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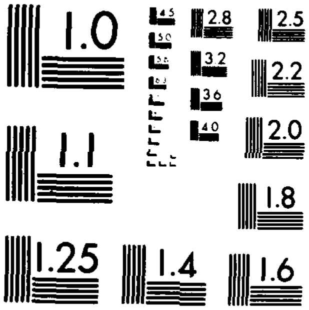

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CORRELATIONS OF SOOT FORMATION IN TURBOJET ENGINES & IN LABORATORY FLAMES

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OCTOBER 1983

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5 JAN 1982 - 28 FEB 1983

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Test data for F101, J79, and TF-41 jet engines were abstracted from the literature and analyzed to determine the correlation between smoke-related engine performance data and laboratory measurements of fuel sooting tendencies. The smoke-related data included smoke number, liner temperature rise, radiation flux, and Smoke Emission Index measurements. The engine data were correlated with the following laboratory measurements of fuel sooting tendencies: fuel hydrogen percent, total fuel aromatic content, polycyclic aromatic content, smoke point, H/C ratio, C/O ratio, and several types of threshold

(Block 20 continued)

sooting indices (TSIs). Rules for estimating TSI values for multicomponent mixtures, such as jet fuels, were developed in order to utilize the existing laboratory data for pure fuels (i.e., single chemical compounds). It was determined that no single laboratory measurement of fuel sooting tendency could be used to correlate all the selected engine test data. Improved results can probably be obtained with more accurate and complete fuel analyses as well as improvements in the procedures for estimating jet fuel TSIs.

PREFACE

This report was prepared by AeroChem Research Laboratories, Inc., P.O. Box 12, Princeton, New Jersey 08542 under Contract No. F08635-82-C-0130 for the Air Force Engineering and Services Center (AFESC), Engineering and Services Laboratory (AFESC/RD), Tyndall Air Force Base, Florida.

This study was a continuation of work performed with AFESC funds under Air Force Office of Scientific Research Contract F49620-77-C-0029. That work was reported in ESL-TR-81-09, February 1981. This study was accomplished between January 1982 and February 1983. Lt Jenkins and Capt Lubozynski (AFESC/RDVS) were the project officers.

This report has been reviewed by the Public Affairs (PA) Office and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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GLOSSARY OF TERMS

Symbol	Meaning
AR%	Volume percent of all aromatic compounds.
C/O	Mole (or atom) ratio of carbon to oxygen metered into the combustor at the test conditions.
EI_s	Smoke Emission Index, the quantity of carbon, in the form of smoke or soot, produced per unit of fuel combusted (g carbon/kg fuel).
F/A	The fuel-to-air ratio metered into the combustor at the test conditions (units: g fuel/kg air).
H%	Weight percent hydrogen.
H/C	Mole (or atom) ratio of hydrogen to carbon.
LTR	Liner temperature rise, the difference (K) between the maximum combustor liner temperature and the inlet air temperature to the combustor.
PCAH	Volume percent of polycyclic aromatic hydrocarbons present.
RF	The radiation flux measured through an optical access port viewing the combustion zone of the combustor (kW m^{-2}).
SN	The SAE Smoke Number measured at the combustor exit.
SP	ASTM smoke point, mm.
SP^{-1}	Inverse of ASTM smoke point, mm^{-1}.
SREPs	Smoke-related engine parameter(s) (RF, LTR, SN, or EI_s).
TSI_{df}	A diffusion flame TSI calculated from the ASTM class analysis of the jet fuel and a diffusion flame mixture rule (Equation (9)).
TSI_{exp}	A diffusion flame TSI calculated from the ASTM smoke point and the molecular weight of the fuel (Equation (2)).
TSI_{pf}	A premixed flame TSI calculated from the ASTM class analysis of the jet fuel and a premixed flame mixture rule (Equation (6)).

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SECTION I

INTRODUCTION

For the foreseeable future, jet aircraft will employ petroleum-derived fuels. However, the chemical nature of these jet fuels is expected to undergo significant changes within the next two decades. The leveling off of petroleum production, coupled with the continued increase in nonmilitary demand for middle-distillates (i.e., the petroleum fraction from which current jet fuels are derived), will result in decreased jet fuel availability (References 1 and 2). It is anticipated that any deficit will be made up from either higher boiling fractions from petroleum feedstock or from coal, shale, or tar sand-derived oil. These alternate sources will undoubtedly result in alterations to the chemical makeup of jet fuels (References 3-5). These considerations have prompted NASA, the US Navy, and the US Air Force to fund programs aimed at optimizing the fuel specifications for aircraft systems. A primary goal of these programs is to investigate the relationships between gas turbine engine performance and fuel composition.

As reported by numerous investigators, the levels of smoke produced by aircraft engines depend upon fuel composition and engine operating condition. Smoke affects engine performance by increasing the heat loading of the combustor section. The service lifetime of the combustor liner is inversely related to its temperature, which is, in turn, greatly increased as the radiation flux from the combustion zone increases. Smoke can become the dominant radiation source as the smoke level (in the primary combustion zone) increases. Increased smoke production also results in increased plume visibility--highly undesirable from both environmental and combat mission viewpoints.

This report summarizes the results of a 14-month program to develop better methods of correlating smoke-related jet engine performance with laboratory measures of fuel sooting or smoking tendencies. The successful development of such correlations would have direct impact on the chemical "design" of future jet fuel composition. Another important benefit of successful correlations would be a reduction in the amount of costly fuel testing on full-scale jet engines.

SECTION II

BACKGROUND

This section will briefly review prior correlation studies of smoke-related engine performance with laboratory measurements of a fuel's sooting tendency. Rather than an exhaustive literature survey and evaluation, which is outside the scope of the present program, this section is intended to provide a brief background in the use of particular laboratory measurements of a fuel's sooting tendency as they have been applied in correlation studies.

A. SMOKE-RELATED ENGINE PERFORMANCE PARAMETERS

It is pertinent to ask which engine performance parameters are important and how smoke levels affect these performance parameters. Four engine performance parameters influenced by engine smoke are: (1) the combustor liner temperature, (2) the flame radiation flux, (3) the SAE Smoke Number (References 6 and 7) and (4) the Smoke Emission Index. The first two parameters are related to the heat load of the combustor section of the jet engine. The last two parameters are related to the level of smoke emissions.

The lifetime of the hot section of an engine is largely determined by the thermal stress and heat cycling of the engine. As the metal gets hotter, it degrades more rapidly and fails sooner. The combustor liner areas most likely to fail are those exposed to the highest temperatures. The liner temperature is determined both by the inlet air temperature and by the additional heat generated by the combustion process. Because the heat load generated by the combustion process is fuel-dependent (see below), the maximum liner temperature rise (equal to the maximum liner temperature minus the inlet gas temperature) is one engine performance parameter of interest in correlation studies.

The construction of most combustor sections of jet engines employs air film cooling of the combustor liner. This air film near the interior surface of the liner effectively reduces the convective transfer of heat from the combustion gases to the liner. The rate of radiative transfer of heat (i.e., radiation flux) to the liner, however, is unaffected by the presence of this air film. There are two main sources of this radiative heat flux. One source is the infrared radiation, emitted primarily from the hot combustion gases, carbon dioxide and water. The second source is the blackbody emission from hot smoke or soot particles. Depending on the amount of smoke within the combustor section, this second source of radiative heating can become the dominant heat load of the combustor liner. Since it is well known that some fuels burn "sootier" than others under identical conditions, it might be anticipated that there would be a fuel dependence to the radiation flux and, in turn, the combustor liner temperature.

The SAE Smoke Number (SN) is an indirect measure of the smoke levels in jet engines. Briefly, a sampling probe inserted into an engine downstream of the combustion zone samples a certain fraction of the gas stream through a filter medium. The diffuse reflectance of the exposed filter paper (Rs) vs. that of a nonexposed filter paper (Rw) is measured, and the Smoke Number is defined as: SN = 1000(1 − (Rs/Rw)). Qualitatively, the SN increases in magnitude as the smoke density increases; however, it is difficult to establish a quantitative relationship between Smoke Number and smoke density (grams of smoke per volume of gas). This is because the size distribution of the smoke particles is dependent upon the combustion processes and this size distribution affects the optical properties (i.e., the reflectance) of the smoke collected. A literature analysis by Champagne (Reference 6) suggests that the smoke density can be estimated to within a factor of 2 using the commonly employed Shaffernocker and Stanforth relationship (Reference 7).

Under given operating conditions the smoke density or smoke levels are expected to depend on the type of fuel used. Laboratory studies of various fuels in premixed or diffusion flames have established that the tendency to soot depends on the fuel molecular structure (References 8 and 9). Thus, the Smoke Number measured at one operating condition of a jet engine should be fuel-related.

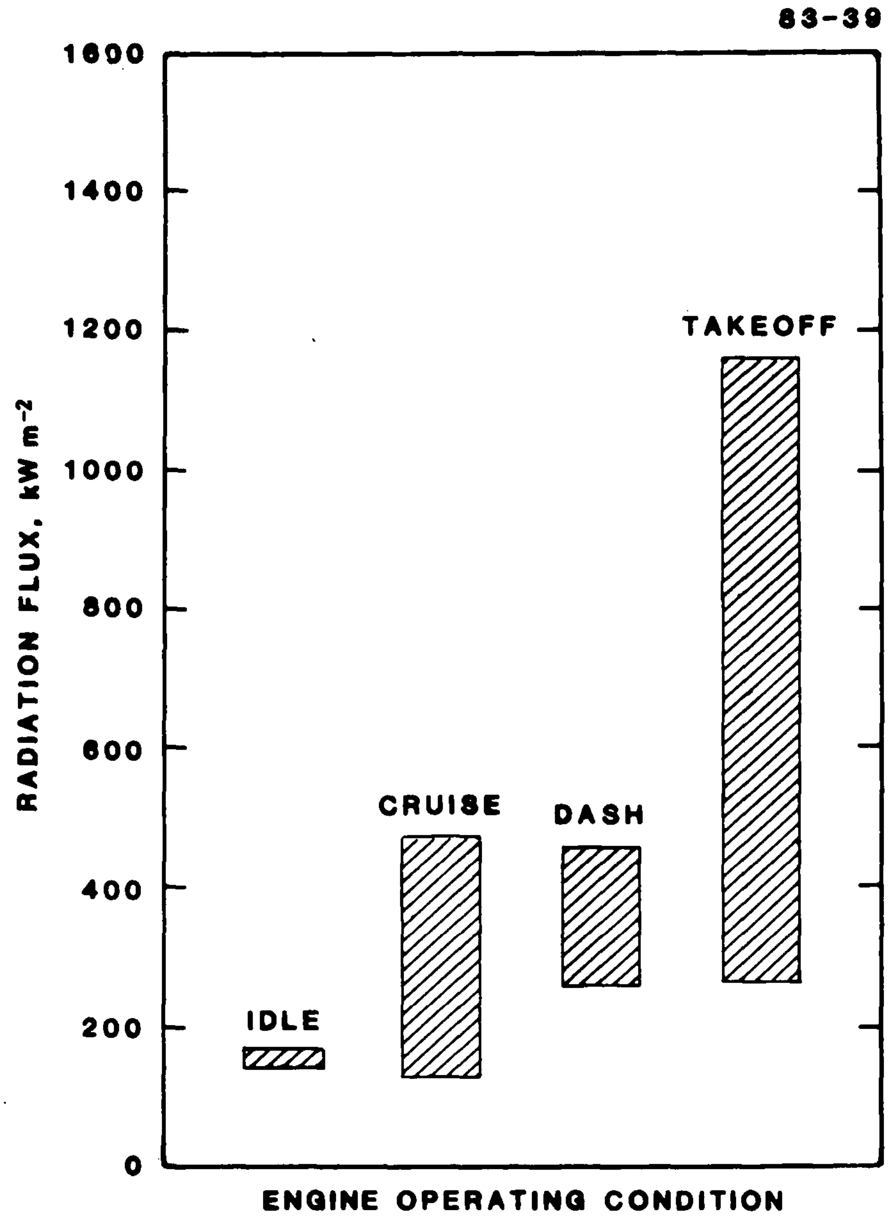
The Smoke Emission Index, EI_s, is the mass of soot produced per unit mass of fuel combusted. This is the "soot yield." The Smoke Emission Index is a derived quantity, calculated (using the Shaffernocker and Stanforth relationship, Reference 7) from the measured Smoke Number. The smoke concentration, the primary fuel-to-air ratio, and the additional air mixed into the combustor prior to the location of the SN measurement, are combined to estimate the mass of smoke or "carbon" produced per unit mass of fuel combusted.

Both the Smoke Number and indirectly, the Smoke Emission Index, are related to the plume visibility at the engine exit. The relationship between plume visibility and the Smoke Number is discussed by Champagne (Reference 6) and by Wood (Reference 10).

B. PREVIOUS CORRELATIONS OF SMOKE-RELATED ENGINE PERFORMANCE TO LABORATORY MEASUREMENTS OF FUEL SOOTING TENDENCIES

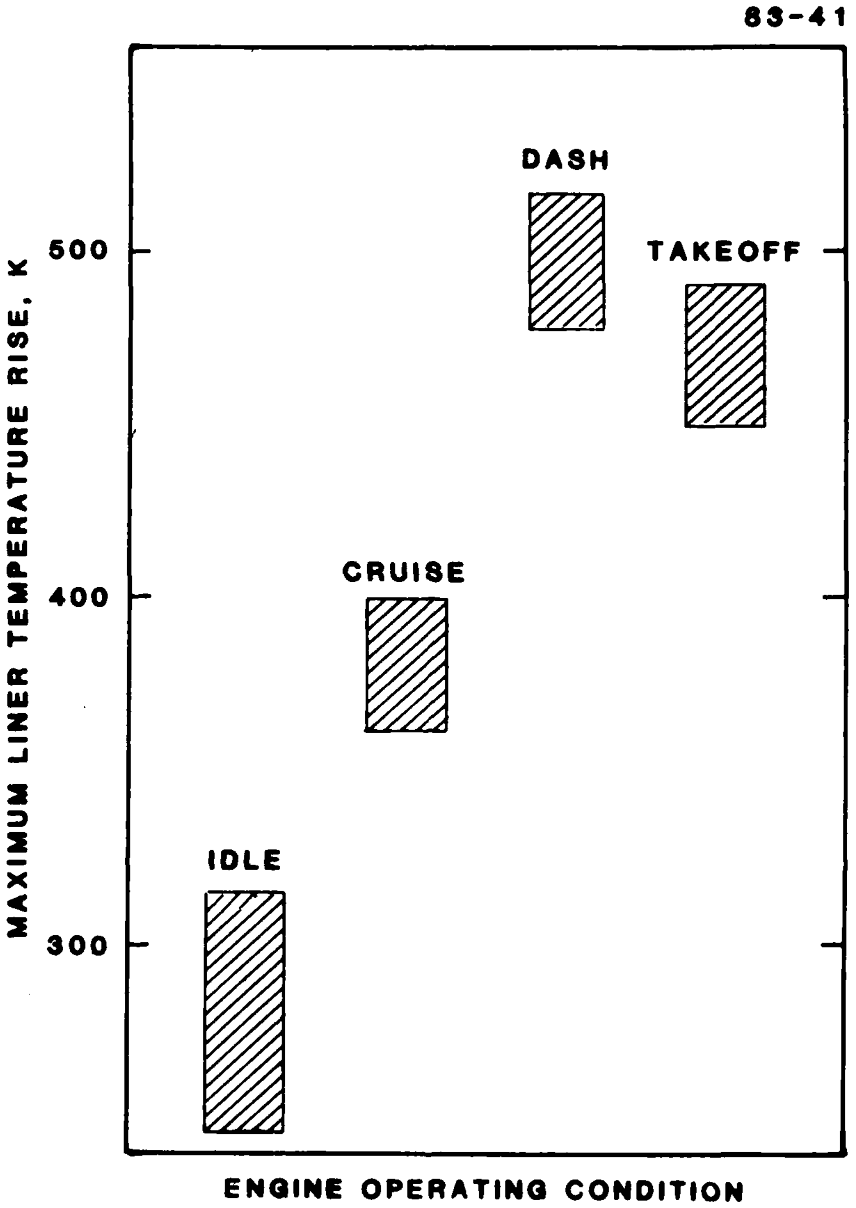
In this section, we briefly summarize the results of several studies which have attempted to correlate the smoke-related engine performance parameters (hereafter referred to as SREPs) with "laboratory measures" of fuel sooting tendencies. These "laboratory measures" of fuel sooting tendencies commonly employed in the correlation studies are not universally used by the combustion community.

The most widely used correlation of SREPs is to the weight percent of hydrogen (H%) in the fuel (References 11-16). The success of this fuel parameter, however, is largely a result of the limited variation of the fuel compositions which have been employed in fuel effects studies of engine performance. To illustrate, two engine studies recently completed on the turbojet J79 (Reference 17) and the turbofan TF-41 (Reference 18) combustors show that H% is not necessarily closely correlated to SREPs in these engines. For the J79 study, four fuels having hydrogen weight percents of 13.0 were studied. Therefore, if H% is a good indicator of smoke production, the SREPs for these four fuels should be very similar at fixed engine operating conditions. Figures 1 to 3 dispel the notion that H% is strongly correlated to these SREPs. Similarly, three fuels in the TF-41 engine study have nearly identical H% (11.9-12.0) yet Figures 4 and 5 show that both the maximum liner temperature rise and the Smoke Number are not constant for each set of operating conditions as would be expected if H% were a good correlating parameter.



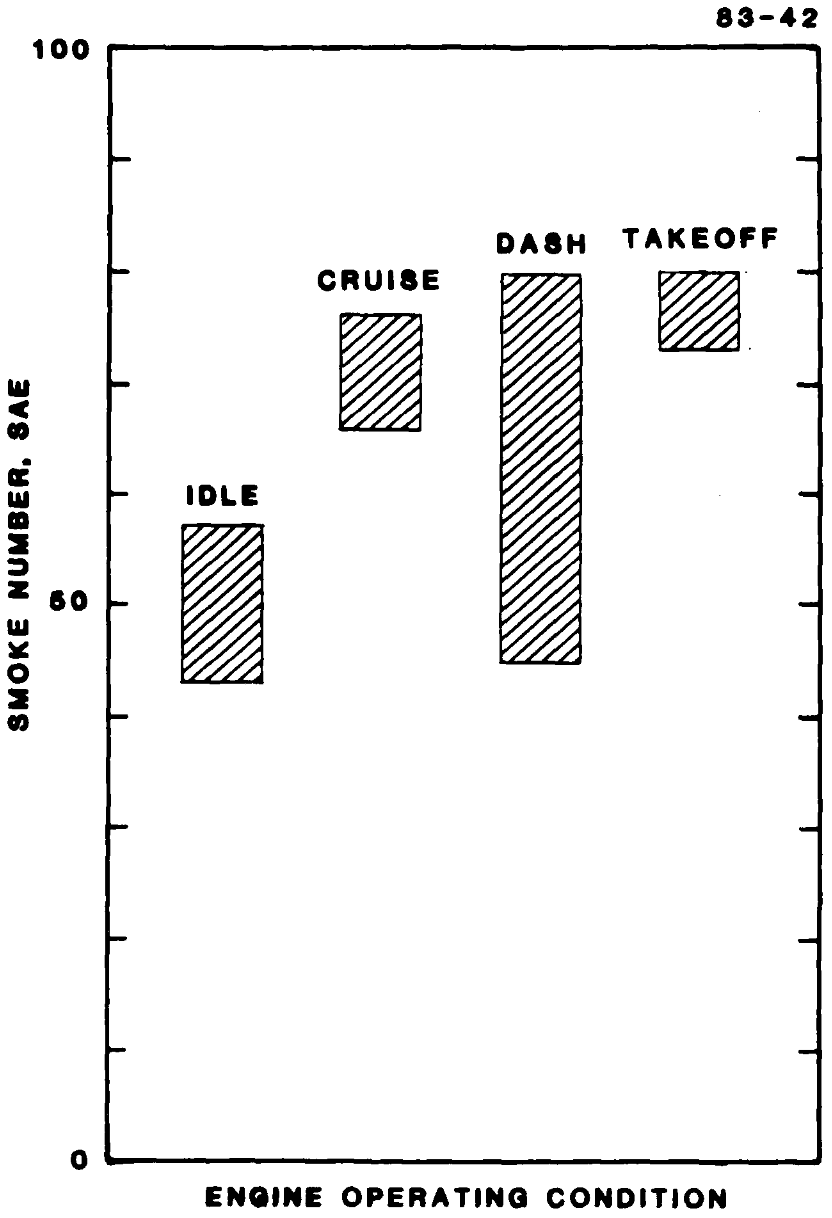
The bars show the range of values obtained using fuels with identical (13 percent) hydrogen content.

