0.86	0.50	0.00	0.01
3. Premixed flame parameters				
TSI _{reg}	0.14	0.15	0.08	0.08
TSI _{unreg}	0.43	0.41	0.05	0.27
$\theta(f_v)$	0.51	0.27	0.08	0.13
T(f_v)	0.02	0.01	0.00	0.01
4. Operating condition parameters				
T _{in}	0.01	0.01	0.02	0.19
P _{in}	0.00	0.12	0.08	0.02
F/A	0.18	0.12	0.05	0.24
C/O	0.22	0.32	0.02	0.31
ϕ_{metered}	0.13	0.00	0.07	0.09
NAPC fuels used in correlations	1-9	1-9	1-9	1-9
95% CL r^2	0.44	0.44	0.44	0.44
99% CL r^2	0.64	0.64	0.64	0.64

TABLE 18. RADIATION FLUX, LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR TF30 COMBUSTOR

<u>Fitting Parameter</u>	<u>Combustor power level</u>		
	<u>Cruise</u>	<u>Sea-level Takeoff</u>	<u>Dash</u>
1. Fuel composition parameters			
Hx	0.59	0.50	0.70
ARx (HPLC)	0.20	0.23	0.44
ARx (FIA)	0.22	0.09	0.31
MCAH	0.00	0.02	0.02
PCAH	0.30	0.43	0.35
2. Diffusion flame parameters			
SP	0.64	0.43	0.67
1/SP	0.63	0.50	0.75
TSI	0.60	0.48	0.69
FCR ₀	0.61	0.46	0.68
Δ FCR	0.11	0.00	0.02
SPE	0.75	0.59	0.80
3. Premixed flame parameters			
TSI _{reg}	0.00	0.02	0.01
TSI _{unreg}	0.32	0.23	0.37
$\phi(f_v)$	0.10	0.41	0.40
T(f _v)	0.18	0.46	0.34
4. Operating condition parameters			
T _{in}	0.00	0.01	0.00
P _{in}	0.51	0.00	0.40
F/A	0.28	0.70	0.21
C/O	0.36	0.71	0.29
$\phi_{metered}$	0.19	0.62	0.09
NAPC fuels used in the correlations			
	1,3-8	1,2,4-8	1,2,4-8
95% CL r^2	0.57	0.57	0.57
99% CL r^2	0.76	0.76	0.76

TABLE 32. SMOKE NUMBER (SAE) LINEAR LEAST SQUARES COEFFICIENTS OF DETERMINATION, r^2 , FOR T53 COMBUSTOR

<u>Fitting parameter</u>	<u>Combustor power level</u>			
	<u>Idle</u>	<u>Cruise</u>	<u>Normal</u>	<u>Military</u>
1. Fuel composition parameters				
Hx	0.63	0.42	0.21	0.26
ARx (HPLC)	0.17	0.31	0.23	0.47
ARx (FIA)	0.25	0.11	0.05	0.14
MCAH	0.00	0.02	0.02	0.03
PCAH	0.19	0.14	0.07	0.24
2. Diffusion flame parameters				
SP	0.46	0.44	0.27	0.30
1/SP	0.62	0.32	0.14	0.19
TSI	0.58	0.39	0.20	0.30
FCR ₀	0.58	0.44	0.26	0.35
Δ FCR	0.00	0.56	0.78	0.48
SPE	0.56	0.15	0.05	0.17
3. Premixed flame parameters				
TSI _{reg}	0.35	0.34	0.18	0.24
TSI _{unreg}	0.79	0.08	0.00	0.00
$\theta(f_v)$	0.59	0.16	0.01	0.14
T(f_v)	0.05	0.01	0.03	0.10
4. Operating condition parameters				
T _{in}	0.00	0.07	0.15	0.00
P _{in}	0.07	0.31	0.01	0.14
F/A	0.05	0.09	0.04	0.35
C/O	0.11	0.14	0.08	0.38
$\theta_{metered}$	0.00	0.02	0.00	0.25
NAPC fuels used in correlations				
	1-10	1-4, 6-10	1-4,6, 7,9,10	1-7, 9,10
95% CL r^2	0.40	0.44	0.50	0.44
99% CL r^2	0.58	0.64	0.70	0.64

TABLE 33. SUCCESSFUL CORRELATIONS FOR SMOKE NUMBER DATA

Fitting parameter	Number of				Average	
	<u>successful correlations</u>				<u>r² for</u>	<u>Average</u>
	TF30	T56	T53	Total	<u>successes</u>	<u>r² for</u>
		(95% CL/99% CL)			95%/99%	<u>all tests</u>
1. Fuel composition parameters						
H*	0/0	3/2	1/1	4/3	0.66/0.71	0.41
AR* (HPLC)	0/0	4/3	1/0	5/3	0.58/0.63	0.36
AR* (FIA)	1/0	0/0	0/0	1/0	0.78/...	0.23
MCAH	0/0	0/0	0/0	0/0	/...	0.11
PCAH	0/0	1/1	0/0	1/1	0.60/0.60	0.22
2. Diffusion flame parameters						
SP	0/0	3/2	2/0	5/2	0.57/0.72	0.45
1/SP	0/0	3/2	1/1	4/3	0.66/0.71	0.42
TSIdf	0/0	3/2	1/1	4/3	0.58/0.64	0.42
FCR ₀	0/0	3/1	2/1	5/2	0.53/0.64	0.43
ΔFCR	0/0	0/0	3/1	3/1	0.61/0.78	0.32
SPE	0/0	3/3	1/1	4/4	0.68/0.68	0.39
3. Premixed flame parameters						
TSIreg	0/0	0/0	0/0	0/0	/...	0.13
TSIunreg	0/0	1/0	1/1	2/1	0.67/0.79	0.22
Ø(f _v)	0/0	0/0	1/1	1/1	0.59/0.59	0.21
T(f _v)	0/0	0/0	0/0	0/0	/...	0.06
4. Operating condition parameters						
T _{in}	0/0	0/0	0/0	0/0	/...	0.10
P _{in}	1/0	0/0	0/0	1/0	0.73/...	0.14
F/A	0/0	0/0	0/0	0/0	/...	0.12
C/O	0/0	0/0	0/0	0/0	/...	0.16
Ø _{metered}	0/0	0/0	0/0	0/0	/...	0.10
Total number of correlations	2	4	4	10		

TABLE 34 SUCCESSFUL FUEL PARAMETER CORRELATIONS

<u>Fitting parameter</u>	<u>Number of times successful</u>				<u>Average r' for all tests</u>
	<u>TF30</u>	<u>T56</u>	<u>T53</u>	<u>TOTAL</u>	
	<u>(95%/99%)</u>				
1. Fuel composition parameters					
Hx	3/1	8/5	7/2	18/8	0.39
ARx (HPLC)	0/0	9/6	2/1	11/7	0.29
ARx (FIA)	1/0	0/0	2/0	3/0	0.20
NCAH	0/0	1/0	0/0	1/0	0.10
PCAH	1/0	2/2	3/1	6/3	0.28
2. Diffusion flame parameters					
SP	4/1	8/5	6/1	18/7	0.39
1/SP	3/2	8/5	6/2	17/9	0.38
TSI	3/1	8/6	6/3	17/10	0.38
FCR ₀	3/0	8/3	9/2	20/5	0.37
ΔFCR	0/0	0/0	4/1	4/1	0.18
SPE	5/3	8/7	4/1	17/11	0.38
3. Premixed flame parameters					
TSI _{reg}	0/0	0/0	1/0	1/0	0.12
TSI _{unreg}	1/0	2/1	3/2	6/3	0.21
θ(f _v)	0/0	1/0	3/1	4/1	0.20
T(f _v)	0/0	0/0	0/0	0/0	0.11
4. Operating condition parameters					
"All"	7/3	1/0	3/1	11/4	0.29 (C/O)
Total number of tests	13	16	16	45	