Figure 1. Radiation Flux for Four Fuels and Four Operating Conditions in a J79 Engine



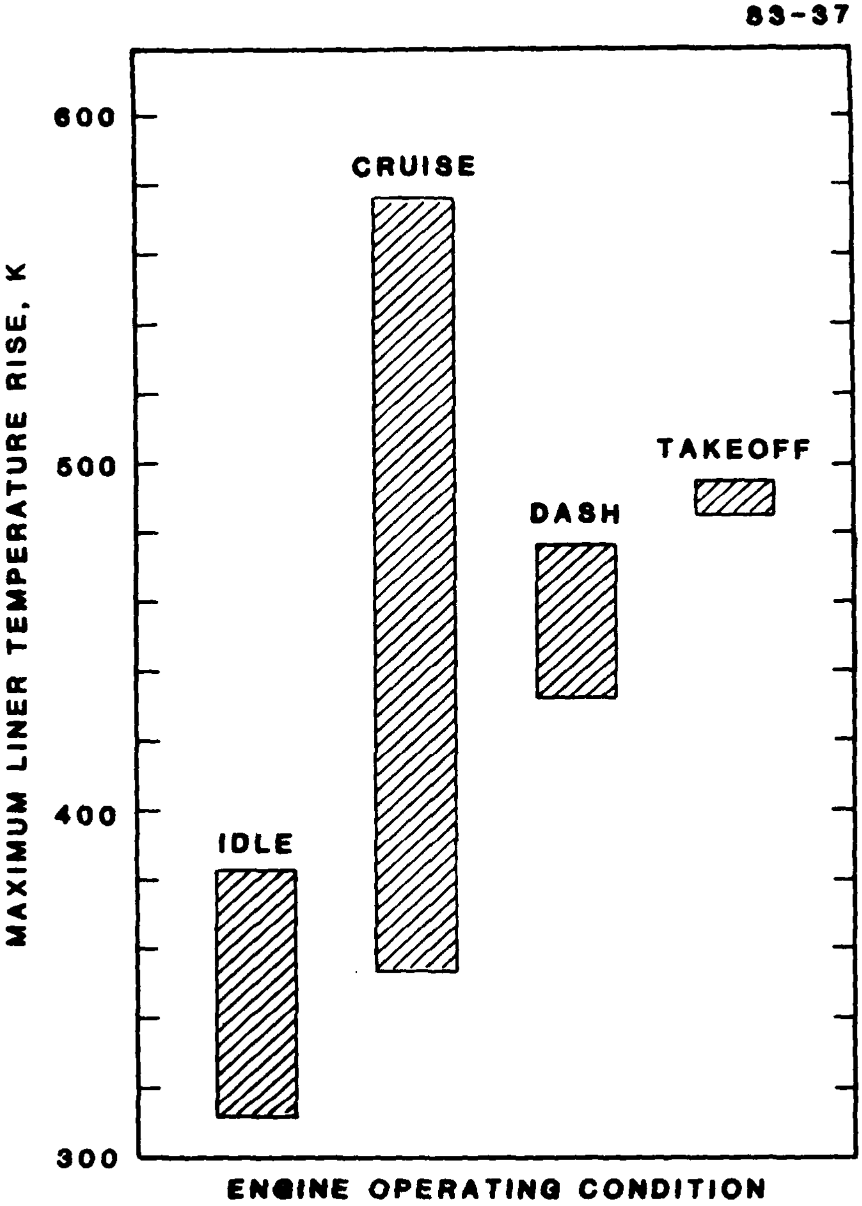
The bars show the range of values obtained using fuels with identical (13 percent) hydrogen content

Figure 2. Maximum Liner Temperature Rise (K) for Four Fuels and Four Operating Conditions in a J79 Engine.



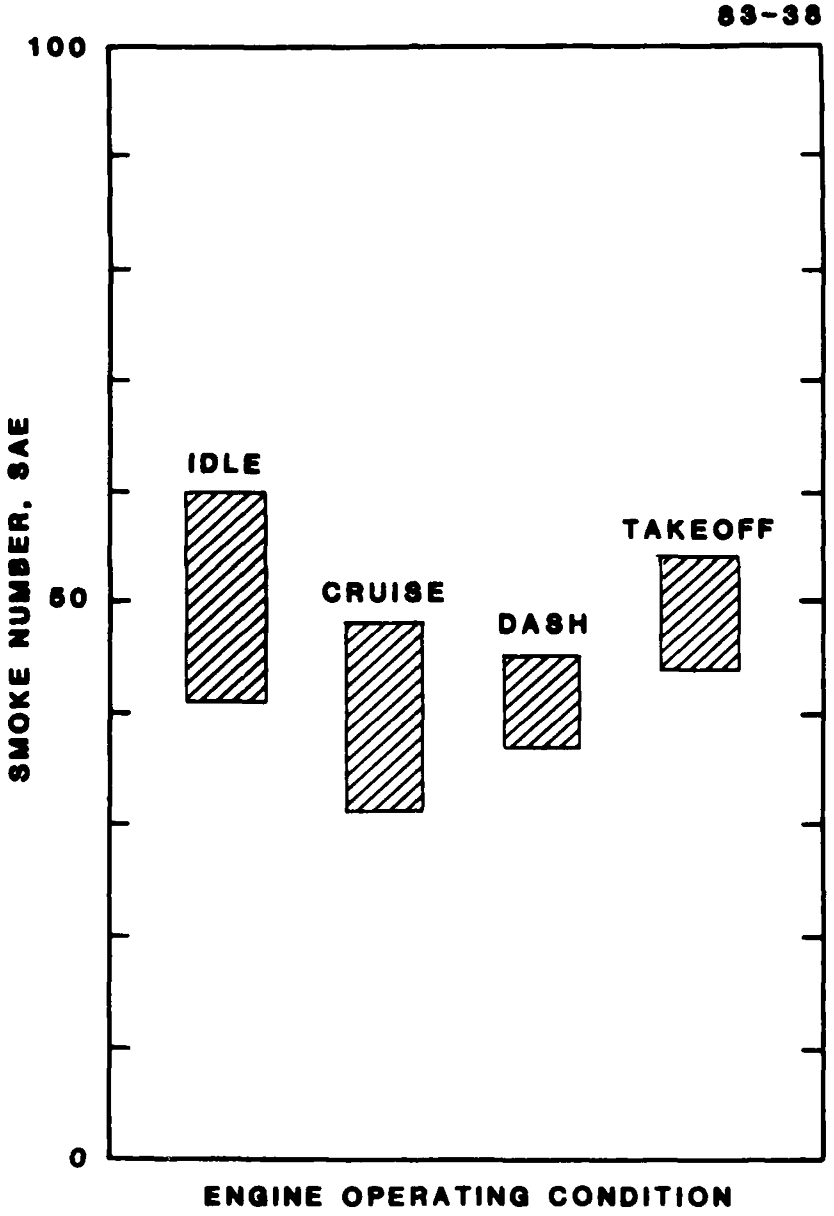
The bars show the range of values obtained using fuels with identical (13 percent) hydrogen content.

Figure 3. Smoke Number at Combustor Exit for Four Fuels and Four Operating Conditions in a J79 Engine.



The bars show the range of values obtained using fuels with similar (11.9-12.0 percent) hydrogen content

Figure 4. Maximum Liner Temperature Rise (K) for Three Fuels and Four Operating Conditions in a TF-41 Engine.



The bars show the range of values obtained using fuels with similar (11 9-12.0 percent) hydrogen content.

Figure 5. Smoke Number for Three Fuels and Four Operating Conditions in a TF-41 Engine.

The hydrogen-to-carbon mole ratio, H/C, has been used by Moses et al. (Reference 19), to correlate engine tests results. This ratio, H/C = 12 H%/ (100 percent - H%), is almost linearly connected with H% because the range of H% over which liquid hydrocarbon fuels are normally varied is restricted to ca. 10-16 percent. Therefore, this parameter correlates as well, or as poorly, as the H% to engine test results.

In laboratory studies of the sooting tendencies of fuels burned in diffusion flames, the minimum flame height for which smoke just escapes from the flame tip is called the smoke point (SP). Minchin (Reference 20) defined the tendency to smoke (or to produce visible soot) as a constant divided by the smoke point. The smoke point (or its inverse) has received limited consideration in correlations of smoke-related engine performance (Reference 21) and thus its usefulness in correlation studies has not been adequately tested.

Laboratory studies of fuel sooting tendencies in premixed flames employ the C/O mole ratio (Reference 22), fuel/air (Reference 23) or fuel/oxygen mole ratios, or their normalized counterparts such as equivalence ratios (References 24 and 25), in illustrating the relationships between the fuel's sooting tendencies and molecular structure (References 8 and 26). The numerical values of these quantities, measured at the threshold for which soot is first observed (i.e., the onset of yellow emission) in premixed flames, are referred to as "critical" ratios. For example, the critical C/O ratio for benzene, as measured in a Bunsen burner, is 0.57. These critical ratios have never been used in correlations of smoke-related engine test results and, therefore, little comment can be made on their utility in correlation studies. These will be treated subsequently in this report.

A general conclusion from laboratory studies of sooting tendencies is that aromatic hydrocarbons, particularly polycyclic aromatic hydrocarbons, have a greater tendency to soot than do paraffinic hydrocarbons. Moses et al. (References 13 and 19) found that total weight percent aromatics (AR%) correlated well with measured flame radiation flux in both a T-63 combustor and a Phillips 2-inch combustor. Friswell (Reference 27) also noted that the Smoke Emission Index correlated well with AR% in a research gas turbine.

In summarizing the results of previous studies on fuel effects on gas turbine SREPs, the hydrogen weight percent is the most commonly used and, possibly the best correlating parameter found to date. In fairness, however, the other laboratory fuel parameters have not been as thoroughly investigated as hydrogen weight percent. It has been concluded from fuel effects studies on SREPs that fuel structure effects are minor (Reference 16). However, fuel structure effects can become important under some operating conditions, as can readily be verified by examining Figures 1-5 (see also (Reference 19)).

SECTION III

PROGRAM APPROACH

This section is devoted to a discussion of the approach followed in this program for correlating the smoke-related engine performance test data to laboratory measurements of fuel sooting or smoking tendencies. The items to be discussed are: (1) the relationship between the combustion process within a jet engine and the laboratory flame data, (2) the types of laboratory data available, (3) the data on fuel effects in the smoke-related engine tests, and (4) the program rationale used in this work.

A. RELATIONSHIP BETWEEN ENGINE COMBUSTION AND LABORATORY FLAMES

Liquid jet fuel is normally injected into the combustor through a fuel nozzle which is placed near the entrance of the combustor and produces a fine spray of fuel droplets. Upstream of the fuel nozzle, a number of air ducts are provided for injecting air into the combustor. The air flow pattern is optimized with respect to a proper balance between rapid mixing of air and fuel spray and the degree of flame stabilization achieved by air flow circulation zones within the combustor.

The similarity between laboratory and engine data lies in the type of combustion zones created. In the fuel-rich zone of the combustor near the fuel nozzle, the combustion process may be diffusion-limited. This process resembles the combustion process in a laboratory diffusion flame. Farther downstream of the fuel jet, where fuel and air have been thoroughly intermixed and the fuel droplets completely vaporized, the combustion process resembles that of a laboratory premixed flame.

Laboratory data on fuel structure effects on soot formation, however, are almost always obtained on laminar flames, whereas in jet engine combustors the flames are highly turbulent. There is little information concerning how turbulence affects the soot formation process in laboratory diffusion flames. Assuming that the effect of turbulence is a minor perturbation on the overall combustion process leading to soot, then the laboratory data on sooting tendencies of different fuels can be used without correction. However, if turbulence is a major perturbation, then the laboratory data may need to be corrected or a different set of data used.

B. LABORATORY DATA

1. Soot Thresholds and Soot Yields

Two types of measurements are generally employed to rank the sooting propensities of fuels. One method is to rank fuels according to the fuel/air conditions necessary for observing soot. For premixed flames the minimum fuel/air ratio (or C/O ratio) for which yellow (soot) emission is observed, is usually employed as an index. In diffusion flames, the minimum flame height at which smoke escapes from the flame tip, is used as an index. The results from either premixed or diffusion flames, are collectively referred to as soot threshold data and have been gathered by a number of investigators in both premixed flames (References 22-25 and 28) and diffusion flames (References 20 and 29-33) for a large number of pure fuels. This extensive data base can be used to judge how fuel molecular structure (e.g., alkanes, alkenes, aromatics, polycyclic aromatics, etc.), influences threshold sooting behavior.

The second method of ranking fuel sooting tendencies is based on the quantity of soot produced per quantity of fuel combusted, i.e., the soot yield. These data are like soot threshold data in that the quantitative soot yields depend on the burning conditions--diffusion flame or premixed flame. Unlike the soot threshold data, only a limited number of fuels have been examined. This severely limits the usefulness of this data base, in a practical sense, for correlating smoke-related engine performance results. For this reason, soot yield data were not used in this correlation study.

Before leaving this section, it should be stressed that either type of laboratory data is expected to be of limited usefulness in correlating smoke-related engine test results. Ideally, one would like an index which includes both types of laboratory information since it is important to know both the minimum fuel/air conditions which produce soot and also how variation of fuel/air conditions alters the soot yield. A ranking of fuel soot production with molecular structure in this manner, i.e., considering soot thresholds and soot yields, should provide a better index for correlating soot-related laboratory and engine test data than an index based upon threshold values alone.

2. Threshold Sooting Indices

The Threshold Sooting Index (TSI) was defined by Calcote and Manos (Reference 8) as a means of removing the dependence of laboratory measurements of fuel sooting tendencies upon the burner and other conditions that vary from study to study. For example, the critical C/O for benzene measured with a Bunsen burner (Reference 34) is 0.57 but the value increases to 0.65 when measured in a premixed flat flame (Reference 35). Similarly, differences in the smoke point measurements in diffusion flames have been found (Reference 8) depending on how the measurement is made. The interesting and useful result from this study was that premixed and diffusion flames could each be correlated, independent of the experimental techniques used to obtain the data, by molecular structure. The TSI scale is normalized such that a particularly sooty fuel (e.g., naphthalene for diffusion flames and 1-methylnaphthalene for premixed flames) has a TSI = 100 and the least sooty fuel (e.g., ethane for diffusion flames and acetylene for premixed flames) has a defined TSI = 0. It is important to note that TSI is a measure of soot threshold and not the soot yield.

The different burning environments in diffusion flames and premixed flames have thus far precluded defining a TSI scale applicable to both. Therefore, Calcote and Manos defined two TSI scales--one for premixed flames and another for diffusion flames. The premixed flame TSI for a fuel was defined as:

$$\mathrm{TSI} = a - b\,(\phi_c). \tag{1}$$

In this equation, the a and b are constants which depend on the burner used to measure the critical equivalence ratio, ϕ_c. This formula requires that the molecular formula of the fuel be known. If it is unknown, the molecular weight and weight percent hydrogen in the fuel can be used to estimate the molecular formula of the fuel. The diffusion flame TSI scale was defined in terms of the smoke point as:

$$TSI = a'(MW/SP) + b'. \tag{2}$$

Note that the molecular weight of the fuel is required. The constants, a' and b', depend upon the diffusion burner employed.

The TSI scale was used in an earlier preliminary correlation study of the fuel effects on smoke-related engine performance (Reference 36). In that work, diffusion flame TSIs were employed in correlating the fuel effects on SREPs. The TSI correlations were no better or worse than the H% correlations but it was believed that if better methods were found to estimate the TSIs for multicomponent jet fuels, better correlations of the data would be obtained.

C. ENGINE TEST DATA ON FUEL STRUCTURE EFFECTS

Early in this program an extensive literature search was carried out to locate sources of engine test data which demonstrated the effect of fuel types, or fuel blends, on smoke-related jet engine performance. The jet engine performance parameters of interest to this correlation study were the Smoke Number, combustor liner temperature, Smoke Emission Index, and radiation flux. These smoke-related engine performance parameters have been discussed in the Background Section II.A.

From a total of about 150 references, 46 reports which contained both a description of the fuel and one or several of the smoke-related engine performance parameters were selected. A short précis of these references is given in Appendix A. These references, which were either original data or reviews of original data, were then subjected to a critical evaluation. The criteria used in this evaluation were: (1) detailed chemical analysis of fuel (i.e., each and every fuel component identified) and (2) specific indication of which data were taken under specific engine operating conditions. None of the references satisfied these dual criteria.

The selection criteria therefore had to be relaxed. Specifically, by relaxing the fuel analysis criterion to require only that fuel analyses be reported in terms of chemical classes (e.g., paraffins, olefins, polycyclic aromatics, cyclic paraffins, etc.), three of the references (References 17, 18, and 37) passed the evaluation. By further relaxing the chemical analysis criterion to require that fuel chemical analyses be reported only in terms of aromatic and paraffin contents, many of the references passed.

It is apparent that the available literature on smoke-related engine performance purporting to establish fuel structure effects is extremely limited in terms of chemical analyses of the fuels investigated. For single chemical compound fuels (i.e., pure fuels such as n-hexane, isooctane, toluene, etc.), the data are essentially nonexistent. Because the fuel compositions have been poorly characterized, it will be extremely difficult to relate fuel structure effects to the smoke-related engine performance results. It is hoped that this major shortcoming will be remedied in future studies of fuel structure effects on engine performance.

D. PROGRAM RATIONALE

AeroChem has reported the results of its previous program on correlating smoke-related engine performance with laboratory measurements of fuel sooting tendencies (Reference 36). In that program, the laboratory measurements used in the correlations were weight percent hydrogen, smoke points, and a sooting threshold scale (diffusion flame, TSIs; see Section III.C). Compositional information on the fuels used in the engine tests was not effectively used. Rather, estimates of the sooting tendencies of the fuels (TSIs) were made based on measured smoke points (ASTM method, Reference 38), and crude molecular weight estimates. At the conclusion of that effort, it was suggested that better correlations of engine data might be achieved if information about the fuel's composition was used.

In the present program, the intent was to locate engine test data containing complete fuel chemical analyses. As mentioned in Section III.C, the best available chemical analyses of fuels actually used in the engine tests are given only in terms of fuel classes. This severely limited the number of engine test reports which could be used in the present correlation work. However, rather than repeat the type of analyses carried out earlier using crude TSI estimation procedures, this program attempted to develop more sophisticated procedures for incorporating fuel structure information into the correlations of smoke-related engine test results.