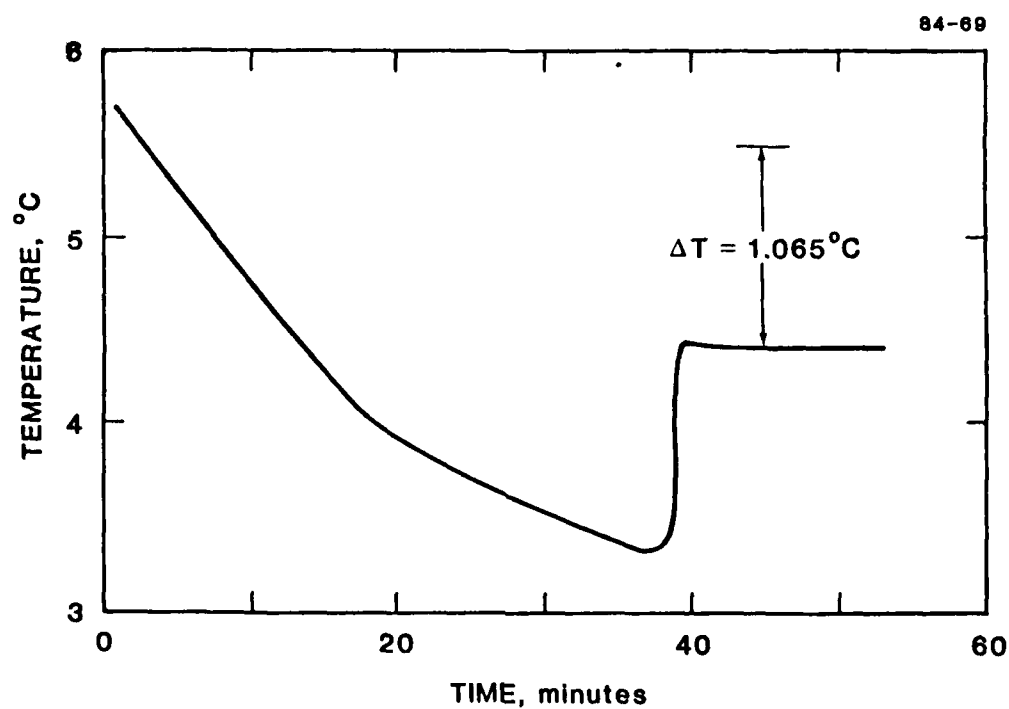


FIGURE 1 FREEZING POINT DEPRESSION CURVE FOR NAPC-6 IN BENZENE

From the observed difference in freezing points, the
MW of NAPC-6 was calculated as 189 g mol^{-1} .