The engine test reports having been selected, the next problem was to decide what correlations to perform. The obvious preference was to use the two most useful laboratory measurements of fuel sooting tendency, soot threshold data and soot yield data, to correlate to the engine test data. However, the laboratory soot yield data could not be used because of the limited number ("a handful") of fuels studied to date. The large number of pure fuels for which soot threshold data are available motivated a combined experimental and analytical approach for estimating jet fuel sooting thresholds (TSIs) based on the jet fuel's composition and the individual sooting thresholds (TSIs) of the chemical components of the jet fuel. This study was the first task of the present program.

In the second task, the jet fuel threshold sooting indices were correlated to the engine test data. In addition, total aromatic content, polycyclic aromatic content, hydrogen percent, and other fuel parameters commonly employed for correlating smoke-related engine performance data (see Section II.B) were correlated to the same engine test data. In this way, the various fuel parameters could be compared in terms of their relative and absolute effectiveness in correlating the engine test data. Thus, if fuel structure effects were important, then sooting tendency parameters sensitive to fuel structure should correlate to the engine test results better than parameters insensitive to fuel structure.

SECTION IV

RESULTS AND DISCUSSION

This section presents the results of this program. Section IV.A details the experiments that aided the development of mixture rules for threshold sooting indices. Section IV.B describes the mixture rules that were validated for use with jet fuels, and the development of some additional correlations which were needed to evaluate TSIs for jet fuels. Section IV.C contains the results of our correlation work on smoke-related fuel effects in three jet engines.

A. DEVELOPMENT OF TSI MIXTURE RULES

The correlation of TSIs to smoke-related jet engine performance requires both diffusion flame smoke points and premixed flame critical equivalence ratios for the fuels used in the jet engine tests. Generally, however, only the smoke points were measured and reported in engine testing programs. Therefore, we set out to determine empirically whether the premixed flame TSI, or diffusion flame TSI, of a fuel blend could be estimated from knowledge of the composition and the TSI values of the fuel blend components. The mathematical relation between the fuel blend's TSI and the TSI values of the fuel's components, we have termed "TSI mixture rules."

The mixture rules developed were based on the results of experiments carried out at AeroChem during this program. Several binary and ternary fuel blends were prepared and both the smoke point (diffusion flame) and the minimum fuel/air ratio for sooting (premixed flames) were measured. These two measured quantities yield an experimental diffusion flame TSI and an experimental premixed flame TSI. These "experimental" TSIs were used to judge the success or failure of the mixture rules.

1. Premixed Flame TSI Mixture Rule

The apparatus used to measure premixed flame soot thresholds has been described previously (Reference 39). Briefly, liquid fuels are metered using a syringe pump, spray vaporized, and the flames stabilized on a heated 2.2 cm diameter multitubular burner. A fuel-rich propane air shroud flame is used to exclude air and reduce heat losses. Air is metered using critical flow orifices. The soot threshold is determined visually by the first appearance of yellow soot emission. The "calibration constants" a and b in Equation (1) are required to convert measured critical fuel air equivalence ratios to TSIs. These were determined in a previous program (Reference 39) by measuring soot thresholds for previously studied fuels: a = 269, b = 118.

Binary and ternary fuel mixtures were prepared, using volumetric measurements and standard laboratory techniques. The burner and vaporizer were operated about 10-20 K above the boiling point of the least volatile component of the mixtures. Care was taken to insure that no condensation occurred in the burner or vaporizer system.

The minimal fuel-to-air ratio required to produce soot was measured on this burner for a series of binary and ternary fuel blends. The fuel composition must be known to calculate the fuel/air equivalence ratio. For example, to burn α moles of Fuel A and β moles of Fuel B, to CO_2 and H_2O in air, the following equation must be satisfied:

$$\alpha\, C_xH_y + \beta\, C_wH_v + \left(\frac{\alpha y + \beta v}{4} + \alpha X + \beta w \right) O_2 \rightarrow \left(\frac{\alpha y + \beta v}{2} \right) H_2O + (\alpha X + \beta w) CO_2 . \qquad (3)$$

The critical equivalence ratio is then defined as:

$$\phi_c = \frac{(\text{fuel/air})_{\text{critical}}}{(\alpha + \beta) \Big/ \left(3.76 \left(\frac{\alpha y + \beta v}{4} + \alpha x + \beta w \right) \right)} .$$

Finally, the critical equivalence ratio was used with the a and b calibration constants to give an experimental premixed flame TSI for the fuel blend.

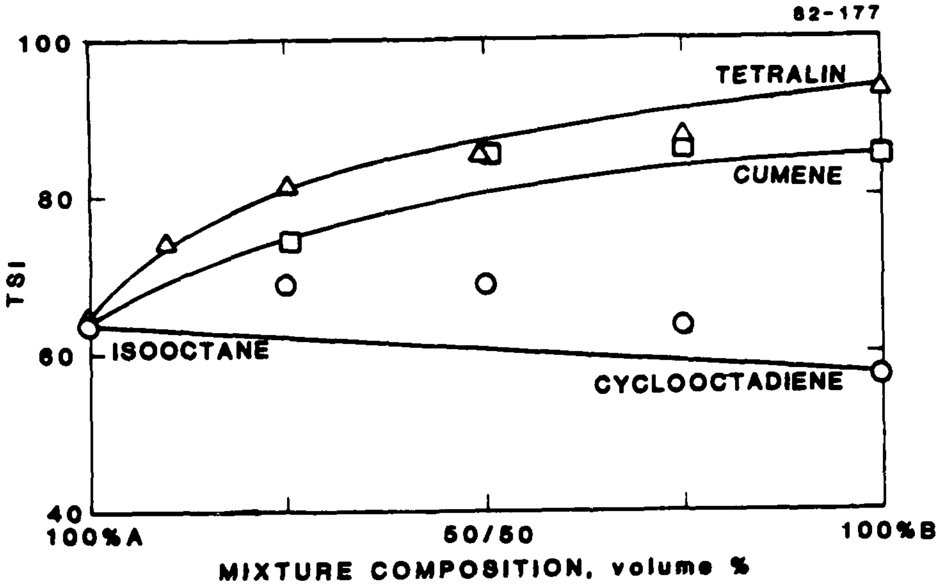
Having established the methodology, experimental TSIs were determined for a series of binary fuel mixtures. The experimental data for the binary fuel blends are given in Figures 6 and 7. On the figures, the points are the experimentally measured TSI values; the lines are calculated from the mixture rule for premixed flames. As noted earlier, this rule was empirically determined:

$$(1.1)^{TSI_{mix}} = \sum_i X_i \, (1.1)^{TSI_i} . \qquad (4)$$

In this equation, TSI_{mix} is the mixture rule estimate for the fuel blend and X_i and TSI_i are the mole fraction and the premixed flame TSI values for pure fuel component i.

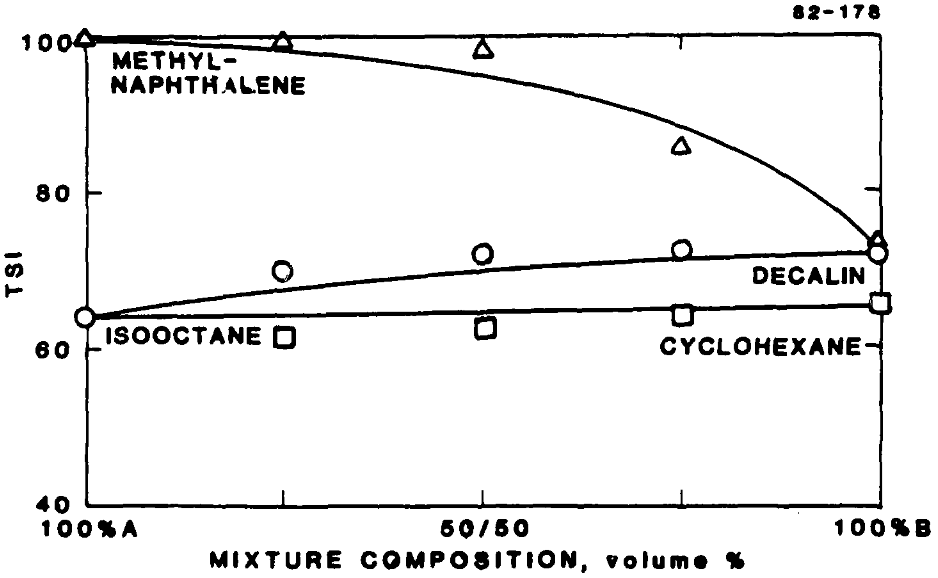
As can be seen in Figures 6 and 7, this rule gives a fairly good fit to the data, i.e., usually within ± 5 percent. Cyclooctadiene/isooctane mixtures are the only example where the fit is poor. Since no detailed analysis was made to identify why these curves are nonlinear with mixture composition, the reasons why the mixture rules fail for cyclooctadienes remain unclear. Possibly this behavior is associated with a flame temperature effect since this is the only case where the second mixture component has a higher flame temperature but a lower TSI than the first component. In any case, 1-5 cyclooctadiene is not likely to be of practical importance in considering jet fuel blends, although the possibility that other fuels could exhibit this characteristic remains and the flame temperature effect merits further consideration.

As a further confirmation of the reliability of the mixture rule, two ternary fuel blends were investigated. The first was prepared by blending a specific amount of a 50/50 (volume percent) isooctane/decalin mixture with pure 1-methylnaphthalene (MeN). The 50/50 mixture is labeled Fuel A and MeN is labeled Fuel B on Figure 8. As before, symbols are the experimentally derived TSI values and the solid line is calculated. Recall that isooctane is often used as a synonym for 2,2,4-trimethylpentane.



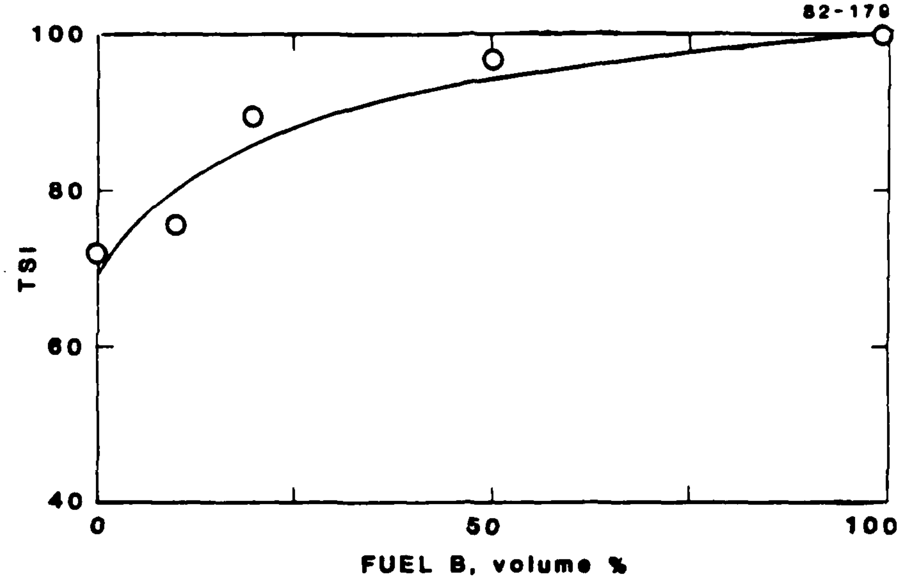
Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 6. Effect of Mixture Composition on Tendency to Soot in Premixed Flames.



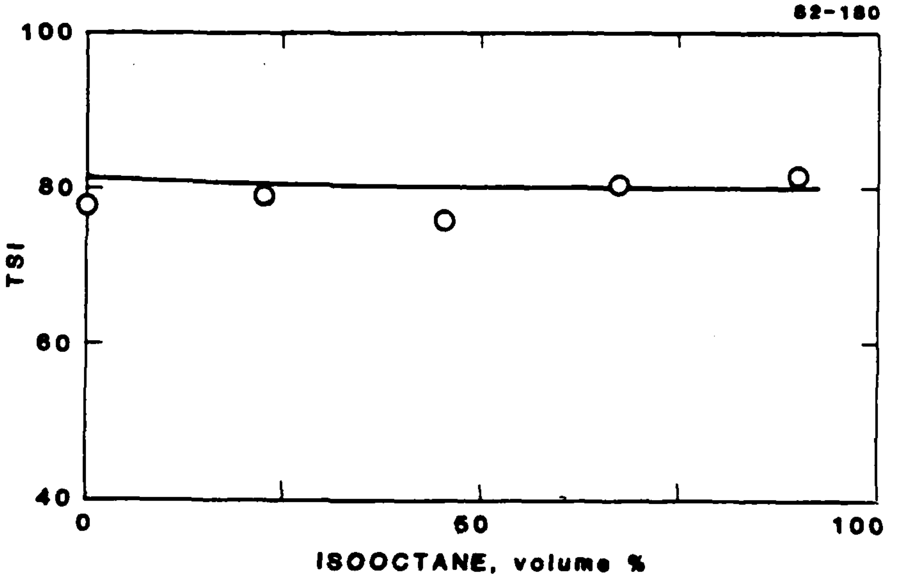
Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 7. Effect of Mixture Composition on Tendency to Soot in Premixed Flames.



Fuel comprised of Fuel A (50/50, v/v, isooctane/decalin mixture) and Fuel B (1-methylnaphthalene). Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 8. Effect of Mixture Composition on Tendency to Soot in Premixed Flames.



Fuel comprised of 10 percent methylnaphthalene and 90 percent of a variable composition binary mixture of isooctane/decalin. Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 9. Effect of Mixture Composition on Tendency to Soot in Premixed Flames.

The second ternary fuel tested was made by blending a mixture of isooctane/decalin (the ratio was varied) with MeN to yield ternary mixtures which contain a constant 10 percent by volume MeN and 90 percent by volume of the variable isooctane/decalin binary mixture. These data are plotted in Figure 9.

The conclusion from these data is that the addition of a small quantity of a very sooty (e.g., aromatic) fuel to a less sooty (e.g., alkane) fuel results in a disproportionately large increase in the sooting tendency of the fuel blend. In other words, "a little goes a long way." The importance of this characteristic is that small quantities of aromatic fuels such as tetralins and naphthalenes can dominate differences between jet fuel blends in which the major constituents are nearly identical.

Although a mixture rule for premixed flame TSI evaluation has been developed, it is important to note that the sooting tendency of pure compounds in premixed flames has not been as extensively investigated as diffusion flames.* This somewhat limits the usefulness of the mixture rule. Where individual TSIs are not available, the only recourse is to estimate the TSIs of the individual components from their structures or to use an experimental determination of a fuel blend's sooting tendency.

2. Diffusion Flame TSI Mixture Rule

The development of a diffusion flame mixture rule followed the same game plan as for premixed flames. Experimental diffusion flame TSIs for several binary and ternary fuel blends were measured and these values were compared with calculated TSIs using a diffusion flame mixture rule. As shown below, a linear sum of mole fraction weighted pure component TSIs provides a very good estimate of the experimental TSI for a fuel blend.

The diffusion flame burner chosen for this work was the ASTM smoke point wick lamp (Reference 38). This lamp was selected because the ASTM apparatus is standardized and is routinely used to gauge the sooting tendency of jet fuels. To determine the calibration constants, a' and b' in Equation (2), smoke points for 11 previously studied pure compounds were measured. TSIs for these fuels were taken from Calcote and Manos for comparison. A least squares analysis of these data (see Table 1) yields the calibration constants a' = +3.39 and b' = -2.53.

The experimental diffusion flame TSI for a fuel blend is calculated using Equation (2). This equation requires the measured smoke point for the fuel blend, the mole-weighted molecular weight of the fuel blend, and the previously determined calibration constants for the lamp.

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* Almost simultaneously with completion of this program AeroChem completed another study in which extensive data were obtained and are thus now available (Reference 39) for comparison with jet engine performance.

TABLE 1. ASTM WICK LAMP CALIBRATION FUELS

Fuel	MW $g\ mol^{-1}$	Smoke Point mm	TSI (Calcote and Manos, Reference 8)	TSI (This Work)
Isooctane (2,2,4-trimethylpentane)	114	43.5	5.6 ± 0.6	6.3
Toluene	92	7.5	50 ± 2	39.1
Benzene	78	7.8	31 ± 0.5	31.4
p-Cymene	134	7.4	62 ± 22	58.9
1-Methylnaphthalene	142	4.9	89 ± 0	95.7
Ethylbenzene	106	6.7	59 ± 3	51.1
p-Xylene	106	7.6	51 ± 8	44.8
Decalin	138	23.7	13 ± 0.5	17.2
Cyclohexene	82	31.4	5.7 ± 0.5	6.3
1-Decene	140	26.8	6.4 ± 0.8	15.2
Tetralin	132	6.8	56 ± 10	63.3

The diffusion flame mixture rule was empirically determined by evaluating the variation of experimental TSIs for six binary fuel blends. The experimental TSIs for these binary fuel blends are represented by the symbols in Figures 10 and 11. Examination of the data points shows that the experimental TSI varies nearly linearly with variation of the composition. Therefore, a linear sum of mole fraction-weighted fuel component TSIs was evaluated as a mixture rule for diffusion flame TSIs. This equation is:

$$TSI_{mix} = \sum_i X_i \, TSI_i , \tag{5}$$

where TSI_{mix} = mixture rule TSI, X_i = mole fraction of fuel component i, and TSI_i = TSI of pure component i. The solid lines in Figures 10 and 11 were calculated using this mixture rule. There is usually little difference between using mole fraction or volume fraction since the densities of most fuel components are similar, but mole fractions are preferred.

As before, the mixture rule for diffusion flames was further verified by investigating three ternary fuel blends. Two of the three ternary fuel blends were mixtures of various proportions of Fuel A, a 50/50 volume percent mixture of isooctane/decalin, with Fuel B, either tetralin or 1-methylnaphthalene. The results of these experiments are represented by the symbols in Figures 12 and 13; the solid lines were calculated by the mixture rule. The third ternary fuel was a mixture of 10 percent by volume of 1-methylnaphthalene and 90 percent by volume of Fuel B, a variable mixture of isooctane and decalin. The experimental TSI for the ternary blend is plotted against the volume percent of isooctane in Figure 14. Again, the solid line is the mixture rule and the symbols are the experimental TSIs.

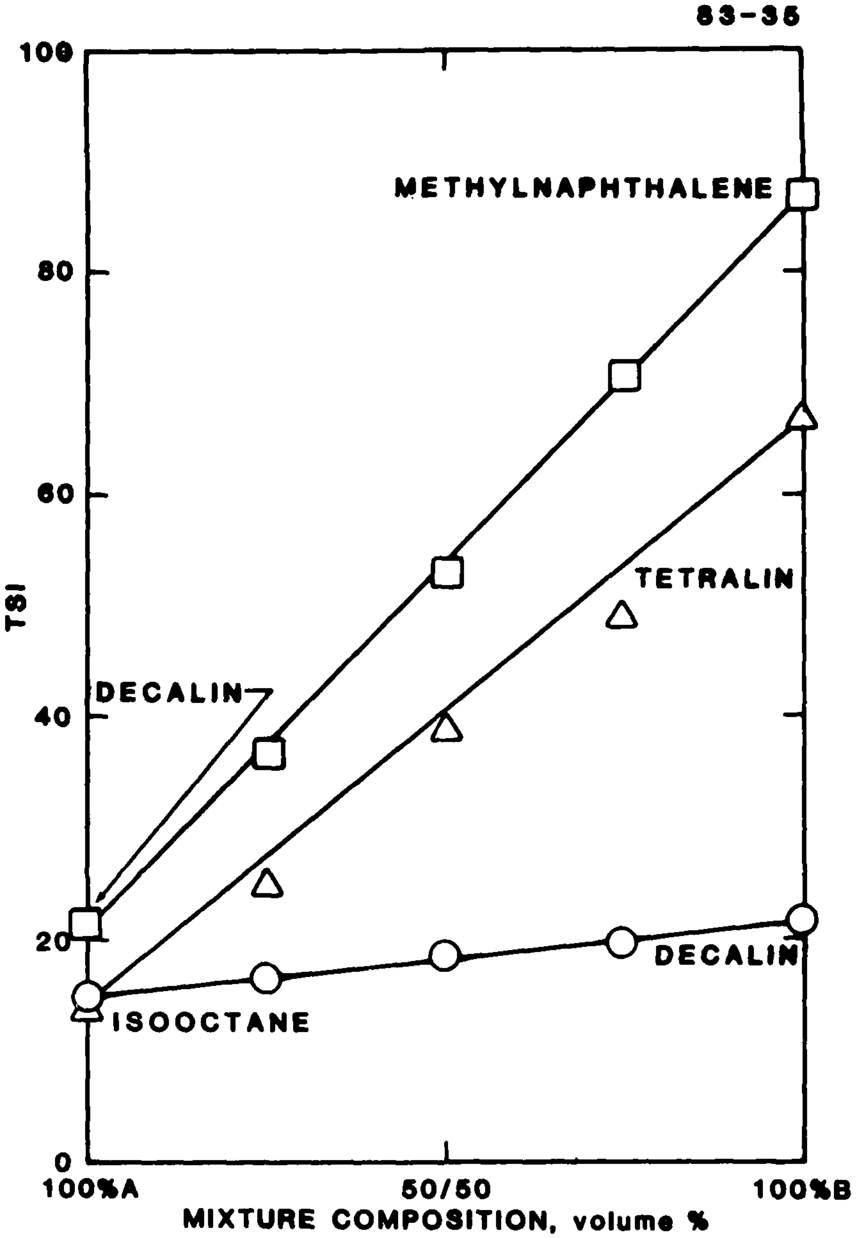


Figure 10. Effect of Binary Mixture Composition on Tendency to Soot in Diffusion Flames

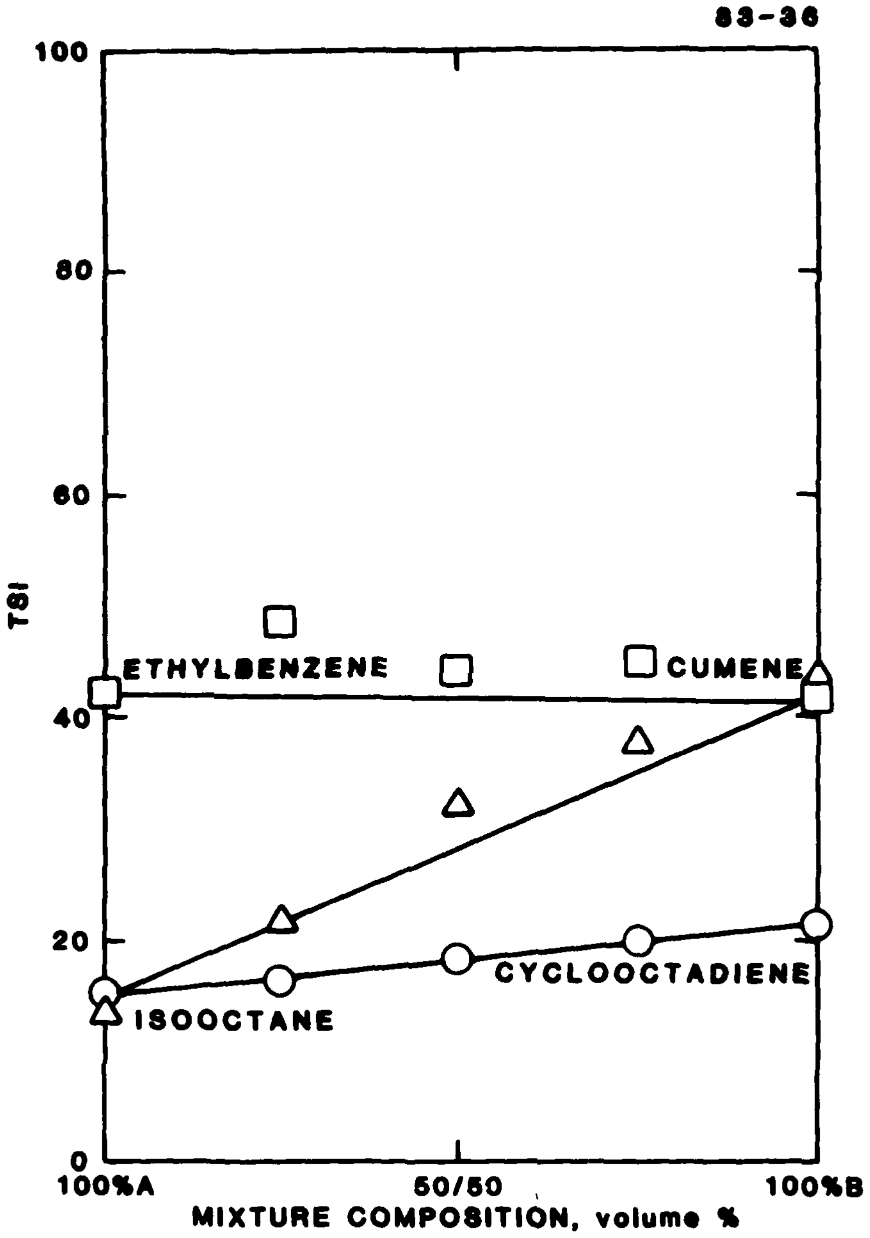
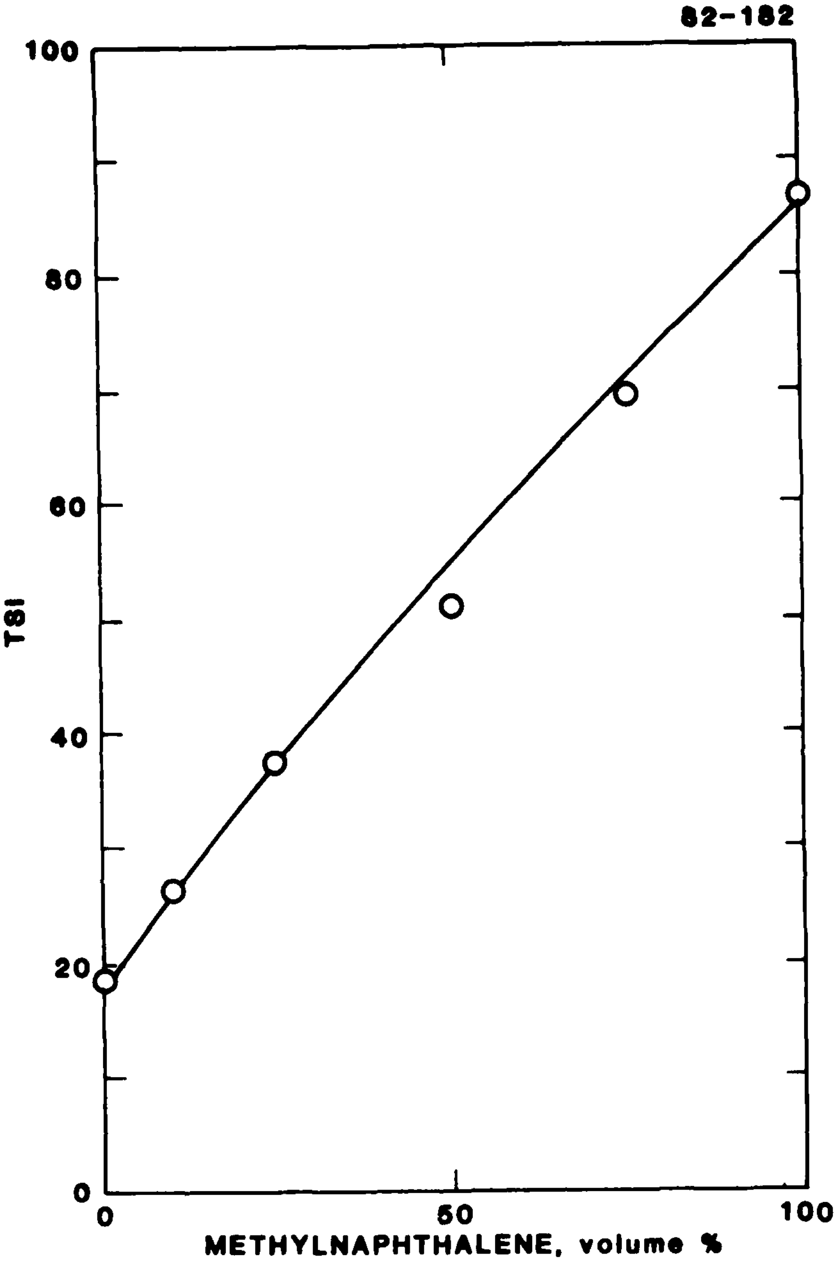
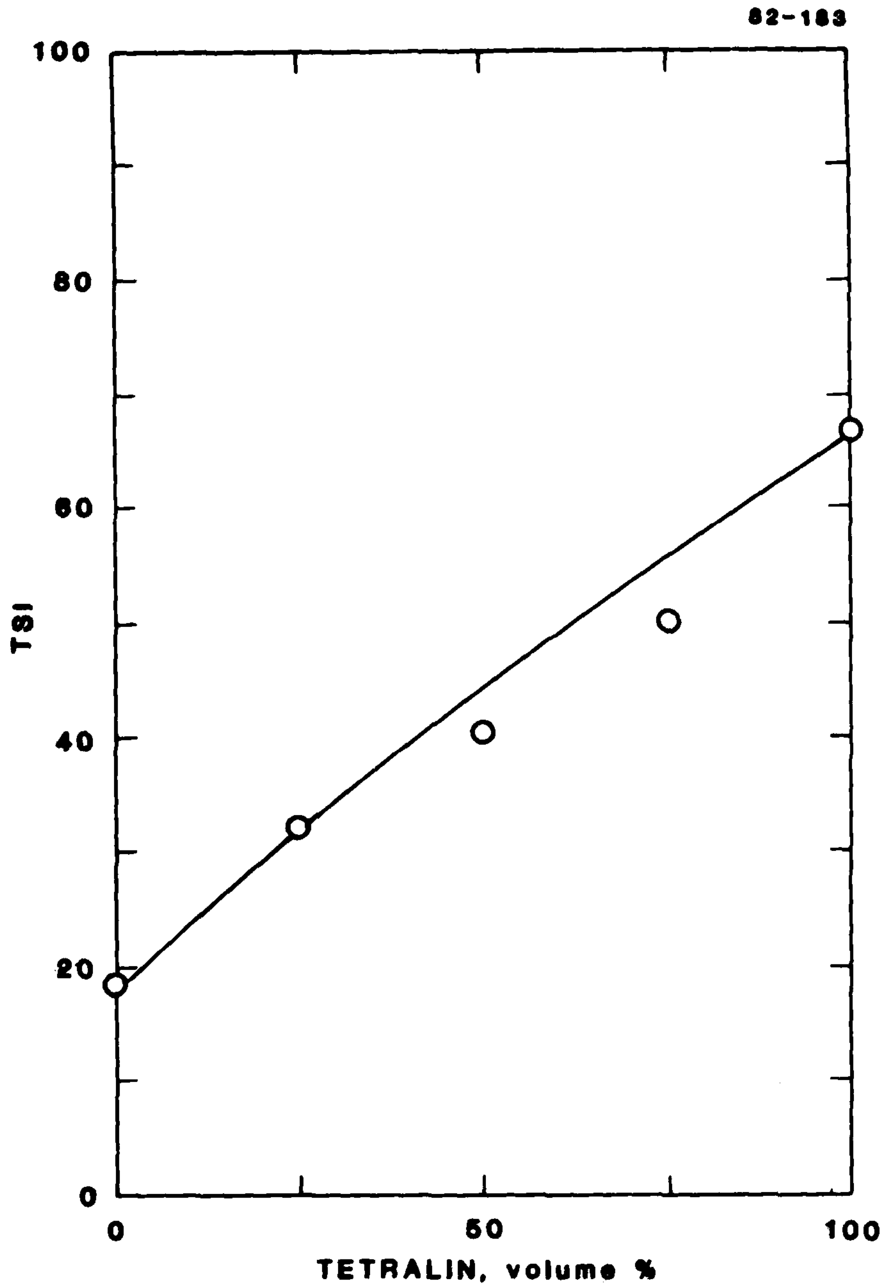


Figure 11. Effect of Binary Mixture Composition on Tendency to Soot in Diffusion Flames.



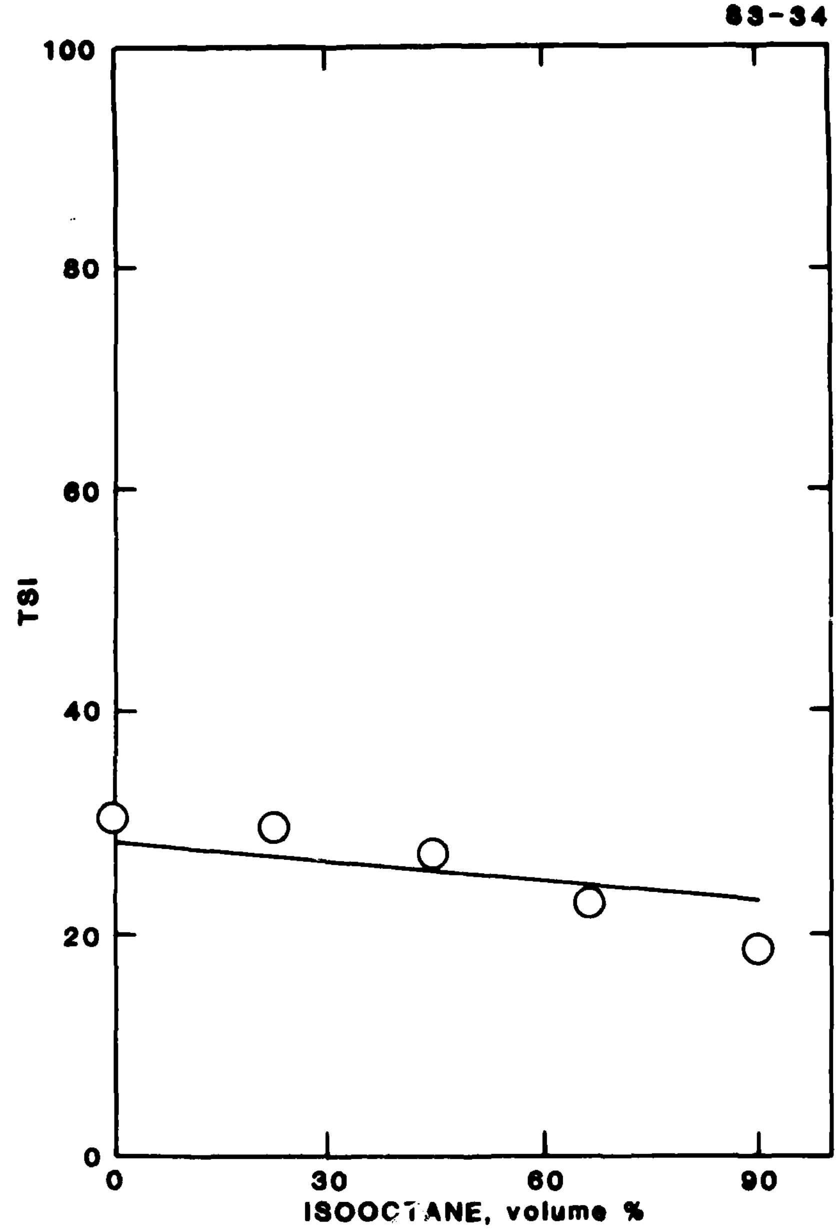
Mixture composed of Fuel A, a binary mixture of isooctane/decalin (50/50, v/v) and Fuel B, 1-methylnaphthalene. Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 12. Effect of Ternary Mixture Composition on Tendency to Soot in Diffusion Flames.



Mixture composed of tetralin and a binary mixture (50/50, v/v, isooctane/decalin). Symbols are experimental TSIs; lines are calculated TSI values using mixing rule.

Figure 13. Effect of Ternary Mixture Composition on Tendency to Soot in Diffusion Flames



Fuel comprised of 10 percent methylnaphthalene and 90 percent of a variable composition binary mixture of isooctane/decalin.

Figure 14. Effect of Mixture Composition on Tendency to Soot in Diffusion Flames.

For the binary and ternary blends tested, the mixture rule appears to provide a reasonable estimate of the experimental TSI values. Thus, if a fuel blend composition is known, its diffusion flame TSI can be reliably estimated using the mixture rule alone. However, for a blend containing components for which the TSI has not been previously reported (Reference 8), the fuel blend's TSI must be determined experimentally by measuring its smoke point. This should not be a serious limitation since diffusion flame TSIs for a large number of compounds have been measured.

B. BENCHMARK TESTS OF TSI MIXTURE RULES

The mixture rules for computing diffusion and premixed flame TSIs were experimentally verified using binary and ternary mixtures. To test the validity of the TSI mixture rules for calculating TSIs for multicomponent fuel blends, samples of analyzed JP-4 and JP-8 jet fuels were obtained from AFWAL, Wright Patterson AFB.* The analysis of these two samples was reported by Smith et al. (Reference 40) who characterized the chemical composition of these fuels by three methods. The ASTM mass spectrometry method (ANSI/ASTM D2789) was used to determine the volume percent of six chemical classes present in the jet fuel (e.g., volume percent alkyl benzenes, volume percent paraffins, volume percent indans and tetralins, etc.). The volume percent of olefins in these samples was determined by the ASTM fluorescent indicator method (ASTM D1319). Lastly, Smith et al. employed capillary column gas chromatography (GC) to measure the weight percent of many individual jet fuel components. Table 2 shows a comparison of the ASTM class analysis with the GC analysis, where the individual components identified by GC have been collected into chemical classes. The agreement is seen to be poor. Thus the fuel composition by chemical classes is highly uncertain.

TABLE 2. CHEMICAL COMPOSITION OF JP-4 AND JP-8 FUEL SAMPLES BY CLASSES

(Reported by Smith et al., Reference 40)

	JP-4		JP-8	
Hydrocarbon Class	ASTM Method Vol. Percent	GC Wt. Percent	ASTM Method Vol. Percent	GC Wt. Percent
Paraffins	61.2	43.2	44.4	25.3
Olefins	1.5	0	2.1	0
Monocyclic Paraffins	24.2	10.7	41.4	3.0
Dicyclic Paraffins	4.9	0	2.6	0
Alkylbenzenes	8.2	12.1	6.7	7.5
Indans/Tetralins	1.1	0	3.4	0
Naphthalenes	0.4	2.1	1.5	6.4
Total	101.5	68.1	102.1	42.2

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* The jet fuel samples were supplied to AeroChem by Major Don Potter of Wright-Patterson AFB, Fuels and Lubrication Branch.

Smith also reported several "physical" properties of these fuels; smoke points were measured with the ASTM Smoke Point Lamp (ANSI/ASTM D1322) and the distillation curve for each fuel was determined using the ASTM method D86.