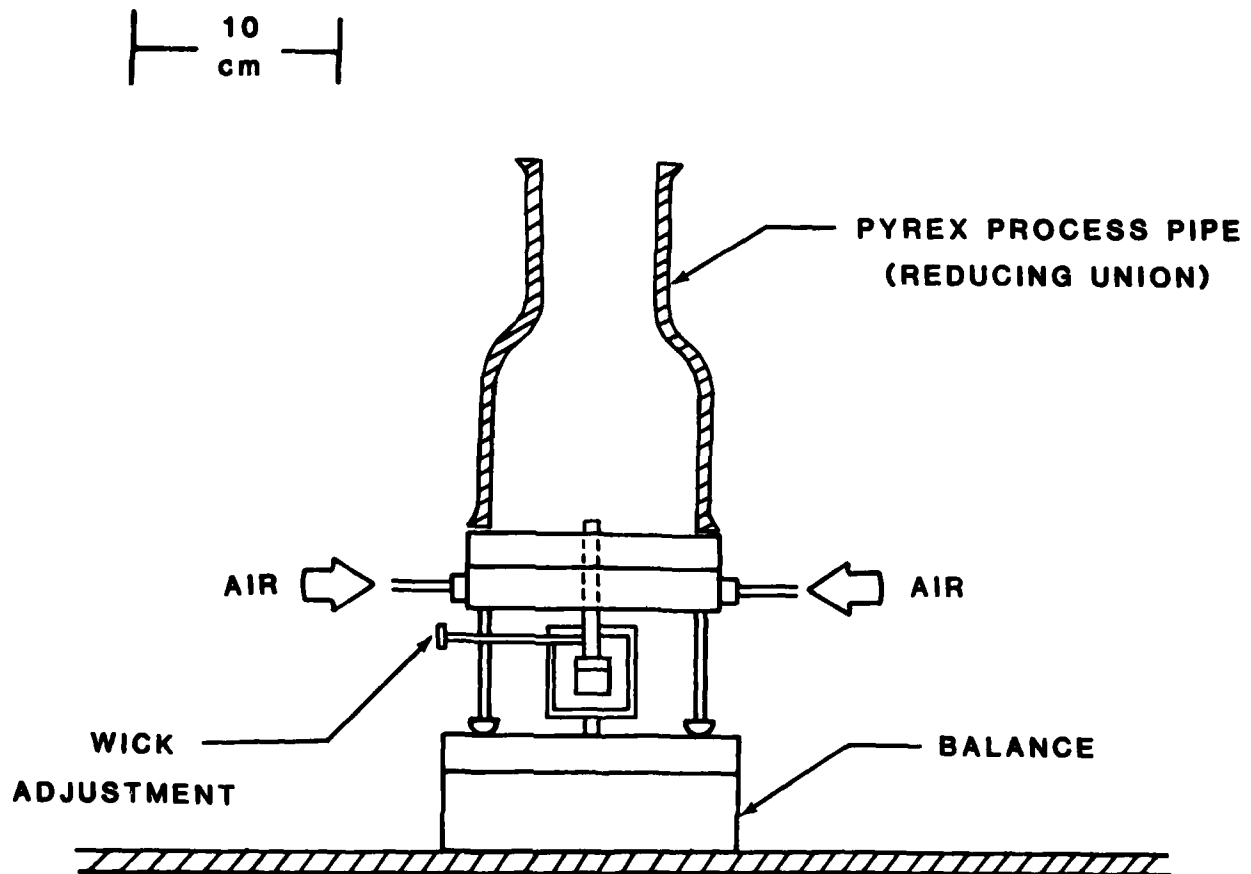


FIGURE 2 DIFFUSION FLAME APPARATUS

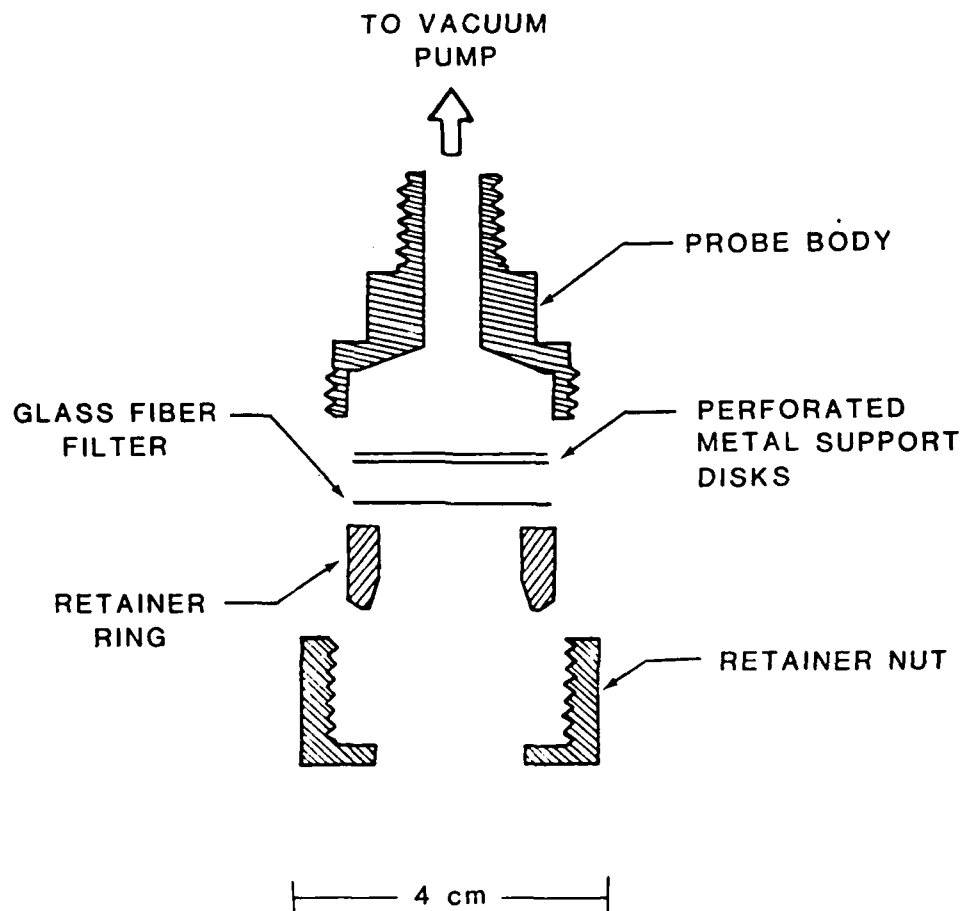


FIGURE 3 SOOT COLLECTION PROBE

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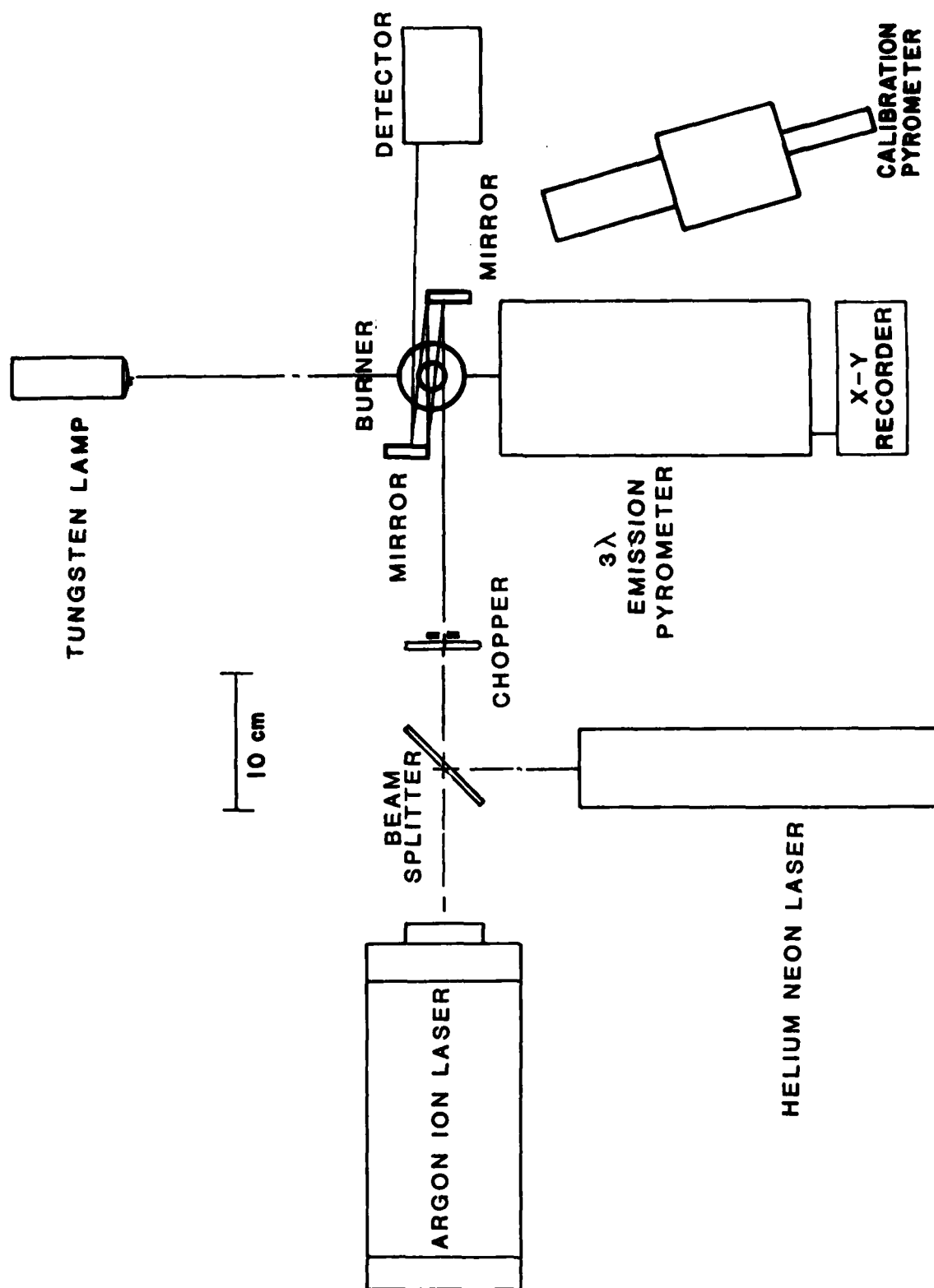


FIGURE 4 PREMIXED FLAME SOOT YIELD AND EMISSION TEMPERATURE APPARATUS

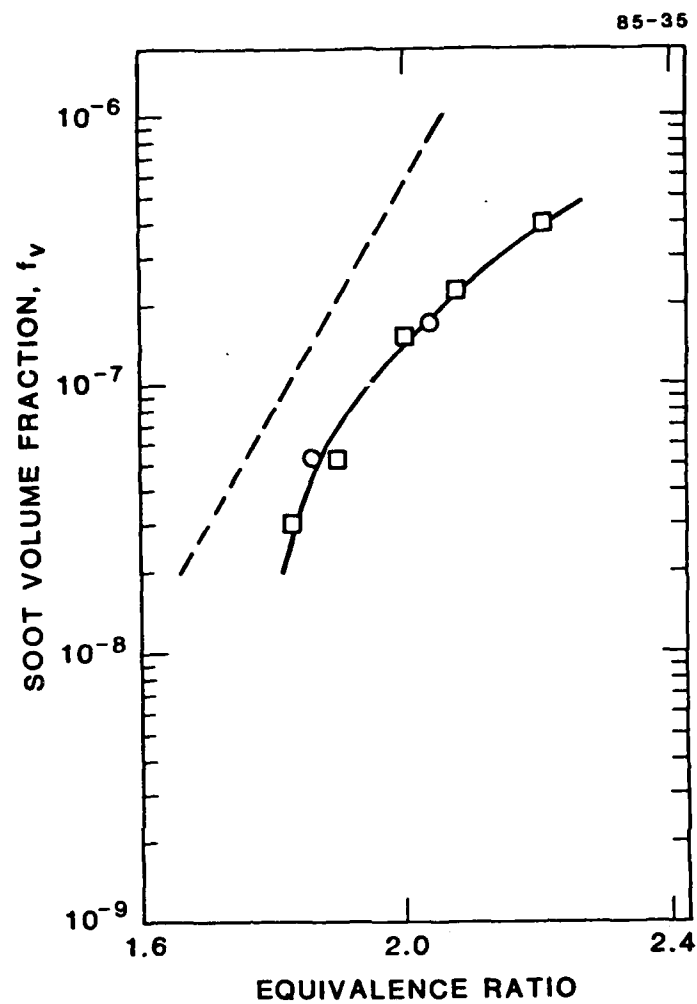


FIGURE 5 PREMIXED FLAME SOOT CONCENTRATIONS
FOR AEROCHEM-A

□ = unregulated burner; ○ = regulated burner;
-- = calculated from mixture rule.

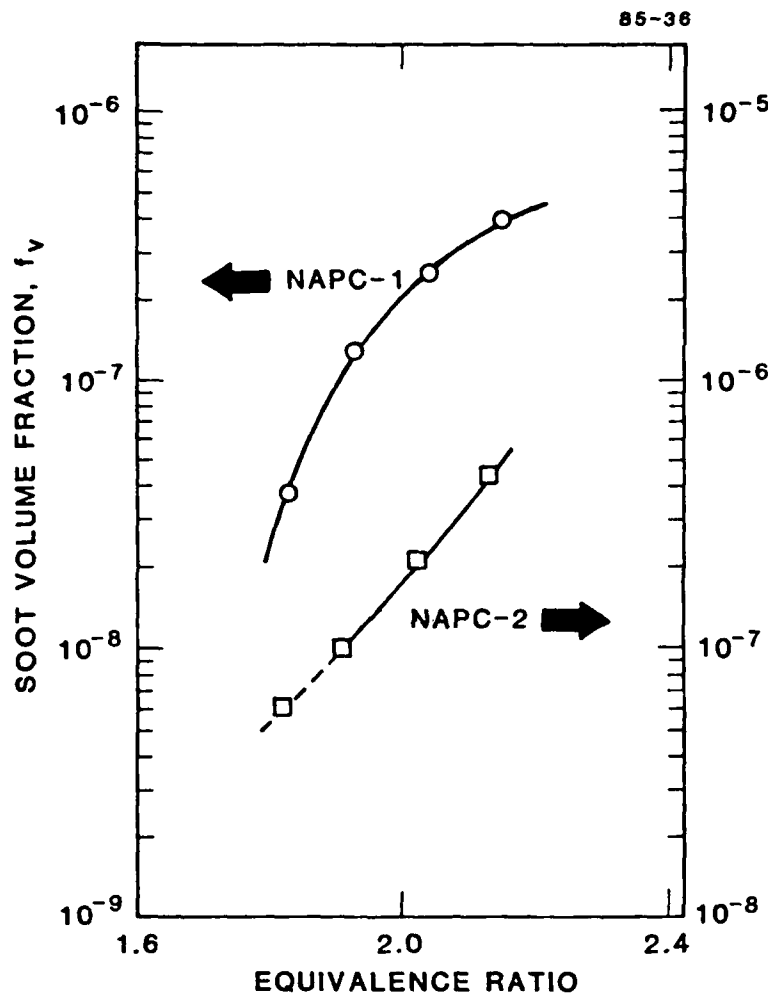


FIGURE 6 PREMIXED FLAME SOOT CONCENTRATIONS FOR NAPC-1 AND NAPC-2

--- Rayleigh estimate; — Mie scattering calculation.