1. Premixed Flame TSIs

The premixed flame TSIs for the JP-4 and JP-8 samples were obtained from both measured ϕ_c for the samples, using estimated molecular weights, and from composition information, using previously measured pure component TSIs and the premixed flame mixture rule. The mixture rule TSIs were calculated, using both the fuel class analyses and the detailed chemical composition from the GC analyses by Smith et al.

a. Experimental Premixed Flame TSIs. In this series of experiments, the fuel-to-air (mole) ratio at which soot is first observed in a premixed flame was measured for the JP-4 and JP-8 fuel samples. The apparatus was the same as employed in developing the premixed flame mixture rule (see Section IV.A.1). These fuel-to-air ratios were converted to critical equivalence ratios using the estimated molecular weight for the fuel (see below) and the reported hydrogen weight percent. Finally, utilizing the previously determined calibration constants for this burner ($a = 269$ and $b = 118$), the critical equivalence ratios (ϕ_c's) for the JP-4 and JP-8 were converted to experimental premixed TSIs via the equation: $TSI = a - b(\phi_c)$. These TSIs are given in Table 3 under the heading "Premixed Flames: Experimental."

b. Premixed Flame Mixture Rule TSI

(1) Class Analysis TSIs. Premixed flame TSIs were calculated using both the ASTM class analyses and the GC analyses of the jet fuels. The premixed flame class averaged TSIs for JP-4 fuel components are listed in Table 4, along with the range of TSI values for specific components identified in each class. A modified mixture rule was used to calculate the JP-4 and JP-8 TSIs, using the class analysis:

$$(1.1)^{TSI_{mix}} = \sum_{classes} V_j \, (1.1)^{TSI_j}, \qquad (6)$$

where V_j is the volume fraction of fuel class j (Table 2) and TSI_j is the average TSI of fuel class j (Table 4). Volume fractions were used since neither mole fractions nor molecular weights were available. The mixture rule TSIs calculated are presented in Table 3 as "Premixed Flame TSIs, Calculated via Class Analysis."

(2) GC Analysis TSIs. As noted, the GC analysis did not identify all components in the jet fuel samples (i.e., the reported species added up to only 68 percent by weight for JP-4 and 43 percent by weight for JP-8). A modified premixed flame mixture rule was therefore employed to normalize the mole fraction to unity. This mixture rule was:

$$(1.1)^{TSI_{mix}} = \frac{\sum X_i \, (1.1)^{TSI_i}}{\sum X_i}, \qquad (7)$$

TABLE 3. COMPARISON OF EXPERIMENTAL AND CALCULATED THRESHOLD SOOTING INDICES FOR JET FUELS

	TSI	
	JP-4	JP-8
Premixed Flames:		
1. Experimental	60	85
2. Calculated via:		
a. Class Analysis	73	75
b. GC Analysis	79	89
Diffusion Flames:		
1. Experimental		
a. ASTM Lamp	14	33
b. AeroChem Lamp	14	30
2. Calculated via:		
a. Class Analysis	11	12
b. GC Analysis	14	32

TABLE 4. CLASS AVERAGE AND RANGE OF PREMIXED FLAME THRESHOLD SOOTING INDICES FOR JP-4 FUEL COMPONENTS

Hydrocarbon Class	Class Average TSI	Range of TSIs[a]
Paraffins	66	57-70
Olefins	64[b]	---
Monocyclic Paraffins	63	56-70
Dicyclic Paraffins	77[b]	---
Alkylbenzenes	88	79-99
Indans/Tetralins	95[b]	---
Naphthalenes	100	100

[a] This range of TSIs represents the minimum and maximum values of the premixed flame TSI for each identified fuel component in the GC analysis.

[b] Estimated. These fuel components were not identified in the GC analysis.

where X_i is the mole fraction of fuel component i and TSI_i is the premixed flame TSI for fuel component i. This procedure assumes the unidentified fuel components have the same average composition as the identified fuel components. Since the GC analysis identified fuel components, mole fractions were available from the reported weight fractions and an estimated average molecular weight for the JP-4 or JP-8 samples (see Section IV.B.2.a for estimation of molecular weight from distillation data). The identified fuel components of the JP-4 and JP-8 samples are reported in Tables 5 and 6. The final results of the calculations for the mixture rule, premixed flame TSIs are given in Table 3 as "Premixed Flame TSIs, Calculated via GC Analysis."

c. Discussion of Premixed Flame TSIs. The mixture rule TSIs and the experimental TSIs are compared in Table 3. The TSIs calculated using both class analysis and GC analysis are in poor agreement with the experimental TSIs for both fuels. The JP-8 results are, however, considerably better than the JP-4 results. This disagreement is not only the result of inadequate fuel analyses, but also of the fact that the premixed flame TSI mixture rule is sensitive to small errors in the composition of those components which have large TSI values. A more complete and accurate fuel analysis would be necessary to provide better mixture rule estimates of jet fuel TSIs. Furthermore, the premixed flame mixture rule should be refined and improved by obtaining experimental premixed flame TSIs for more complicated fuel blends than the binary and ternary blends used to develop the present form of the mixture rule. Finally, many of the premixed flame TSI values assigned to the fuel components of JP-4 and JP-8 were estimated from the limited literature data on molecular structure vs. TSI trends (Reference 8). The lack of experimental TSIs for pure components and the uncertainty range of TSIs for fuel classes makes the failure to obtain accurate agreement between calculated and observed values hardly surprising.

2. Diffusion Flame TSIs

Diffusion flame TSIs for the two jet fuel samples were estimated using two basic approaches similar to those used for premixed flame TSIs. Experimentally, the smoke points were measured, molecular weights estimated, and the TSIs computed with Equation (2). The other approach combined the results of the chemical analysis and the diffusion flame mixture rule to estimate the TSIs.

a. Experimental Diffusion Flame TSIs. Smoke points for the two analyzed jet fuels were measured on the ASTM lamp. With this apparatus, the JP-4 smoke point (mm) was 28.4 and the JP-8 smoke point was 17.6. The calibration constants for the ASTM lamp were given in Section IV.A.2.

In addition, a custom wick lamp (AeroChem lamp, Reference 39) was used to evaluate the jet fuels' TSIs. With this lamp, the mass consumption rate of fuel ($\dot{m}$, g s^{-1}) is measured at the smoke point. Since the mass consumption rate of fuel in a diffusion flame is, theoretically and experimentally, linearly proportional to the flame height, the diffusion flame definition given earlier (Equation (2)), can be rewritten as:

$$TSI = a'' \frac{MW}{\dot{m}} + b''. \qquad (8)$$

TABLE 5. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-4 SAMPLE

Fuel Component	Weight Percent (Reference 40)	Molecular Weight $g\ mol^{-1}$	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
n-Butane	0.12	58	0.29	1.4	57
Isobutane	0.66	58	1.59	2.2	55[a]
n-Pentane	1.06	72	2.05	1.3	63
2,2-Dimethylbutane	0.10	86	0.17	3.7	62[a]
2-Methylpentane	1.28	86	2.07	2.9	65
3-Methylpentane	0.89	86	1.43	2.8	65[a]
n-Hexane	2.21	86	3.57	2.5	64
Methylcyclopentane	1.16	84	1.92	4.9	56[a]
2,2-Dimethylpentane	0.25	100	0.35	3.6[a]	65[a]
Benzene	0.50	78	0.94	31	80
Cyclohexane	1.24	84	2.06	3.2	70[a]
2-Methylhexane	2.35	100	3.27	3.2	65[a]
3-Methylhexane	1.97	100	2.74	3.2	65[a]
trans-1,3-Dimethylcyclopentane	0.36	98	0.52	6.3[a]	56[a]
cis-1,3-Dimethylcyclopentane	0.34	98	0.48	6.3[a]	56[a]
cis-1,2-Dimethylcyclopentane	0.54	98	0.76	6.3[a]	56[a]
n-Heptane	3.67	100	5.11	2.7	69[a]
Methylcyclohexane	2.27	98	3.23	4.4	70[a]
2,2,3,3-Tetramethylbutane	0.24	114	0.29	7.2[a]	60[a]
Ethylcyclopentane	0.26	98	0.38	4.9[a]	56[a]
2,5-Dimethylhexane	0.37	114	0.45	3.6[a]	65[a]
2,4-Dimethylhexane	0.58	114	0.71	3.6[a]	65[a]
1,2,4-Trimethylcyclopentane	0.25	112	0.30	7.8[a]	56[a]
3,3-Dimethylhexane	0.26	114	0.32	3.6[a]	65[a]
1,2,3-Trimethylcyclopentane	0.25	112	0.30	7.8[a]	56[a]
Toluene	1.33	92	2.02	50	83
2,2-Dimethylhexane	0.71	114	0.86	3.6[a]	65[a]
2-Methylheptane	2.70	114	3.29	3.5	65[a]
4-Methylheptane	0.92	114	1.13	4.0	65[a]
cis-1,3-Dimethylcyclohexane	0.42	112	0.53	7.4[a]	70[a]
3-Methylheptane	3.04	114	3.72	3.7	65[a]

[a] Indicates an estimated TSI value for the component.

TABLE 5. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-4 SAMPLE (CONTINUED)

Fuel Component	Weight Percent (Reference 40)	Molecular Weight g mol^{-1}	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
1-Methyl-3-ethylcyclohexane	0.17	126	0.18	6.2[a]	70[a]
1-Methyl-2-ethylcyclohexane	0.39	126	0.43	6.2[a]	70[a]
Dimethylcyclohexane	0.43	124	0.48	6.2[a]	70[a]
n-Octane	3.80	114	4.63	3.2	72[a]
1,3,5-Trimethylcyclohexane	0.99	126	1.10	7.8[a]	70[a]
1,1,3-Trimethylcyclohexane	0.48	126	0.53	7.8[a]	70[a]
2,5-Dimethylheptane	0.52	128	0.57	5.0[a]	60[a]
Ethylbenzene	0.37	106	0.48	59	92[a]
m-Xylene	0.96	106	0.15	51	91
p-Xylene	0.35	106	0.46	51	91
3,4-Dimethylheptane	0.43	128	0.47	6[a]	70[a]
4-Ethylheptane	0.18	128	0.19	5[a]	70[a]
4-Methyloctane	0.86	128	0.93	5[a]	70[a]
2-Methyloctane	0.88	128	0.96	5[a]	70[a]
3-Methyloctane	0.79	128	0.86	5[a]	70[a]
o-Xylene	1.01	106	1.32	51	91
1-Methyl-4-ethylcyclohexane	0.48	126	0.53	7.4[a]	70[a]
n-Nonane	2.25	128	2.45	4.1	70[a]
Isopropylbenzene	0.30	120	0.35	63	85
n-Propylbenzene	0.71	120	0.82	65[a]	83[a]
1-Methyl-3-ethylbenzene	0.49	120	0.57	60[a]	90[a]
1-Methyl-4-ethylbenzene	0.43	120	0.50	60[a]	90[a]
1,3,5-Trimethylbenzene	0.42	120	0.48	47	99[a]
1-Methyl-2-ethylbenzene	0.23	120	0.27	60[a]	90[a]
1,2,4-Trimethylbenzene	1.01	120	1.16	50[a]	99[a]
n-Decane	2.16	142	2.12	4.3	70[a]
n-Butylcyclohexane	0.70	140	0.69	8[a]	70[a]
1,3-Diethylbenzene	0.46	134	0.47	60	91[a]
1-Methyl-4-propylbenzene	0.40	134	0.41	65[a]	83[a]
1,3-Dimethyl-5-ethylbenzene	0.61	134	0.64	60[a]	91[a]
1-Methyl-2-i-propylbenzene	0.29	134	0.30	65[a]	85[a]
1,4-Dimethyl-2-ethylbenzene	0.70	134	0.73	60[a]	99[a]

TABLE 5. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-4 SAMPLE (CONCLUDED)

Fuel Component	Weight Percent (Reference 40)	Molecular Weight g mol^{-1}	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
1,2-Dimethyl-4-ethylbenzene	0.77	134	0.80	60[a]	99[a]
n-Undecane	2.32	156	2.07	4.3	70[a]
1,2,3,4-Tetramethylbenzene	0.75	134	0.78	50[a]	100[a]
Naphthalene	0.50	128	0.54	100	100[a]
2-Methylundecane	0.64	170	0.53	5.8[a]	70
n-Dodecane	2.00	170	1.65	4.8	70[a]
2,6-Dimethylundecane	0.71	184	0.54	7.2[a]	70[a]
2-Methylnaphthalene	0.56	142	0.55	89	100[a]
1-Methylnaphthalene	0.78	142	0.76	89	100
n-Tridecane	1.52	184	1.15	5.2	70[a]
2,6-Dimethylnaphthalene	0.25	156	0.22	98	100[a]
n-Tetradecane	0.73	198	0.52	5.4	70[a]
Total	68.08		83.19		

TABLE 6. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-8 SAMPLE

Fuel Component	Weight Percent (Reference 40)	Molecular Weight g mol^{-1}	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
n-Heptane	0.03	100	0.05	2.7	69[a]
n-Octane	0.09	114	0.14	3.2	72[a]
1,3,5-Trimethylcyclohexane	0.06	126	0.09	7.8[a]	70[a]
1,1,3-Trimethylcyclohexane	0.06	126	0.09	7.8[a]	70[a]
m-Xylene	0.06	106	0.10	51	91
3-Methyloctane	0.04	128	0.06	5.0	70[a]
2,4,6-Trimethylheptane	0.07	142	0.09	7.3[a]	60[a]
o-Xylene	0.06	106	0.10	51	91
cis-1-Ethyl-3-methylcyclohexane	0.10	126	0.14	7.4[a]	70[a]
n-Nonane	0.31	128	0.44	4.1	70[a]
n-Propylcyclohexane	0.14	126	0.20	7.0[a]	65[a]
1,2,4-Trimethylbenzene	0.27	120	0.41	50[a]	99[a]

[a] Indicates an estimated TSI value for the component.

TABLE 6. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-8 SAMPLE (CONTINUED)

Fuel Component	Weight Percent (Reference 40)	Molecular Weight $g\ mol^{-1}$	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
n-Decane	1.31	142	1.68	4.3	70[a]
n-Butylcyclohexane	0.74	140	0.97	8.0[a]	65[a]
1,3-Dimethyl-5-ethylbenzene	0.62	134	0.84	60[a]	91[a]
1,4-Dimethyl-2-ethylbenzene	0.56	134	0.76	60[a]	91[a]
2-Methyldecane	0.41	156	0.48	5.3[a]	70[a]
1-Ethylpropylbenzene	0.99	148	1.22	75[a]	90[a]
n-Undecane	4.13	156	4.83	4.3	70[a]
2,6-Dimethyldecane	0.66	170	0.71	6.8[a]	70[a]
1,2,3,4-Tetramethylbenzene	1.12	134	1.53	50[a]	100[a]
Naphthalene	1.14	128	1.62	100	100
2-Methylundecane	1.16	170	1.24	5.8[a]	70
n-Dodecane	4.72	170	5.06	4.8	70[a]
1,3,5-Triethylbenzene	0.60	162	0.68	60[a]	99[a]
2,6-Dimethylundecane	2.06	184	2.04	7.2[a]	70[a]
1,2,4-Triethylbenzene	0.99	162	1.11	50[a]	99[a]
n-Hexylcyclohexane	0.93	168	1.01	10[a]	65[a]
2-Methylnaphthalene	1.46	142	1.88	89	100[a]
1-Methylnaphthalene	1.84	142	2.36	89	100
1-Tridecene	0.73	182	0.73	6.6[a]	67[a]
Phenylcyclohexane	0.87	160	0.99	72	87
n-Tridecane	4.43	184	4.39	5.2	70[a]
n-Heptylcyclohexane	1.00	182	1.00	11[a]	65[a]
n-Heptylbenzene	0.25	176	0.26	77[a]	90[a]
Biphenyl	0.63	130	0.89	50[a]	99[a]
1-Ethylnaphthalene	0.33	156	0.39	89[a]	100[a]
2,6-Dimethylnaphthalene	1.34	156	1.57	98	100[a]
n-Tetradecane	2.99	198	2.75	5.4	70[a]
2,3-Dimethylnaphthalene	0.36	156	0.42	98	100[a]

TABLE 6. COMPONENTS AND THRESHOLD SOOTING INDICES FOR JP-8 SAMPLE (CONCLUDED)

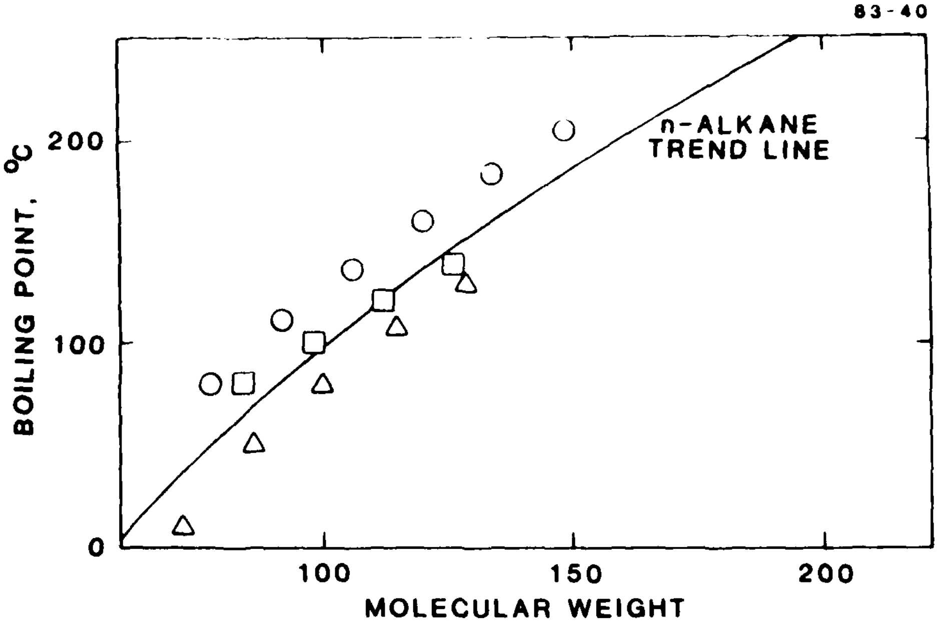
Fuel Component	Weight Percent (Reference 40)	Molecular Weight g mol^{-1}	Mole Percent	Diffusion Flame TSI (Reference 8)	Premixed Flame TSI (Reference 8)
n-Octylbenzene	0.61	190	0.59	80[a]	90[a]
n-Pentadecane	1.61	212	1.38	5.5[a]	70[a]
n-Hexadecane	0.45	226	0.36	5.7[a]	76
n-Heptadecane	0.08	240	0.06	5.8[a]	70[a]
n-Octadecane	0.02	254	0.02	6.0[a]	70[a]
Total	42.43		47.73		

The calibration constants were determined by burning several pure compounds, measuring the mass consumption rate for each fuel at the smoke point, and performing a least-squares fit to the Calcote and Manos diffusion flame TSI values. The calibration constants so determined are (Reference 39): $a'' = 1.09 \times 10^{-4}$ mol s^{-1} and $b'' = 0.28$. The mass consumption rates at the smoke points for the JP-4 and JP-8 fuels on the AeroChem lamp were 1.07×10^{-3} and 0.667×10^{-3} g s^{-1}.

To convert the smoke points, or the mass consumption rates at the smoke points, to experimental diffusion flame TSIs requires one more piece of information, namely, the average molecular weights of the jet fuels, which are almost never reported. Smith et al. did not report the average molecular weights but they did report the distillation curves for the fuels. A rough estimate of the average molecular weight of a hydrocarbon fuel blend can be made using the distillation curve (References 41 and 42).

Inspection of the boiling points for a homologous series of hydrocarbons (e.g., n-alkanes, 1-n-alkylbenzenes, etc) reveals a smooth and monotonic increase as the molecular weight increases. As examples of this, the boiling points of the n-alkanes, 2,2-dimethylalkanes, and a few members of the n-alkane substituted benzenes are given in Figure 15. Branched paraffins and cyclic paraffins have lower boiling points than corresponding n-alkanes containing the same number of carbon atoms. However, the polycyclic hydrocarbons, indans, tetralins, and decalins have higher boiling points than the corresponding n-alkanes with the same number of carbon atoms.