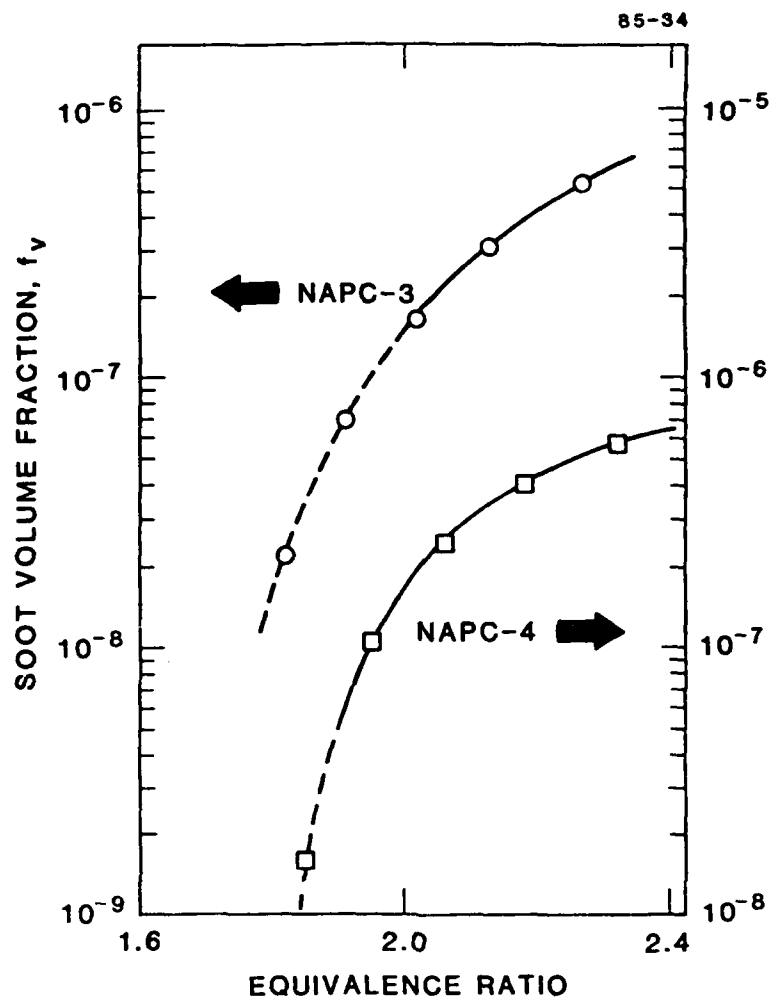


FIGURE 7 PREMIXED FLAME SOOT CONCENTRATIONS FOR NAPC-3 AND NAPC-4

Curves as in Fig. 6.

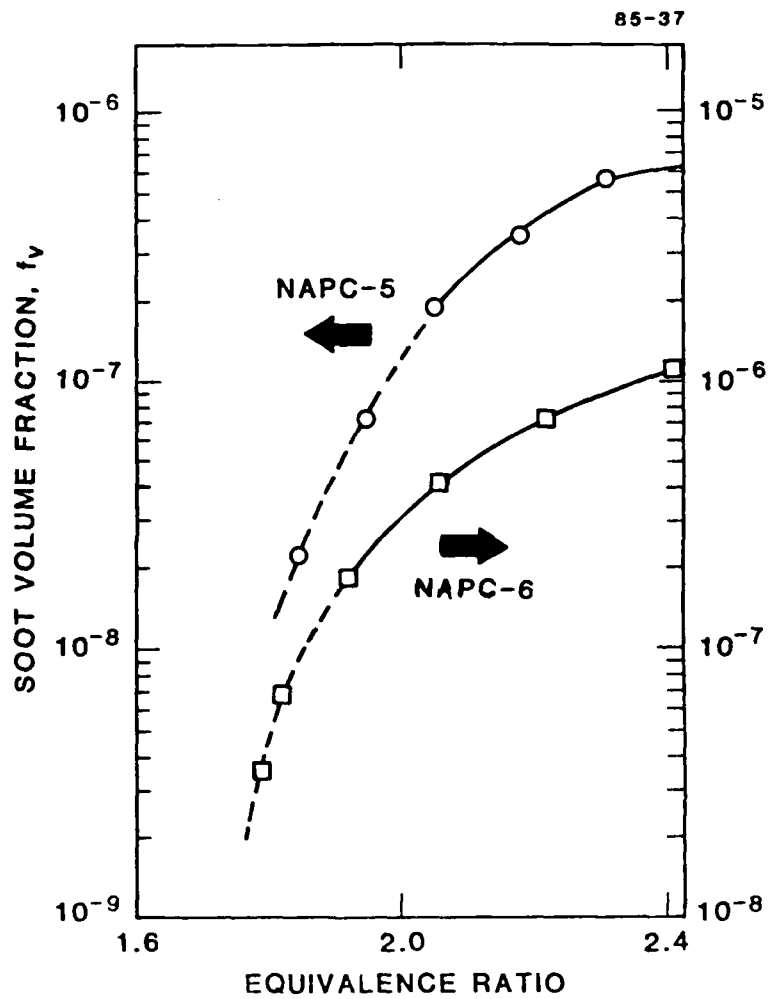


FIGURE 8 PREMIXED FLAME SOOT CONCENTRATIONS FOR NAPC-5 AND NAPC-6
Curves as in Fig. 6.

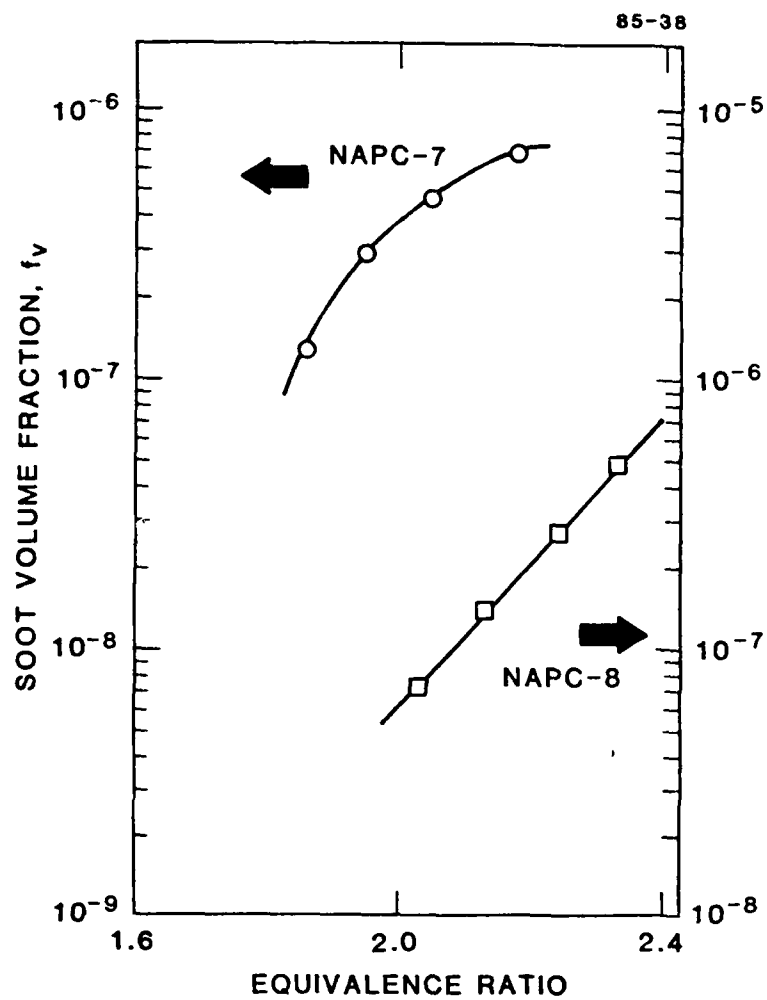


FIGURE 9 PREMIXED FLAME SOOT CONCENTRATIONS FOR NAPC-7 AND NAPC-8
Curves as in Fig. 6.