A typical jet fuel contains considerable amounts of all these hydrocarbon types, but the largest fraction of its composition is comprised of paraffins. Therefore, the correlation between the boiling point and molecular weight for the n-alkanes was used to estimate the molecular weight for each jet fuel distillation fraction. The following equation was fitted to the n-alkane homologous series: boiling point (°C) = $-974 + 234 \ln(MW)$. The overall molecular weight of the jet fuel was then calculated by summing the volume fraction weighted molecular weights of the distillation fractions. The estimated average molecular weight of JP-4 is thus 140 and of JP-8, 180 g mol^{-1}.



△ 2,2 dimethyl substituted n-alkanes; ○ n-alkane substituted benzenes; □ multiple methyl substituted cyclohexanes

Figure 15. Variation of Boiling Point (°C) with Fuel Molecular Weight for Homologous Series.

Experimental diffusion flame TSIs were then calculated. The ASTM lamp smoke points yielded a TSI = 14 for JP-4 and a TSI = 33 for the JP-8. The AeroChem lamp estimates a TSI = 14 for JP-4 and a TSI = 30 for JP-8. These TSIs are tabulated under "Diffusion Flames: Experimental" in Table 3.

b. Mixture Rule Diffusion Flame TSIs

(1) Class Analysis TSIs. The fuel class compositions, determined by the ASTM mass spectrometry method and the ASTM fluorescent indicator method, provide one way to calculate the jet fuel diffusion flame TSIs. The mixture rule was used in the form:

$$\mathrm{TSI} = \sum_i V_i \, \mathrm{TSI}_i, \tag{9}$$

where now V_i is the volume fraction of the hydrocarbon class and TSI_i is the average TSI for the hydrocarbon class. The substitution of volume fractions for mole fractions in the mixture rule introduced some uncertainty in the TSI values. This substitution was necessary because only volume fractions were reported in the mass spectrometric analysis of the jet fuel by the ASTM method (Table 2). In a few cases, it was verified that the TSIs calculated using volume fractions for binary and ternary fuel blends (the blends of Section IV.A.2) were within 3-5 percent of the mole fraction weighted value.

The average TSI for each hydrocarbon class was found by averaging the TSI values for all individual fuel components identified in the GC analysis of JP-4 which were members of the fuel class. The same class-averaged TSI values were used to calculate the JP-8 diffusion flame TSI by the "class" mixture rule. The class-averaged diffusion flame TSIs for the JP-4 sample are listed in Table 7. The JP-4 and JP-8 mixture rule TSIs calculated using the class analyses are found in Table 3 under "Diffusion Flames: Calculated via Class Analysis."

TABLE 7. CLASS AVERAGE AND RANGE OF DIFFUSION FLAME THRESHOLD SOOTING INDICES FOR JP-4 FUEL COMPOUNDS

Hydrocarbon Class	Class Average TSI	Range of TSIs[a]
Paraffins	3.5	1.4-5.4
Olefins	4.9[b]	---
Monocyclic Paraffins	5.7	5-8
Dicyclic Paraffins	13[b]	---
Alkylbenzenes	54	31-65
Indans/Tetralins	73[b]	---
Naphthalenes	93	89-100

[a] This range of TSIs represents the minimum and maximum values of the premixed flame TSI for each identified fuel component in the GC analysis.

[b] Estimated. These fuel components were not identified in the GC analysis.

(2) GC Analysis TSIs. The mixture rule for calculating the diffusion flame TSI for a fuel blend was given in Section IV.A.2. The gas chromatographic analysis of the jet fuels was incomplete; only 0.84 mole fraction of the JP-4 components and 0.48 mole fraction of the JP-8 components were accounted for. Thus a modified form of the mixture rule (Equation (2)) was employed. This form is:

$$TSI_{mix} = \frac{\sum x_i TSI_i}{\sum x_i} . \qquad (10)$$

Physically, this equation assumes that the unidentified fuel components are identical to the identified fuel components and present in the same proportion. The weight percents, mole percent, and diffusion flame TSIs for the identified components of the JP-4 and JP-8 are listed in Tables 5 and 6, respectively. The TSIs for the JP-4 and JP-8 using the GC analysis and the last relationship are listed under "Diffusion Flames: Calculated via GC Analysis" in Table 3.

c. Discussion of Diffusion Flame TSIs. The criterion used to judge the success of the TSI mixture rule was that it reproduce the experimental TSI values for the JP-4 and JP-8 fuels. Experimental TSI values for each fuel measured using the two apparatuses are nearly identical (Table 3). The modified (Equation (9)) mixture rule TSI using the fuel composition determined by GC analysis reproduces the experimental TSI value for both fuels. The class analysis TSI value for JP-4 is ≈ 20 percent low (11 vs. 14) and the class analysis TSI for JP-8 is ≈ 60 percent low (12 vs. 32).

Two sources of error can account for inaccuracies in mixture rule TSIs using the class analysis fuel composition. First, the TSI calculation was based on the assumption that the reported class analysis was correct. For the JP-8 fuel, the GC analysis indicated that at least 5.3 percent of the fuel was naphthalenes whereas the ASTM class analysis for naphthalenes gave 1.5 percent (Table 2). This raises the question of the reliability of the class analysis reported by Smith et al. (Reference 40). The second and possibly major source of error can be the fact that, for a given fuel class (e.g., paraffins, alkylbenzenes , naphthalenes, etc.), a large range of TSI values can be assigned to its members. This makes the assignment of an average TSI value to an individual fuel class somewhat arbitrary. The range of diffusion flame TSI values for the members of the fuel classes is listed in Table 7.

The "accuracy" of the mixture rule is highly dependent upon the completeness of the fuel composition analysis. Based on the comparison of the experimental and mixture rule TSI values (for diffusion flames), a class analysis is a very poor substitute for a gas chromatographic analysis of a jet fuel containing 100 or more components.

C. CORRELATIONS OF SMOKE-RELATED ENGINE PERFORMANCE

The goal of this program was to find better methods of correlating laboratory measures of fuel sooting tendencies to smoke-related engine tests. To provide a fair comparison of these correlations, each of the laboratory measurements of sooting tendency (see Section II.B), was correlated to a smoke-related engine performance parameter (SREPs; see Section II.A for discussion) measured for each fuel under one engine operating condition (i.e., either idle, cruise, dash, or takeoff). We are interested in the influence of fuel composition on SREPs rather than the effects of engine operating conditions, although, of course, these affect the SREPs (Reference 43).

1. Threshold Sooting Indices

Very little compositional information was found in the reports of the engine testing programs. It was thus impossible to calculate experimental premixed flame TSIs since ϕ_C was not reported for the fuels tested. An experimental diffusion flame TSI was calculated from reported ASTM smoke points, using the a' and b' calibration constants obtained in this program and estimating the molecular weights from the reported distillation curves.

The mixture rules were employed to the extent possible to calculate TSIs from the fuel composition. However, the fuel composition was not determined by GC analysis; rather, only the ASTM class analyses were given. As noted earlier, the fuel composition determined by class analysis provides a very poor basis for calculating mixture rule TSIs. Thus it can immediately be recognized that insufficient data are available for good correlations with TSIs.

The threshold sooting indices used in the correlations were therefore limited to: (1) the experimental diffusion flame TSI based on the ASTM smoke point, TSI_{exp}; (2) the mixture rule diffusion flame TSI using the class analysis, TSI_{df}; and (3) the mixture rule premixed flame TSI using the class analysis, TSI_{pf}. These TSIs were calculated using the identical methods used for the JP-4 and JP-8 samples (see Section IV.B). The fuel parameters, TSIs, and molecular weights estimated for the fuels used in the J79 and F101 engine testing programs of Gleason et al. (References 17 and 37) are listed in Table 8. The fuel parameters estimated for the TF-41 engine testing program of Vogel et al. (Reference 18) are listed in Table 9.

2. Nomenclature

The large number of laboratory sooting tendency parameters that can be correlated to the smoke-related engine test parameters leads to a communication difficulty. For brevity, as well as clarity, the abbreviations listed in the Glossary of Terms will be used to communicate our findings.

3. Sources of Engine Test Data

Section III.D gives the rationale for selecting engine test data. As a result of this process, smoke-related engine test data were taken from three recent fuel effects engine test programs for detailed study. The turbojet J79 engine and the fan-assisted turbojet F101 engine test data were taken from Gleason, et al. (References 17 and 37). The turbofan TF-41 engine test data were taken from Vogel et al. (Reference 18). For all three engines, measurements were made of the SAE Smoke Number (SN) measured at the combustor exit and the maximum combustor liner temperature rise (LTR, units K) above the air inlet temperature. For the J79 engine, the radiation flux (RF, units kW m^{-2}), measured through an optical access port, and the Smoke Emission Index (EI_s, units g kg^{-1}), were also reported. For the J79 and F101 engine data the operating conditions of: idle, subsonic cruise, takeoff, and supersonic dash in this work were referred to in the report of Gleason et al. as the data taken at Test Points 3, 5, 7, and 9, respectively. For the TF-41 engine, the test results were reported under the titles of operating conditions.

4. Functional Form of Correlations

The correlations between the SREPs and the fuel or engine operating parameters were of the linear form: $y = a + bx$. That is, for a single operating condition (idle, cruise, dash, or takeoff), the y values (y = SN, LTR, RF, or EI_s) measured for the fuel set were correlated to either the properties of the fuels tested (x = H%; SP; SP^{-1}; AR%; PCAH; H/C; C/O; TSI_{exp}; TSI_{df}; or TSI_{pf}) or to the actual engine operating conditions employed for testing each individual fuel (x = F/A; inlet air temperature at combustor, K; or inlet air pressure to combustor, kPa). The latter three independent variables were correlated against SREPs to determine if the operating conditions were truly held constant during the measurement of a single SREP for the entire fuel set.

The linear fits were not the only functional forms of fitting equations considered. Some preliminary efforts were made to explore other forms such as logarithmic ($y = a \ln(bx)$), exponential ($y = a e^{bx}$), and some multiparameter linear forms. In all cases, the alternate fitting functions were only either as good or worse than the linear, one-parameter functional form.

TABLE 8. ESTIMATED FUEL PARAMETERS FOR JET FUELS USED IN J79 AND F101 TEST PROGRAMS

Fuel No.[a]	Fuel Description	MW	H%[b]	SP,[b] mm	TSI_{exp}	TSI_{df}	TSI_{pf}
1	JP-4	139	14.5	32.5	12	11	74
2	JP-8	179	14.0	26.5	20	13	76
3	JP-8 + GMSO[c]	184	13.9	24.3	23	12	75
4	JP-8 + 2040[d]	179	12.0	12.5	46	37	89
5	JP-8 + Xylene Bottoms[e]	165	13.0	20.5	25	21	79
6	JP-8 + Xylene Bottoms	157	12.0	13.5	37	30	82
7	JP-8 + 2040	178	13.0	17.0	33	23	83
8	JP-4 + 2040	154	12.0	12.0	41	35	88
9	JP-4 + 2040	149	13.0	15.0	31	24	84
10	JP-4 + Xylene Bottoms	136	12.0	13.0	33	31	83
11	JP-4 + Xylene Bottoms	138	13.0	18.0	24	23	80
12	JP-4 + 2040 + Xylene Bottoms	153	14.0	25.0	18	13	75
13	Diesel Fuel Oil No. 2	211	13.1	18.0	37	18	80

[a] Fuel numbers used in the engine test reports of Gleason et al. (References 17 and 37).

[b] Measured by Gleason et al. (References 17 and 37). All other fuel parameters listed were estimated or calculated in this work.

[c] GMSO = Gulf Mineral Seal Oil, a high paraffin content fuel blending agent.

[d] 2040 = 2040 Solvent, a high naphthalenes content fuel blending agent.

[e] Xylene Bottoms = a high monocyclic aromatic hydrocarbon, fuel blending agent.

TABLE 9. ESTIMATED FUEL PARAMETERS FOR JET FUELS USED IN TF-41 TEST PROGRAM

Fuel No.[a]	Fuel Description	MW	H% [b]	SP[b] mm	TSI_{exp}	TSI_{df}	TSI_{pf}
1	JP-4	133	14.4	38.0	9	10	72
2	JP-4 + 2040[c]	161	12.0	12.0	43	36	89
3	JP-4 + 2040	146	12.9	14.0	33	25	85
4	JP-4 + Xylene Bottoms[d]	137	11.9	11.0	40	33	83
5	JP-4 + Xylene Bottoms	145	13.0	14.0	33	23	80
6	JP-4 + Xylene Bottoms + GMSO[e]	150	13.9	23.0	20	14	75
7	JP-8	178	13.9	24.0	23	13	76
8	JP-8 + 2040	176	11.9	12.0	47	35	88
9	JP-8 + 2040	175	12.9	16.0	35	24	84
10	JP-8 + Xylene Bottoms	164	12.0	12.0	44	31	83
11	JP-8 + Xylene Bottoms	170	12.9	18.0	30	22	80
12	JP-8 + GMSO	186	13.9	25.0	23	13	76

[a] Fuel numbers used in the engine test report of Vogel et al. (Reference 18).

[b] Fuel parameters reported by Vogel et al. (Reference 18). All other fuel parameters listed were estimated or calculated in this work.

[c] 2040 = Solvent, a high naphthalenes content fuel blending agent.

[d] Xylene Bottoms = a high monocyclic aromatic hydrocarbon fuel blending agent.

[e] GMSO = Gulf Mineral Seal Oil--a high paraffin content fuel blending agent.

5. Goodness-of-Fit Criterion

The degree to which a fuel parameter or engine operating condition is successful in correlating the engine test data for a given operating condition is measured by the magnitude of the correlation coefficient, R (Reference 44). In the tables, the value of R^2 is given because it ranges from 0 to +1. If $R^2 = 0$ the x parameter is not related to the y parameter. If $R^2 = 1$, the x parameter is "perfectly" related to the y parameter.

To graphically illustrate the meaning of R^2, the linear correlations of maximum liner temperature rise (LTR; J79 engine data) to TSI_{df}, TSI_{exp}, and F/A are shown in Figures 16-18, respectively. The values of R^2 are 0.90, 0.67, and 0.23, respectively, for the linear correlations (solid lines) to the individual data points obtained for the fuels tested under cruise conditions. It is clear that the larger values of R^2 are indicative of the ability of the x parameter, as employed in the linear fitting equation, to correlate the actual measured value of the LTR. Although the engine operating conditions were supposedly held constant for each fuel tested under cruise conditions, it is apparent from the abscissa of Figure 18 that the fuel-to-air ratio was varied somewhat (F/A = 13.0 to 14.2) between the fuel tests. It should thus be apparent why SREP data were also fitted to engine operating condition parameters.

6. Results and Discussion of Correlations

The results of the correlation tests are summarized in Tables 10-17. Rather than individually discuss the voluminous amount of information contained in these tables, it is more instructive to compare the results for each set

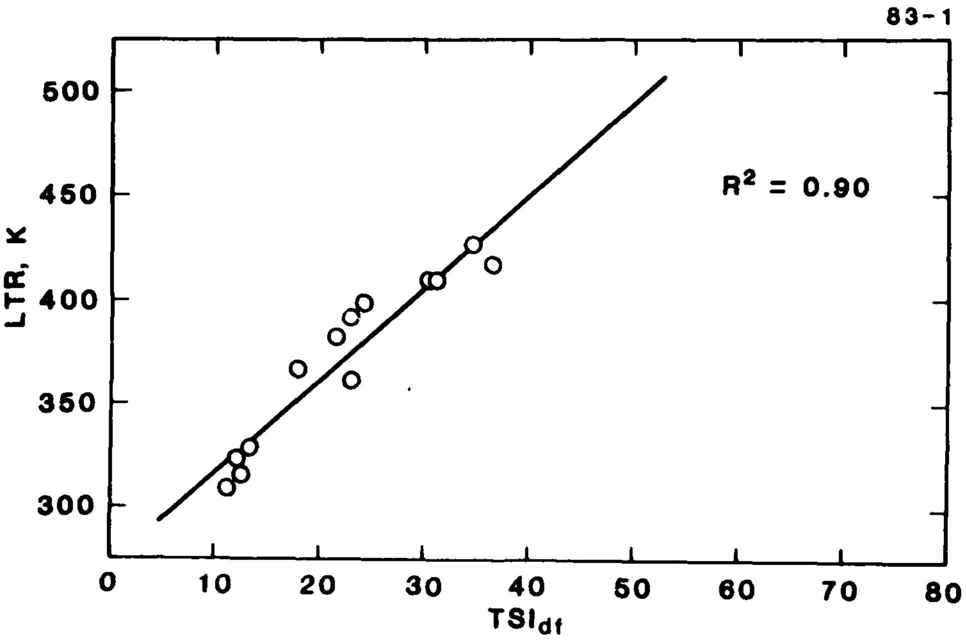


Figure 16. Linear Correlation of Maximum Liner Temperature Rise to Mixture Rule Diffusion Flame TSI for J79 Engine at Cruise Conditions

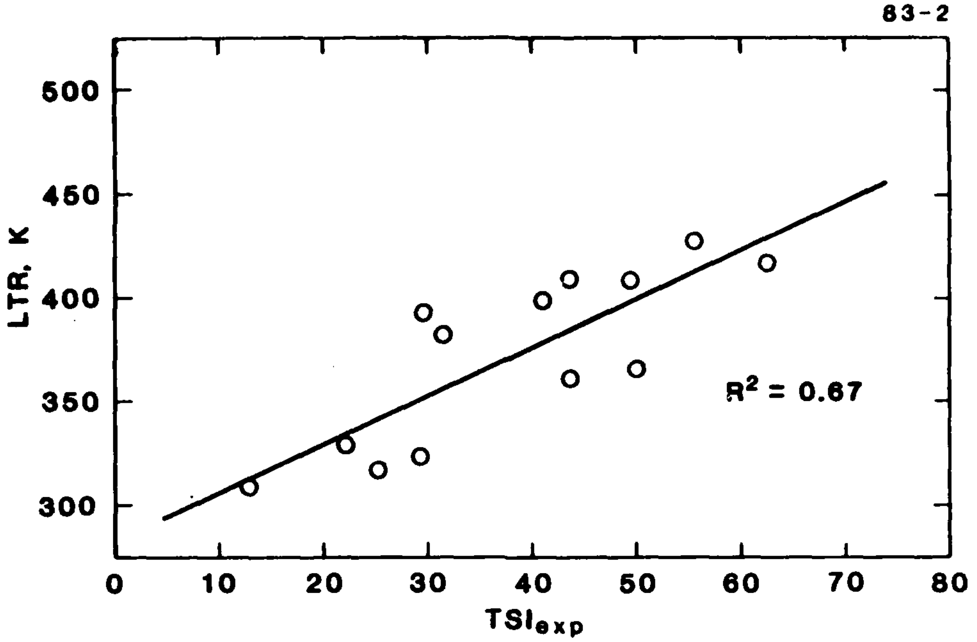


Figure 17. Linear Correlation of Maximum Liner Temperature Rise to Experimental Diffusion Flame TSI for J79 Engine at Cruise Conditions

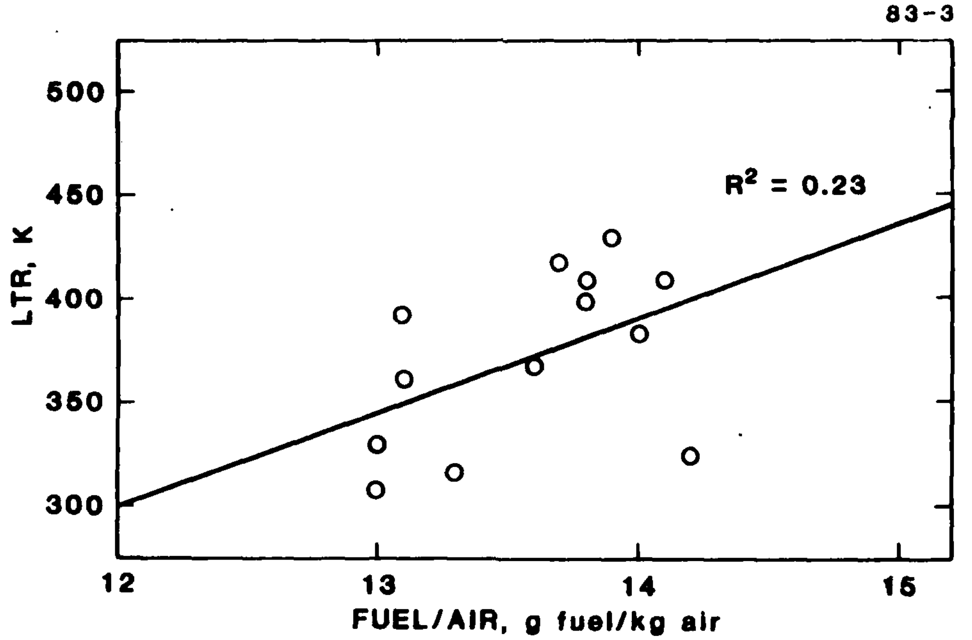


Figure 18. Linear Correlation of Maximum Liner Temperature Rise to Fuel-to-Air Ratio for J79 Engine at Cruise Conditions

TABLE 10. SMOKE NUMBER (SN) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR J79 TURBOJET ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$[a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.87	0.93	0.37	0.04	0.55	*
SP	0.88	0.95	0.48	0.02	0.58	**
SP^{-1}	0.81	0.93	0.52	0.03	0.57	*
AR%	0.67	0.74	0.26	0.16	0.46	
PCAH	0.17	0.30	0.26	0.16	0.22	
H/C	0.87	0.93	0.37	0.04	0.55	*
TSI_{exp}	0.67	0.74	0.29	0.00	0.43	
TSI_{df}	0.74	0.89	0.39	0.01	0.51	*
TSI_{pf}	0.67	0.83	0.46	0.01	0.49	*
C/O	0.07	0.32	0.11	0.05	0.14	
Engine:						
Inlet Temperature	0.00	0.01	0.05	0.14	0.05	
Inlet Pressure	0.08	0.04	0.08	0.00	0.05	
F/A	0.01	0.14	0.05	0.04	0.06	

[a] Average correlation coefficient.

[b] ** = Best average correlation.
* = 85% of best average correlation.

TABLE 11. SMOKE NUMBER (SN) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR F101 ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$ [a]	Rating[b]
	Idle	Cruise	Dash	Takeoff		
Fuel:						
H%	0.56	0.44	0.05	0.61	0.42	
SP	0.58	0.41	0.06	0.58	0.41	
SP^{-1}	0.48	0.46	0.08	0.61	0.41	
AR%	0.37	0.19	0.00	0.34	0.23	
PCAH	0.26	0.60	0.34	0.37	0.39	
H/C	0.56	0.44	0.05	0.61	0.42	
TSI_{exp}	0.52	0.60	0.19	0.73	0.51	**
TSI_{df}	0.55	0.56	0.10	0.62	0.46	*
TSI_{pf}	0.59	0.63	0.14	0.63	0.50	*
C/O	0.15	0.42	0.07	0.24	0.22	
Engine:						
Inlet Temperature	0.01	0.01	0.02	0.18	0.06	
Inlet Pressure	0.21	0.01	0.04	0.02	0.07	
F/A	0.00	0.32	0.06	0.02	0.10	

[a] Average correlation coefficient.

[b] ** = Best average correlation.

* = 85% of best average correlation.

TABLE 12. SMOKE NUMBER (SN) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR TF-41 ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$[a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.77	0.28	0.27	0.52	0.46	**
SP	0.61	0.18	0.28	0.32	0.35	
SP^{-1}	0.75	0.31	0.25	0.52	0.46	**
AR%	0.59	0.28	0.24	0.41	0.38	
PCAH	0.28	0.04	0.02	0.12	0.12	
H/C	0.77	0.28	0.27	0.52	0.46	**
TSI_{exp}	0.77	0.32	0.21	0.44	0.44	*
TSI_{df}	0.80	0.28	0.23	0.51	0.46	**
TSI_{pf}	0.70	0.22	0.24	0.43	0.40	*
C/O	0.30	0.15	0.32	0.40	0.29	
Engine:						
Inlet Temperature	0.04	0.07	0.08	0.01	0.05	
Inlet Pressure	0.00	0.02	0.16	0.09	0.07	
F/A	0.16	0.07	0.30	0.25	0.20	

[a] Average correlation coefficient.

[b] ** = Best average correlation.

* = 85% of best average correlation.

TABLE 13. MAXIMUM LINER TEMPERATURE RISE (LTR) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR J79 TURBOJET ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$ [a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.61	0.92	0.72	0.63	0.72	**
SP	0.73	0.89	0.65	0.61	0.72	**
SP^{-1}	0.66	0.90	0.59	0.51	0.67	*
AR%	0.41	0.74	0.56	0.49	0.55	
PCAH	0.16	0.31	0.13	0.10	0.18	
H/C	0.62	0.92	0.72	0.63	0.72	**
TSI_{exp}	0.52	0.67	0.60	0.46	0.56	
TSI_{df}	0.49	0.90	0.63	0.51	0.63	*
TSI_{pf}	0.51	0.81	0.48	0.41	0.55	
C/O	0.03	0.43	0.58	0.91	0.49	
Engine:						
Inlet Temperature	0.00	0.04	0.00	0.14	0.05	
Inlet Pressure	0.13	0.07	0.11	0.06	0.09	
F/A	0.00	0.23	0.45	0.82	0.38	

[a] Average correlation coefficient.

[b] ** = Best average correlation.

* = 85% of best average correlation.

TABLE 14. MAXIMUM LINER TEMPERATURE RISE (LTR) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR F101 ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$ [a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.37	0.24	0.33	0.42	0.34	*
SP	0.46	0.21	0.20	0.27	0.29	
SP^{-1}	0.31	0.31	0.25	0.34	0.30	
AR%	0.34	0.07	0.19	0.31	0.23	
PCAH	0.03	0.35	0.12	0.13	0.16	
H/C	0.38	0.24	0.33	0.41	0.34	*
TSI_{exp}	0.25	0.37	0.41	0.40	0.36	*
TSI_{df}	0.28	0.28	0.32	0.42	0.33	*
TSI_{pf}	0.27	0.29	0.24	0.28	0.27	
C/O	0.03	0.35	0.63	0.49	0.38	**
Engine:						
Inlet Temperature	0.00	0.03	0.00	0.03	0.02	
Inlet Pressure	0.22	0.01	0.36	0.15	0.19	
F/A	0.04	0.31	0.62	0.26	0.31	

[a] Average correlation coefficient.

[b] ** = Best average correlation.

* = 85% of best average correlation.

TABLE 15. MAXIMUM LINER TEMPERATURE RISE (LTR) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR TF-41 ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$[a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.12	0.19	0.47	0.45	0.31	*
SP	0.12	0.10	0.23	0.19	0.16	
SP^{-1}	0.09	0.13	0.35	0.39	0.24	
AR%	0.01	0.02	0.18	0.37	0.15	
PCAH	0.19	0.37	0.62	0.21	0.35	*
H/C	0.11	0.19	0.47	0.44	0.30	
TSI_{exp}	0.15	0.26	0.44	0.31	0.29	
TSI_{df}	0.13	0.21	0.55	0.49	0.35	*
TSI_{pf}	0.16	0.27	0.60	0.40	0.36	**
C/O	0.15	0.26	0.51	0.43	0.34	*
Engine:						
Inlet Temperature	0.03	0.02	0.00	0.03	0.02	
Inlet Pressure	0.14	0.09	0.01	0.05	0.07	
F/A	0.14	0.24	0.45	0.33	0.29	

[a] Average correlation coefficient.

[b] ** = Best average correlation.

* = 85% of best average correlation.

TABLE 16. SOOT EMISSION INDEX (EI_s) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR J79 TURBOJET ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$[a]	Rating[b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.82	0.92	0.29	0.04	0.52	*
SP	0.73	0.85	0.35	0.07	0.50	*
SP^{-1}	0.78	0.94	0.41	0.09	0.56	**
AR%	0.76	0.81	0.26	0.00	0.46	
PCAH	0.13	0.29	0.13	0.60	0.29	
H/C	0.82	0.92	0.29	0.04	0.52	*
TSI_{exp}	0.53	0.67	0.16	0.14	0.38	
TSI_{df}	0.74	0.94	0.30	0.13	0.53	*
TSI_{pf}	0.58	0.79	0.30	0.30	0.49	*
C/O	0.05	0.34	0.16	0.00	0.14	
Engine:						
Inlet Temperature	0.03	0.02	0.04	0.30	0.10	
Inlet Pressure	0.06	0.04	0.06	0.00	0.04	
F/A	0.00	0.16	0.10	0.02	0.07	

[a] Average correlation coefficient.

[b] ** = Best average correlation.
 * = 85% of best average correlation.

TABLE 17. RADIATION FLUX (RF) CORRELATIONS TO FUEL AND ENGINE PARAMETERS FOR J79 TURBOJET ENGINE

Correlating Parameters	Correlation Coefficient (R^2)				$\overline{R^2}$ [a]	Rating [b]
Fuel:	Idle	Cruise	Dash	Takeoff		
H%	0.14	0.36	0.21	0.23	0.24	
SP	0.20	0.42	0.41	0.38	0.35	
SP^{-1}	0.14	0.48	0.37	0.39	0.35	
AR%	0.03	0.11	0.04	0.04	0.06	
PCAH	0.53	0.85	0.80	0.93	0.78	**
H/C	0.14	0.36	0.21	0.23	0.24	
TSI_{exp}	0.22	0.71	0.46	0.56	0.49	
TSI_{df}	0.24	0.56	0.36	0.42	0.40	
TSI_{pf}	0.44	0.72	0.68	0.71	0.64	
C/O	0.04	0.06	0.25	0.02	0.09	
Engine:						
Inlet Temperature	0.25	0.36	0.05	0.02	0.17	
Inlet Pressure	0.27	0.52	0.17	0.01	0.24	
F/A	0.07	0.20	0.03	0.00	0.08	

[a] Average correlation coefficient.

[b] ** = Best average correlation.
* = 85% of best average correlation.

of SN, LTR, RF, and EI_s collectively. The Smoke Number correlations (Tables 10-12) reveal that the fuel parameters H%, SP, SP^{-1}, H/C,* or any TSI, are equally good (or equally poor) predictors of the SN measured under a given operating condition. This can best be seen in the averaged correlation coefficients, $\overline{R^2}$, for each fuel parameter in each table. Also shown are relative ratings in terms of the best average correlation and 85 percent of the best $\overline{R^2}$. Further inspection of the Smoke Number correlations shows that, for one or two of the operating conditions (dash or takeoff) of each engine type, all fuel parameters correlated poorly with the measured SN values.

The maximum liner temperature rise (LTR) for the J79, F101, and TF-41 engines is poorly correlated to the fuel parameters (Tables 13, 14, and 15, respectively). For these engines, the correlation with F/A ratio (an engine operating condition) is almost as good as the correlation with the best fuel parameters. For the J79 engine (Table 13), under any given operating conditions, the fuel parameters H%, SP, SP^{-1}, or TSIs correlate fairly well with the measured LTR values (i.e., R^2's are > 0.5).

The Smoke Emission Index (EI_s), as calculated for the J79 engine (Table 16), correlates well with the fuel parameters H%, SP, SP^{-1}, or TSIs under idle or cruise conditions. No fuel parameter correlates to EI_s under dash operation, but the PCAH is the single fuel parameter which correlates well with EI_s under takeoff conditions. Engine parameters correlate poorly to the Smoke Emission Index under all operating conditions.

Finally, the radiation flux data for Fuels 2-7 and 9 of the J79 engine test data, Table 17, are best correlated to the PCAH content of the fuels; only one other parameter comes close. The TSI_{pf} fuel parameter gives only a good RF correlation.

It is interesting to further consider the data in Tables 10 through 17 in an attempt to quantify and rank the relative usefulness of the fuel parameters in correlating the engine data. To do this, we rate each fuel parameter considering only those correlations where R^2 is at least 85 percent of the best R^2 for a given test.

To evaluate fuel parameters' overall ability to correlate all of the SREPs at all of the operating conditions (idle, cruise, dash, and takeoff) we use the $\Sigma \overline{R^2}$ values from Tables 10 through 17 and the number of times (out of a possible eight) that any particular fuel parameter had $\overline{R^2} \geq 85$ percent of the best $\overline{R^2}$. The results are summarized in Table 18. TSI_{df} and H% are the best correlating parameters, "useful" in seven and six instances (out of eight total), respectively. Another way to quantify the usefulness of fuel parameters in correlating SREPs is to compare their average $\overline{R^2}$'s; this is done in the last column of Table 18 (note that the average only considers the "useful" cases). As previously noted (Figures 16 through 18), these low R^2 values indicate a poor correlation.

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* For these data H/C is equivalent to H% so only H% will be considered further in these discussions.

TABLE 18. RATING OF FUEL PARAMETERS FOR OVERALL USEFULNESS IN CORRELATIONS[a]

Fuel Parameter	$\overline{\Sigma R^2}$	Rank	Number of Times Useful[b]	Rank	Average $\overline{R^2}$
TSI_{df}	3.27	1	7	1	0.47
H%	2.90	2	6	2	0.48
SP^{-1}	2.26	3	4	4	0.57
TSI_{pf}	2.24	3	5	3	0.45
SP	1.80	4	3	5	0.60

[a] This analysis considers only correlations where $\overline{R^2} \geq 0.85$ of best $\overline{R^2}$.

[b] Out of a possible eight.

The ratings for the four separate operating conditions are given in Tables 19 through 22. These tables treat correlation with SN, LTR, EI_s, and RF as equivalent. The ability of any fuel parameter to correlate cruise conditions is rather good; it is less satisfactory for idle, and approaches uselessness for dash or takeoff, the two conditions of interest. These poor correlations may very well be due to the inadequacy of the data base. Based on the available data, the above analysis indicates that no fuel parameter stands out as superior to any other. The most generally useful are TSI_{df}, SP, and H% in that order.

Finally, we consider the ability or usefulness of the laboratory parameters in correlating SN or LTR for the three engines tested. The correlations with SN (Table 23) for idle for the J79 and TF-41 engines are reasonably good. Only H% for idle and TSI_{df} for cruise were applicable, by our 85 percent test, to all three engines. However, neither idle nor cruise gives a satisfactory correlation for the F101, and the cruise correlation for the TF-41 is unacceptable. No good correlations are found for dash or takeoff. Each condition has a different top-rated laboratory parameter. This should not be surprising because the combustion process must change for each condition. It may be an indication of the complexity of the problem of ranking fuels for turbojet engine performance.

The ability to correlate fuel parameters with LTR is presented in Table 24. Cruise and takeoff for the J79 engine are very well correlated, and idle and dash for the J79 engine are reasonably correlated. C/O is shown to be the best correlating parameter for takeoff and is a top contender for all three engines.

A few additional observations concerning the results can be made. As noted earlier (Section II.B), the H% and H/C ratio are closely related. This is confirmed by the correlation coefficients for these fuel parameters--H% and H/C give similar R^2 values. Second, although the TSI_{exp} is linearly related to the inverse smoke point (SP^{-1}), there are significant differences in the ability of these two parameters to correlate to SREPS, probably due to the molecular weight "correction" in the TSI_{exp} definition (Equation (2)). This points out a need for experimental molecular weight determinations of jet fuels to determine the adequacy or inadequacy of TSI_{exp} in correlation studies. Lastly, the correlation results, as well as inspection of the engine test reports (References 17 and 18), show that the engine operating conditions should be held rigorously constant during a test. In a few isolated cases discussed here, the engine operating conditions correlated almost as well as the fuel dependent parameters, but it is clearly demonstrated that the fuel plays a dominant role in controlling smoke-related engine parameters.

TABLE 19. RATING OF FUEL PARAMETERS FOR USEFULNESS IN CORRELATING FOR IDLE CONDITIONS[a]

Fuel Parameter	ΣR^2	Rank	Number of Times Useful[b]	Rank	Average R^2
SP	3.38	1	5	1	0.68
H%	3.02	2	4	2	0.76
SP^{-1}	3.00	2	4	2	0.75
TSI_{df}	2.09	3	3	3	0.70

[a] This analysis considers only correlations where $R^2 \geq 0.85$ of best R^2.

[b] Out of a possible eight.

TABLE 20. RATING OF FUEL PARAMETERS FOR USEFULNESS IN CORRELATING FOR CRUISE CONDITIONS[a]

Fuel Parameter	ΣR^2	Rank	Number of Times Useful[b]	Rank	Average R^2
TSI_{df}	3.57	1	5	1	0.71
SP^{-1}	3.08	2	4	2	0.77
H%	3.05	2	4	2	0.76
TSI_{pf}	2.99	3	4	2	0.75
SP	2.69	4	3	3	0.90

[a] This analysis considers only correlations where $R^2 \geq 0.85$ of best R^2.

[b] Out of a possible eight.

TABLE 21. RATING OF FUEL PARAMETERS FOR USEFULNESS IN CORRELATING FOR DASH CONDITIONS[a]

Fuel Parameter	ΣR^2	Rank	Number of Times Useful[b]	Rank	Average R^2
SP	1.76	1	4	1	0.44
PCAH	1.76	1	3	2	0.59
TSI_{pf}	1.74	1	3	2	0.58
TSI_{df}	1.18	2	2	3	0.59
H%	0.99	3	2	3	0.50

[a] This analysis considers only correlations where $R^2 \geq 0.85$ of best R^2.

[b] Out of a possible eight.

TABLE 22. RATING OF FUEL PARAMETERS FOR USEFULNESS IN CORRELATING FOR TAKEOFF CONDITIONS[a]

Fuel Parameter	ΣR^2	Rank	Number of Times Useful[b]	Rank	Average R^2
TSI_{df}	2.04	1	4	1	0.51
C/O	1.83	2	3	2	0.61
PCAH	1.69	3	3	2	0.56

[a] This analysis considers only correlations where $R^2 \geq 0.85$ of best R^2.

[b] Out of a possible eight.

TABLE 23. MEASURE OF ABILITY TO CORRELATE SN
(Value is R^2 from Ref. Table.)

Engine/Table	Idle		Cruise		Dash		Takeoff	
J79/10	SP	0.88	SP	0.95	SP^{-1}	0.52	PCAH	0.16
	H%	0.87	H%	0.93	SP	0.48	AR%	0.16
	SP^{-1}	0.81	SP^{-1}	0.93	TSI_{pf}	0.46	Inlet Temp.	0.14
	--		TSI_{df}	0.89	--		--	
	--		TSI_{pf}	0.83	--		--	
F101/11	TSI_{pf}	0.59	TSI_{pf}	0.63	PCAH	0.34	TSI_{exp}	0.73
	SP	0.58	TSI_{exp}	0.60	--		TSI_{df}	0.62
	H%	0.56	PCAH	0.60	--		--	
	TSI	0.55	TSI_{df}	0.56	--		--	
	TSI_{exp}	0.52	--		--		--	
TF-41/12	TSI_{df}	0.80	TSI_{exp}	0.32	C/O	0.32	H%	0.52
	H%	0.77	SP^{-1}	0.31	F/A	0.30	SP^{-1}	0.52
	TSI_{exp}	0.77	H%	0.28	SP	0.28	TSI_{df}	0.51
	SP^{-1}	0.75	AR%	0.28	H%	0.27	TSI_{exp}	0.44
	TSI_{pf}	0,70	TSI_{df}	0.28	--		--	
Order of preference (Value = ΣR^2)								
	H%	2.20	TSI_{df}	1.73	SP	0.76	TSI_{exp}	1.17
	SP^{-1}	1.56	TSI_{pf}	1.46	--		TSI_{df}	1.13
	SP	1.46	SP^{-1}	1.24	--		--	
	TSI_{df}	1.35	H%	1.21	--		--	
	TSI_{pf}	1.29	TSI_{exp}	0.92	--		--	
	TSI_{exp}	1.29	--		--		--	

TABLE 24. MEASURE OF ABILITY TO CORRELATE LTR
(Value is R^2 from Ref. Table.)