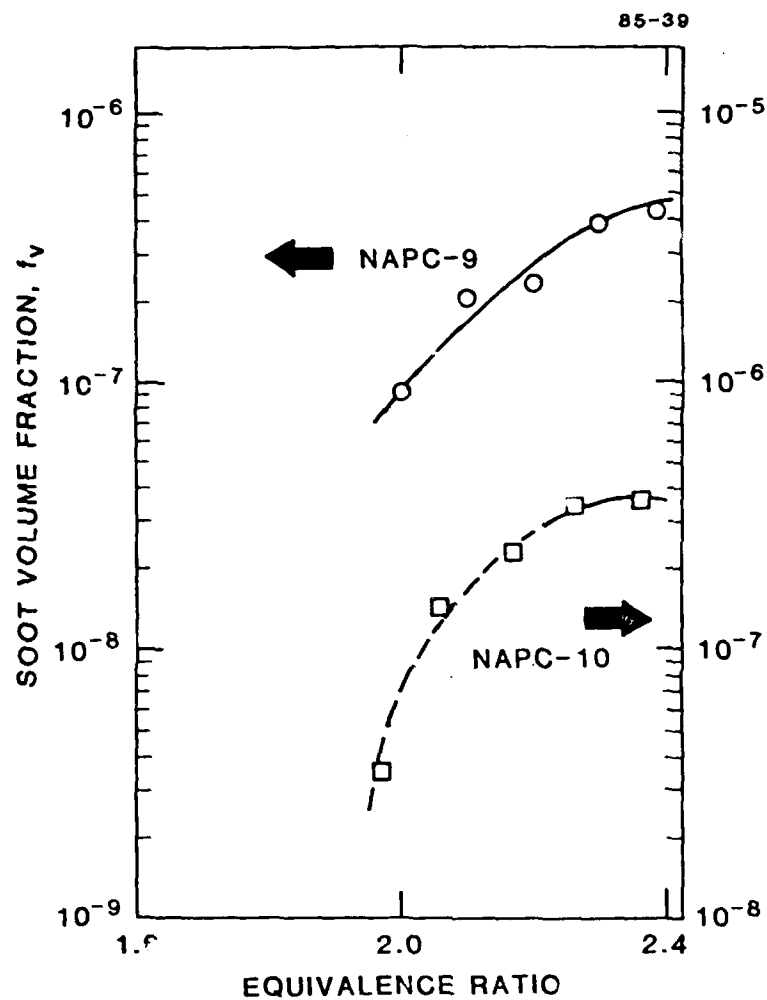


FIGURE 10 PREMIXED FLAME SOOT CONCENTRATIONS FOR NAPC-9 AND NAPC-10
Curves as in Fig. 6

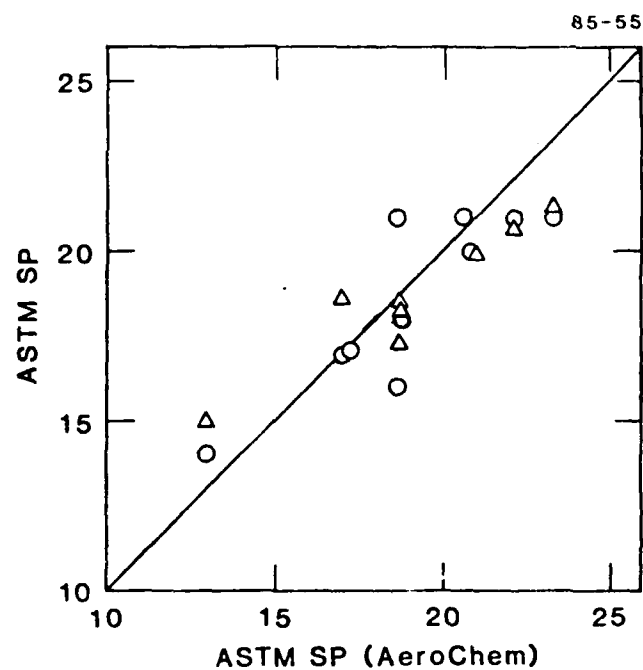


FIGURE 11 COMPARISON OF ASTM SMOKE POINTS

○ = NAPC data; △ = NRL data.

The line represents the desired perfect correlation.

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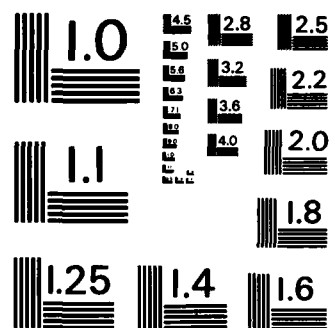
R J GILL ET AL. AUG 85 AEROCHEM-TP-451 N00014-83-C-2311

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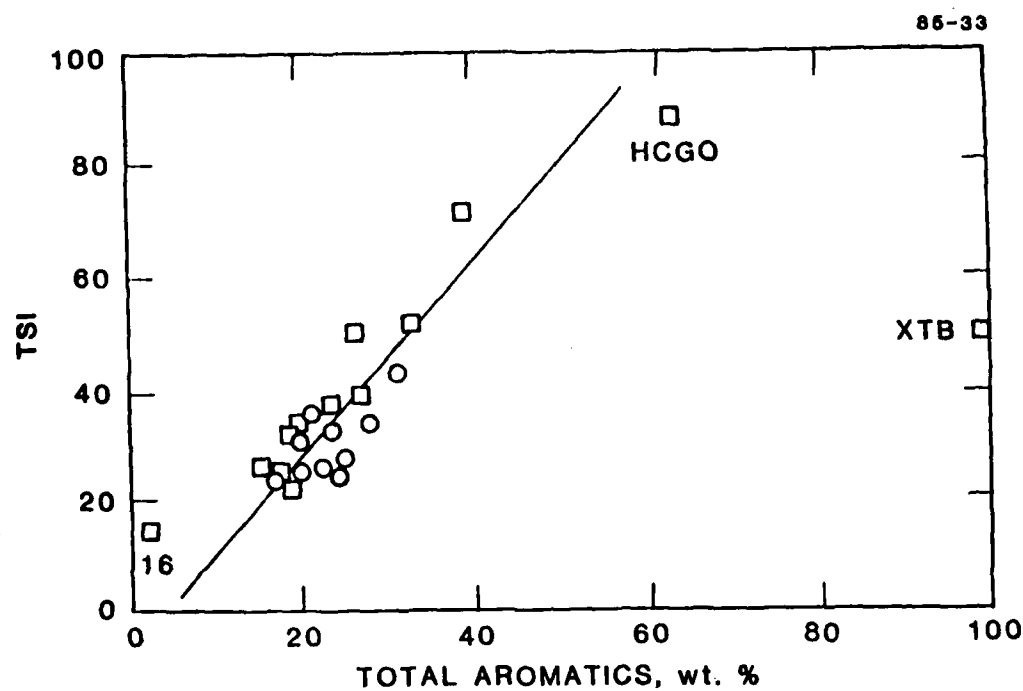


FIGURE 12 VARIATION OF THRESHOLD SOOTING INDICES
WITH TOTAL AROMATIC CONTENT

○ = NAPC 1-10; □ = other NAPC fuels (see Table 1).
The fitted line disregards NAPC-16, HCGO, and XTB
and has $r^2 = 0.72$.

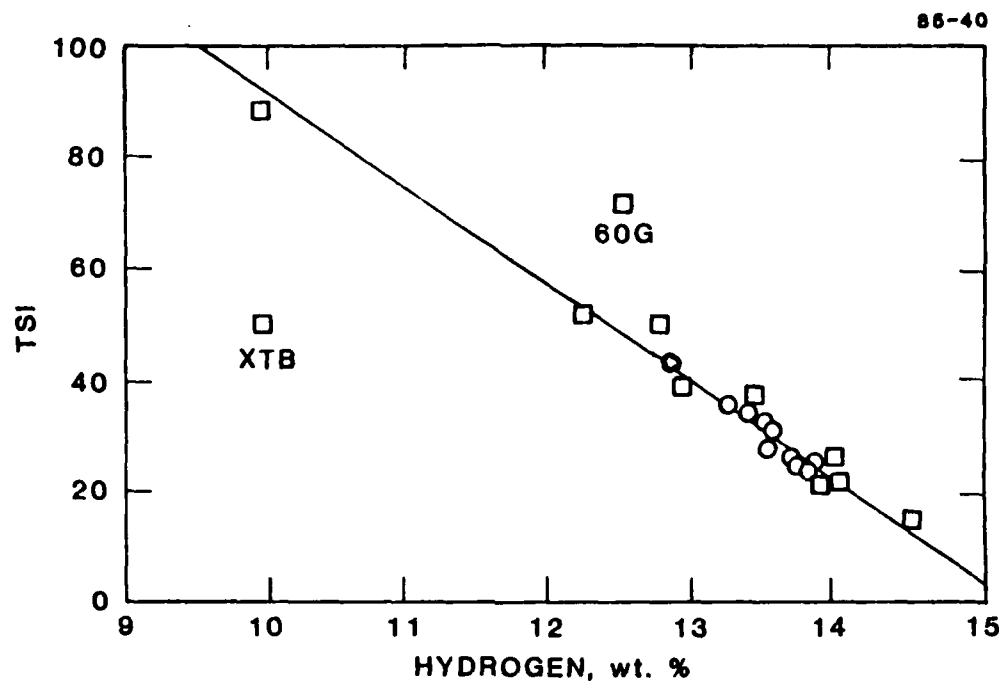


FIGURE 13 DIFFUSION FLAME TSI's vs. H% for NAPC FUELS
The fitted line disregards 60G and XTB and has $r^2 = 0.93$.
Symbols as in Fig. 12

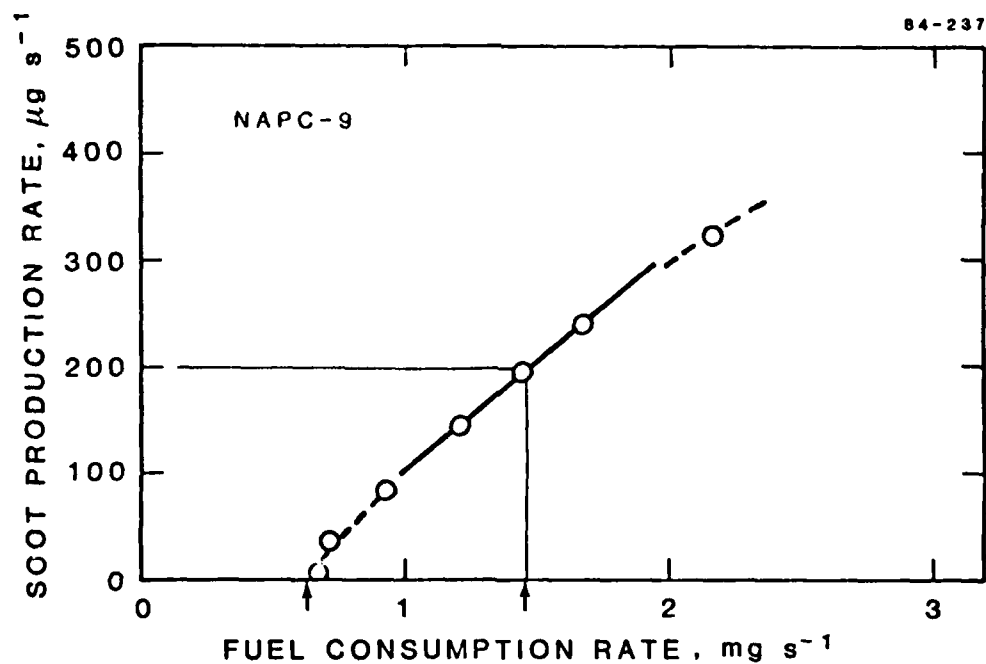


FIGURE 14 DIFFUSION FLAME SOOT PRODUCTION RATES
OF NAPC-9

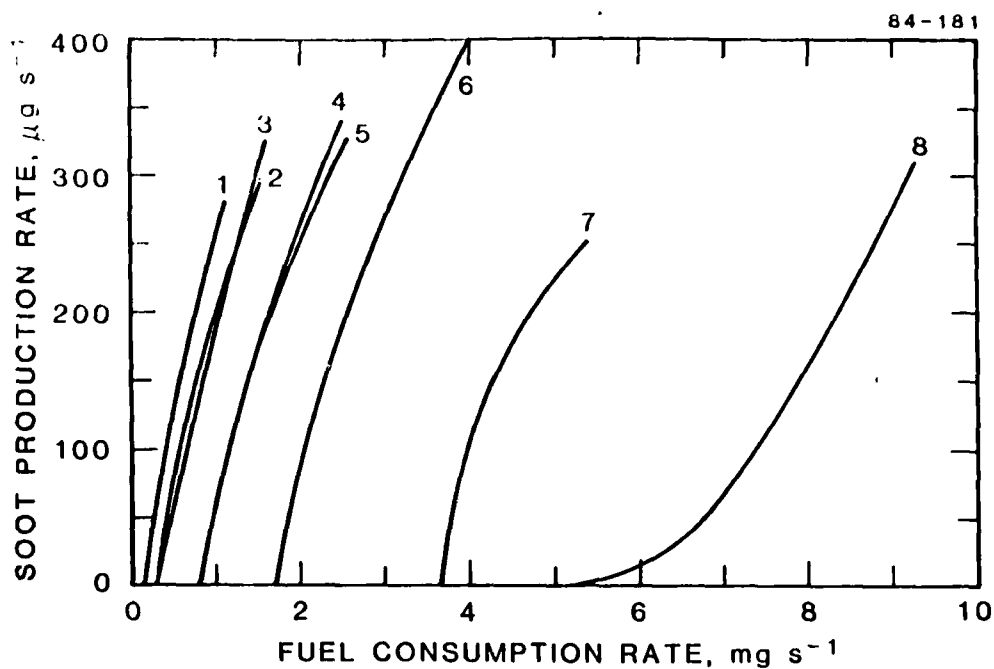


FIGURE 15 SOOT PRODUCTION IN DIFFUSION FLAMES

Key: (1) 1-methylnaphthalene; (2) toluene; (3) tetralin; (4) decalin; (5) AeroChem-A (fuel mixture); (6) isooctane (2,2,4-trimethylpentane); (7) n-tetradecane; and (8) n-heptane.

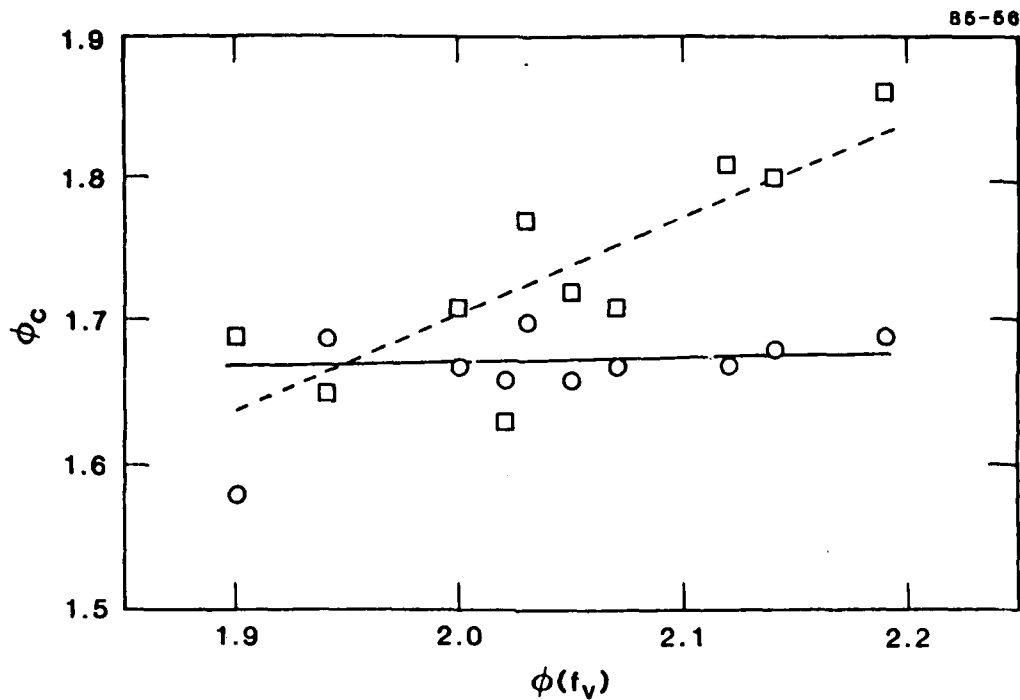


FIGURE 16 THE EQUIVALENCE RATIO AT $f_v = 2 \times 10^{-7}$ COMPARED WITH THE SOOT THRESHOLD EQUIVALENCE RATIO

○ = unregulated burner data; □ = regulated burner data.

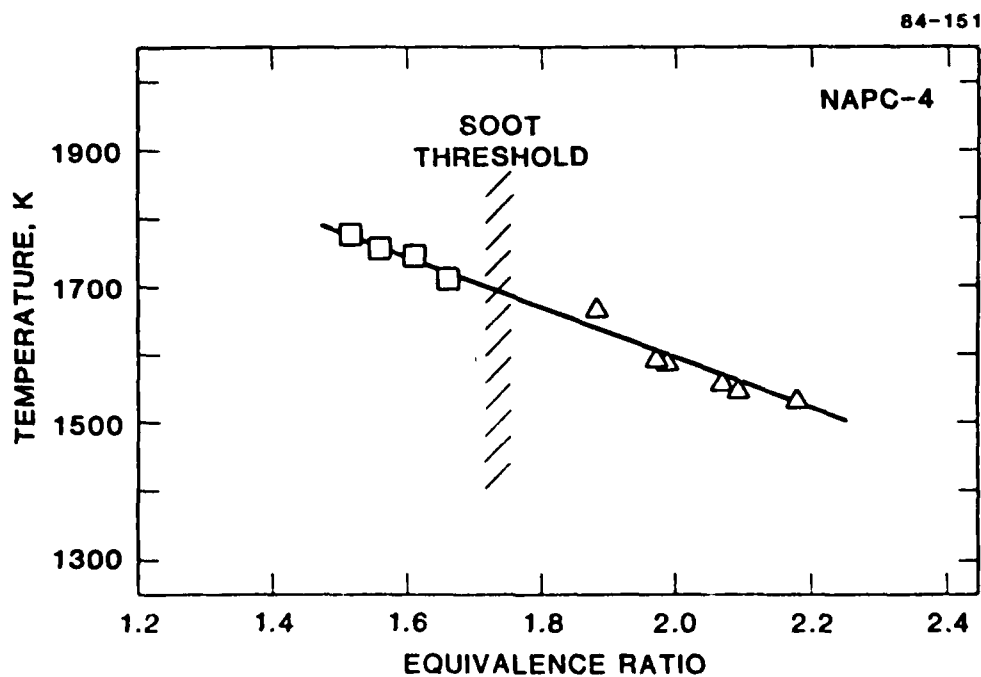


FIGURE 17 FLAME TEMPERATURES FOR NAPC-4 AT 2.0 CM ABOVE BURNER SURFACE

□ = thermocouple data; Δ = 3λ emission pyrometer data.

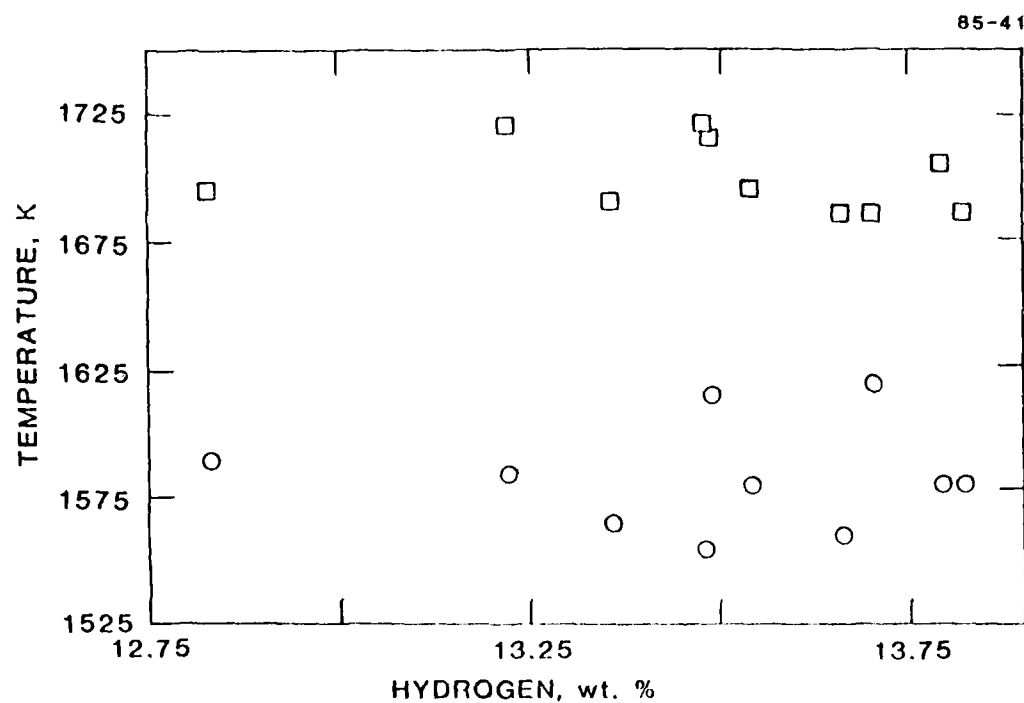


FIGURE 18 PREMIXED FLAME TEMPERATURES FOR NAPC 1-10

□ = flame temperature at soot threshold, ϕ_c ;
○ = flame temperature at soot volume fractions of 2×10^{-7} , $\phi(f_v)$.

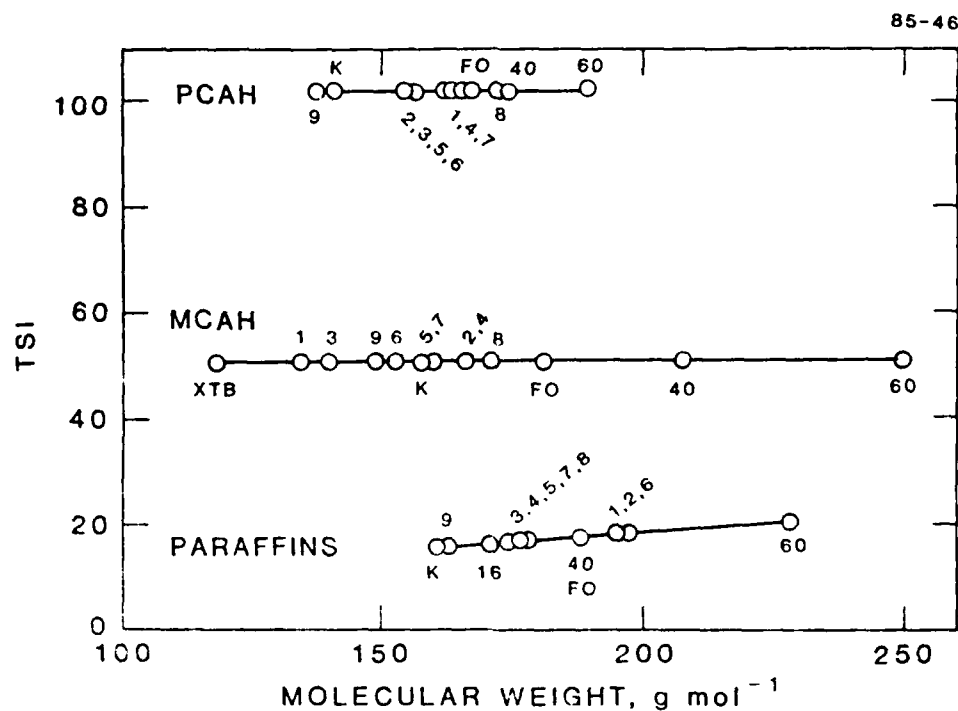


FIGURE 19 ESTIMATED TSIs FOR HYDROCARBON CLASS FRACTIONS OF NAPC FUELS

The estimated molecular weights are from Ref. 38. The numbers identify NAPC fuels. Other codes are: K = kerosene, FO = fuel oil, 40 = 40 Golden, 60 = 60 Golden, XTB = xylene tower bottoms. These data were used to calculate the results given in Fig. 20. Other estimated TSIs for these classes are possible and are probably more realistic.

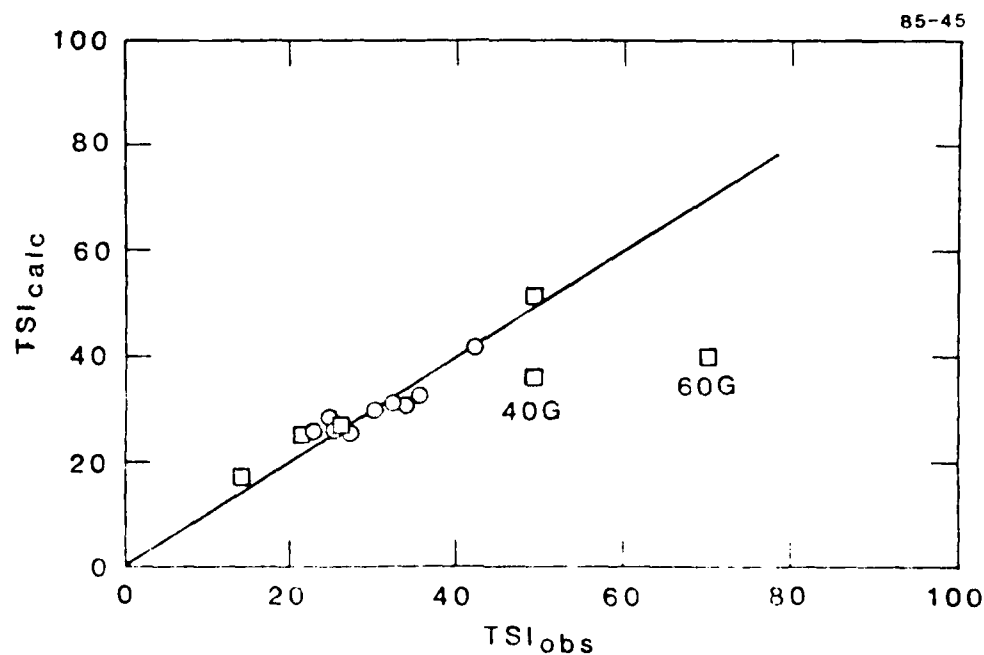


FIGURE 20 CALCULATED TSI VALUES COMPARED WITH EXPERIMENTAL TSIs

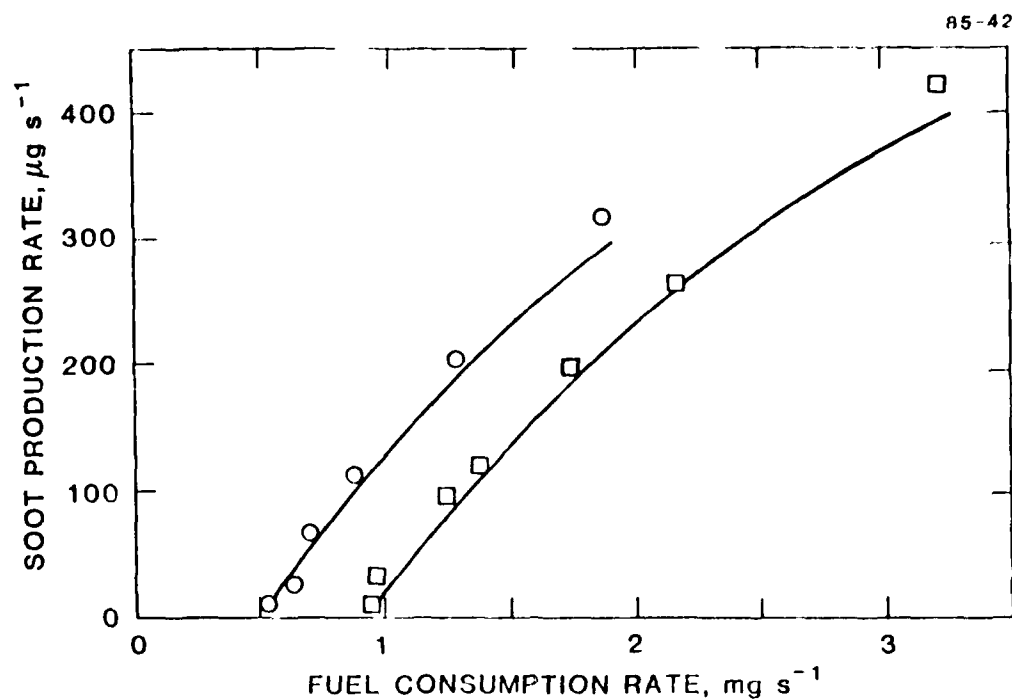


FIGURE 21 SOOT PRODUCTION RATE MIXTURE RULE TESTS

○ = 40%/60% by volume toluene/isooctane; □ = 15%/85% by volume toluene/isooctane.
Lines calculated using mixture rule.

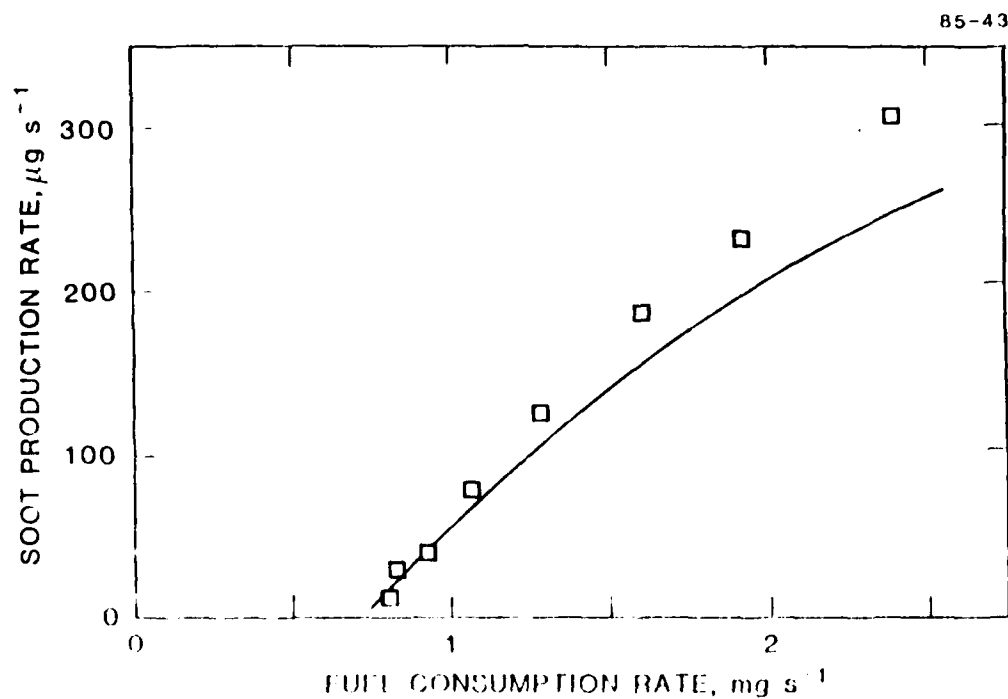


FIGURE 22 SOOT PRODUCTION RATE MIXTURE RULE TEST FOR AEROCHEM-A

The line was calculated using the mixture rule.

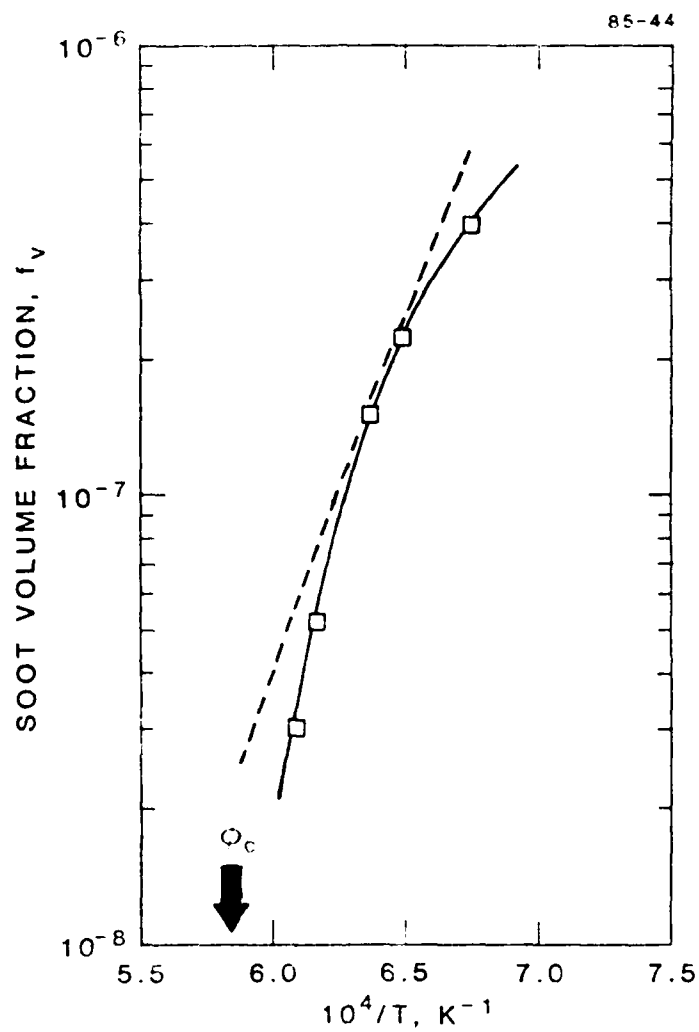


FIGURE 23 EXPERIMENTAL AND CALCULATED SOOT VOLUME FRACTIONS FOR AEROCHEM-A

— $\square$ = experimental data, unregulated burner;
--- = mixture rule calculated values, see text.

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