Engine/Table	Idle		Cruise		Dash		Takeoff	
J79/13	SP	0.73	H%	0.92	H%	0.72	C/O	0.91
	SP^{-1}	0.66	SP^{-1}	0.90	SP	0.65	F/A	0.82
	--		TSI_{df}	0.90	TSI_{df}	0.63	--	
	--		SP	0.89	--		--	
	--		TSI_{pf}	0.81	--		--	
F101/14	SP	0.46	TSI_{exp}	0.37	C/O	0.63	C/O	0.49
	--		PCAH	0.35	F/A	0.62	H%	0.42
	--		C/O	0.35	--		TSI_{df}	0.42
	--		SP^{-1}	0.31	--		--	
TF-41/15	--		PCAH	0.37	PCAH	0.62	TSI_{df}	0.49
	--		--		TSI_{pf}	0.60	H%	0.45
	--		--		TSI_{df}	0.55	C/O	0.43
Order of preference (Value = ΣR^2)								
	SP	1.19	SP^{-1}	1.21	TSI_{df}	1.18	C/O	1.83

SECTION V

SUMMARY AND RECOMMENDATIONS

The ability of 10 individual fuel parameters (several of which are interrelated), inlet air temperature, C/O ratio, and F/A ratio to correlate with four smoke-related engine parameters for four engine operating conditions has been evaluated for engine test data reported in the available literature.

The fuel parameters included: weight percent hydrogen; ASTM smoke point; inverse ASTM smoke point, weight percent aromatics; weight percent polycyclic aromatic hydrocarbons; molar ratio of hydrogen to carbon; a threshold soot index, TSI_{exp}, based on the ASTM smoke point and an estimated molecular weight; a TSI_{df} calculated from the ASTM class analysis of the jet engine fuel and the average of the individual TSIs from diffusion flame measurements using a mixture rule developed in this program; and a TSI_{pf} calculated from the ASTM class analysis of the jet engine fuel and the average of the individual TSIs from premixed flame measurements using a mixture rule developed in this program. The smoke-related engine parameters included: SAE Smoke Number measured at the combustor exit; the Smoke Emission Index (the quantity of soot (smoke) produced per unit of fuel combusted (g carbon per kg fuel)); the radiation flux to the combustor wall; and the combustor liner temperature increase over the inlet air temperature. The four engine conditions were: idle, cruise, dash, and takeoff.

In order to use TSI data on individual fuel components, mixture rules were developed from a series of experiments on binary and ternary fuel blends for both premixed and diffusion flames. For diffusion flames, the mixture rules give a TSI dependent on the mole percent composition of the mixture; for premixed flames, the greater TSI components make a larger contribution to the TSI of the mixture than do the ingredients with lower TSIs.

This study was limited to tests on three engines (J79, F101, and TF-41) because of the limited available information on the composition of the fuels tested in jet engine programs aimed at evaluating the effects of fuel structure. Even for the three engine testing programs analyzed, inadequate information was provided on individual fuel components; the fuel composition was presented as classes of compounds, e.g., paraffins, aromatics, naphthalenes, etc. Unfortunately, within a fuel class, e.g., aromatics, the TSI can vary over about 45 percent of the total range of TSIs.

Nevertheless, some of the correlations were excellent with $R^2 > 0.9$ but the correlating parameters which were useful varied with the engine conditions or with the smoke-related engine parameter being correlated. This may not be a valid conclusion; the data base may be inadequate.

This study does not support the use of any single fuel parameter, such as weight percent hydrogen, or the ASTM smoke point, as a means of evaluating smoke-related engine parameters. It does, however, demonstrate that the fuel composition plays a dominant role in determining smoke-related engine parameters.

It is recommended that:

1. An attempt be made to obtain samples of the fuels used in the many previous fuel effects studies and that these fuels be analyzed by, e.g., gas chromatography-mass spectrometry, for the individual fuel component concentrations.
2. In any current or future studies of the effects of fuel composition on smoke-related engine parameters, the fuels should be analyzed as above.
3. The study reported here should be extended to include soot yield information on the fuel components as a correlating parameter. This information has only recently become available and would be expected to give better correlations than soot threshold data which were employed in this study.
4. The study reported here should be extended to analyze the data made available by Recommendations 1 and 2.
5. The effect of turbulence on the relationship between molecular structure and the threshold soot index and the soot yield index for both premixed and diffusion flames should be obtained.

REFERENCES

1. *Energy: Global Prospects 1985-2000*; Workshops on Alternative Energy Strategies, McGraw-Hill, New York, 1977.

2. Longwell, J.P. and Grobman, J., "Alternative Aircraft Fuels," *J. Eng. Power*, vol. 101, pp. 155-161, 1979.

3. Lowndes, J.C., "NASA Readies Help to Meet Fuel Quality," *Aviation Week* and Space Technology, pp 70-73, 5 May 1980.

4. Grobman, J. and Reck, G.M., *The Impact of Fuels on Aircraft Technology Through the Year 2000*, NASA TM-81492, May 1980.

5. *Aircraft Research and Technology for Future Fuels*, NASA CP-2146, July 1980.

6. Champagne, D.L., "Standard Measurement of Aircraft Gas Turbine Engine Exhaust Smoke," *ASME Paper 71-GT-88*, March 1971.

7. Shaffernocker, W.M. and Stanforth, C.M., "Smoke Measurement Techniques," *SAE Trans.*, vol. 77, Paper No. 680346, 1968.

8. Calcote, H.F. and Manos, D.M., "Effect of Molecular Structure on Incipient Soot Formation," *Combust. Flame*, vol. 49, pp. 289-304, 1983.

9. Haynes, B.S. and Wagner, H.Gg., "Soot Formation," *Prog. Energy Combust. Sci.*, vol. 7, pp. 229-273, 1981.

10. Wood, A.D., "Correlation Between Smoke Measurements and the Optical Properties of Jet Engine Smoke," *SAE Paper No. 751119*, November 1975.

11. Blazowski, W.S., "Dependence of Soot Production on Fuel Blend Characteristics and Combustion Conditions," *ASME Paper 79-GT-155*, March 1979.

12. Jackson, T.A. and Blazowski, W.S., *Fuel Hydrogen Content as an Indicator of Radiative Heat Transfer in an Aircraft Gas Turbine Combustor*, AFAPL-TR-79-2014, Air Force Aero Propulsion Laboratory, February 1979.

13. Moses, C.A. and Naegeli, D.W., "Fuel Property Effects on Combustor Performance," *ASME Paper 79-GT-178*, March 1979.

14. Blazowski, W.S., "Future Jet Fuel Combustion Problems and Requirements," *Prog. Energy Combust. Sci.*, vol. 4, pp. 177-199, 1978.

15. Jackson, T.A., "Fuel Property Effects on Air Force Gas Turbine Engines-Program Genesis," *J. Energy*, vol. 6, pp. 376-383, 1982.

16. Bahr, D.W., "Impacts of Broadened-Specification Fuels on Aircraft Turbine Engine Combustors," *J. Energy*, vol. 6, pp. 392-398, 1982.

17. Gleason, C.C., Oller, T.L., Shayeson, M.W., and Bahr, D.W., *Evaluation of Fuel Character Effects on J79 Engine Combustion System*, AFAPL-TR-79-2015, CEEDO-TR-79-06, Air Force Aero Propulsion Laboratory, and Civil and Environmental Engineering Development Office, June 1979.

18. Vogel, R.E., Troth, D.L., and Verdouw, A.J., Fuel Character Effects on Current, High Pressure Ratio, Can-Type Turbine Combustion Systems," AFAPL-TR-79-2072, ESL-TR-79-20, Air Force Aero Propulsion Laboratory, and Civil and Environmental Engineering Development Office, April 1980.

19. Naegeli, D.W., Dodge, L.G., and Moses, C.A., "The Sooting Tendency of Fuels Containing Polycyclic Aromatics in a Research Combustor," AIAA Paper 82-0299, January 1982.

20. Minchin, S.T., J. Inst. Petrol., vol. 17, p. 102, 1931.

21. Naegeli, D.W. and Moses, C.A., "Effect of Fuel Molecular Structure on Soot Formation in Gas Turbine Engines," ASME Paper 80-GT-62, March 1980.

22. Wright, F.J., "The Formation of Carbon under Well-Stirred Conditions," Twelfth Symposium (International) on Combustion, pp. 867-875, The Combustion Institute, Pittsburgh, 1969.

23. Street, J.C. and Thomas, A., "Soot Formation in Premixed Flames," Fuel, vol. 34, pp. 4-36, 1955.

24. Calcote, H.F. and Miller, W.J., Ionic Mechanisms of Carbon Formation in Flames, AeroChem TP-371, AFOSR-TR-78-1082, AeroChem Research Laboratories, Inc., May 1978.

25. Blazowski, W.S., "Dependence of Soot Production on Fuel Structure in Backmixed Combustion," Combust. Sci. Technol., vol. 21, pp. 87-96, 1980.

26. Homann, H., "Carbon Formation in Premixed Flames," Combust. Flame, vol. 11, pp. 265-287, 1967.

27. Friswell, N.J., "The Influence of Fuel Composition on Smoke Emissions from Gas-Turbine-Type Combustors: Effect of Combustor Design and Operating Conditions," Combust. Sci. Technol., vol. 19, pp. 119-127, 1979.

28. Grumer, J., Harris, M.E., and Rowe, F.R., Fundamental Flashback, Blowoff, and Yellow-Tip Limits of Fuel Gas-Air Mixtures, RI 5225, Bureau of Mines, 1956.

29. Clarke, A.E., Hunter, T.G., and Garner, F.H., "The Tendency to Smoke of Organic Substances on Burning. Part I," J. Inst. Petrol., vol. 32, pp. 627-642, 1946.

30. Hunt, R.A., "Relation of Smoke Point to Molecular Structure," Ind. Eng. Chem., vol. 45, pp. 602-606, 1953.

31. Schalla, R.L. and McDonald, G.E., "Variation in Smoking Tendency Among Hydrocarbons of Low Molecular Weight," Ind. Eng. Chem., vol. 45, pp. 1497-1500, 1953.

32. Van Treuren, K.S., "Sooting Characteristics of Liquid Pool Diffusion Flames," MS Thesis, Princeton University, July 1978.

33. Schug, K.P., Manheimer-Timnat, Y., Yaccarino, P., and Glassman, I., "Sooting Behavior of Gaseous Hydrocarbon Diffusion Flames and the Influence of Additives," Combust. Sci. Technol., vol. 22, pp. 235-250, 1980.

34. Street, J.C. and Thomas, A., "Carbon Formation in Premixed Flames," Fuel, vol. 34, pp. 4-36, 1955.

35. Haynes, B.S., Jander, H., and Wagner, H.Gg., "Optical Studies of Soot Formation Processes in Premixed Flames," Ber. Bunsenges. Phys. Chem., vol. 84, pp. 585-592, 1982 .

36. Gould, R.K. Olson, D.B., and Calcote, H.F., Correlation of Soot Formation in Turbojet Engines and in Laboratory Flames, AeroChem TP-407, ESL-TR-81-08, AeroChem Research Laboratories, Inc., February 1981.

37. Gleason, C.C., Oller, T.L., Shayeson, M.W., and Bahr, D.W., Evaluation of Fuel Character Effects on the F101 Engine Combustion System, AFAPL-TR-79-2018, CEEDO-TR-79-07, Air Force Aero Propulsion Laboratory, and Civil and Environmental Engineering Development Office, June 1979.

38. Standard Test Method for Smoke Point of Aviation Turbine Fuels, ANSI/ASTM D1322-75 (Reapproved 1980).

39. Olson, D.B., Soot Formation in Synfuels, Final Report, AeroChem TP-433, DOE/PC/30304-5, AeroChem Research Laboratories, Inc., June 1983.

40. Smith, J.H., Harper, J.C., and Jaber, H., Analysis and Environmental Fate of Air Distillate and High Density Fuels, ESL-TR-81-54, Engineering and Services Laboratory, Air Force Engineering and Services Center, October 1981.

41. Hodgson, F.N. and Tobias, J.D., Analysis of Aircraft Fuels and Related Materials, AFAPL-TR-79-2016, p. 209, Air Force Aero Propulsion Laboratory, March 1979.

42. Shriner, R.L., Fuson, R.C., and Curtin, D.Y., The Systematic Identification of Organic Compounds, 5th ed., pp. 40-43, Wiley, New York, 1964.

43. Grobman, J.S., "Effect of Operating Variables on Pollutant Emissions from Aircraft Turbine Engine Combustors," in Emissions from Continuous Combustion Systems, W. Cornelius and W.G. Agnew, Eds. pp. 279-303, Plenum Press, New York, 1972.

44. Bevington, P.R., Data Reduction and Error Analysis for the Physical Sciences, pp. 119-133, McGraw-Hill, New York, 1969.

APPENDIX A

LITERATURE SURVEY

An extensive literature on the results of engine testing programs exists. This literature was searched to locate reports that describe the results of fuel structure effects on gas turbine or jet engine performance. A précis of each of the reports evaluated is given in this appendix.

1. Air Force Aero Propulsion Laboratory, T.R.A.C.E., Fuel Mainburner/Turbine Effects, AFWAL-TR-81-2081, General Electric Co., September 1982.

   Two combustors, F100 and TF33, were tested. Smoke and NO_x emissions, radiation flux, and liner temperatures were measured for 10 fuels. The results show that lower fuel hydrogen content is correlated to increased smoke emissions, NO_x emissions, and radiation flux. However, one of the fuels tested suggests that naphthalene fuel content is also important in raising smoke and radiation levels.

2. Bahr, D.W., "Impacts of Broadened-Specification Fuels on Aircraft Turbine Engine Combustors," ASME Paper 81-GT-2, March 1981.

   This paper reviews the data on smoke emission levels, NO_x levels, and combustor dome and liner temperatures which result from testing broadened specification fuels. The results (graphs) presented for CF6-6, CF6-50, F101/CFM56, and J79/CJ805 engines are related to fuel hydrogen percent. Aromatic, naphthalene, and hydrogen contents are listed for the fuels reported.

3. Bauserman, G.W., Spengler, C.J., and Cohn, A., "Combustion Effects of Coal Liquid and Other Synthetic Fuels in Gas Turbine Combustors. Part II. Full Scale Combustor and Corrosion Tests," ASME Paper 80-GT-68, March 1980.

   A full-scale combustor, typically employed in the Westinghouse W-251 and W-501 engines was tested with coal liquids and shale oils. NO_x, smoke emissions, and combustor and dome temperatures were measured. Fuel composition is reported in terms of hydrogen content and total aromatics.

4. Blazowski, W.S., "Future Jet Fuel Combustion Problems and Requirements," Progr. Energy Combust. Sci., vol. 4, p. 177, 1978.

   Jet engine design problems (emissions, ignition/relight envelope, liner temperature, etc.) are reviewed. Selected results on fuel effects on smoke emissions, liner temperatures, and radiation flux are related to fuel hydrogen contents in the form of graphs.

5. Blazowski, W.S., "Research Needs in Alternate Fuel Combustion," paper presented at 1976 AFOSR Contractors Meeting on Air-Breathing Combustion Dynamics, Wright Patterson AFB, 11-13 August 1976.

   The results of earlier engine test data are reviewed. Correlations, in graphic format, between liner temperature rise, Smoke Number, or NO_x emissions with fuel hydrogen content or combustor inlet temperature are given without reference to engine type or fuel composition.

6. Blazowski, W.S. and Henderson, R.E., Assessment of Pollutant Measurement and Control Goals for Military Aircraft Engines, AFAPL-TR-72-102, Air Force Aero Propulsion Laboratory, November 1972.

   Aircraft emission studies with particular emphasis on NO_x, combustor efficiency, and smoke emission levels are reviewed. Fuel effects are not discussed but engineering approaches to reducing emissions are suggested.

7. Blazowski, W.S. and Jackson, T.A., Evaluation of Future Jet Fuel Combustion Characteristics, AFAPL-TR-77-93, Air Force Aero Propulsion Laboratory, July 1978.

   Results are given of engine tests on a T56 combustor employing JP-4, JP-5, and several fuel blends. Smoke Numbers, liner temperatures, and NO_x emission measurements are reported. The jet fuels were analyzed only in terms of total aromatic and olefin contents. Smoke points are not reported.

8. Butze, H.F. and Ehlers, R.C., Effect on Fuel Properties of Performance of a Single Aircraft Turbojet Combustor, NASA TM X-71789, 1975.

   Liner temperatures, smoke emissions, and NO_x emissions are reported for sixteen fuels including pure chemical compounds and jet fuel blends under idle and cruise test conditions of a JT8D combustor. Smoke points are not reported. Compositions of jet fuels are reported as total aromatic content and hydrogen content. Results are correlated to hydrogen content and fuel/air ratio.

9. Clark, J.A., "Fuel Property Effects on Radiation Intensities in a Gas Turbine Combustor," AIAA J., vol. 20, p. 274, 1982.

   A research gas turbine combustor was operated over a limited range of pressures (3-12 atm) and temperatures (600-700 K) with seven test fuels. Radiation flux measurements are correlated to the fuel hydrogen, single ring aromatic, or polycyclic aromatic content. Smoke points and fuel components are not reported.

10. Clark, J.A., "Gas Turbine Combustor Soot and Radiation Studies," PhD Thesis, Purdue University, 1981.

    A more complete report of the results given in 9 above. No detailed chemical analysis of the fuels is given. Soot volume fractions and radiation flux are reported for pressures, 3-12 atm, and temperatures, 600 to 700 K. Correlations of the data to hydrogen, single ring, and multiple-ring aromatics are presented.

11. Claus, R.W., Spectral Flame Radiance from a Tubular-Can Combustor, NASA TP-1722, February 1981.

    A JT8D single can combustor was studied to determine the effect of fuel type, inlet air pressure, and fuel/air ratio on flame radiation levels. Only two fuels, Jet A and an ERBS fuel, were used in this work. With Jet A fuel, increasing pressure increased flame temperature and soot concentration (vide infra). Increasing fuel/air ratio for Jet A increased flame radiation in some combustor sections.

12. DeCorso, S.M., Pillsbury, P.W., Bauserman, G., Mulik P.R., Ambrose, M. J., and Stein, T.R., Gas-Turbine Combustor Performance on Synthetic Fuels, Final Report, AP-1623, Vol. 2, Westinghouse Electric Corp., June 1981.

    A modified B-4 combustor and a combustor section typical of the Westinghouse W-251 and W-501 engines were tested with several coal-derived and shale-derived liquids. The fuels were characterized by hydrogen content, total aromatics, and boiling range. The NO_x emissions were dependent upon combustor gas outlet temperatures and fuel-bound nitrogen levels. The smoke emissions were dependent upon fuel hydrogen content and combustor gas outlet temperatures.

13. DeCorso, S.M., Pillsbury, P.W., Bauserman, G., and Mulik, P.R., Gas Turbine Combustor Performance in Synthetic Fuels, EPRI-AP-1623, Westinghouse Electric Corp., November 1980.

    Both full-scale and half-diameter versions of a Westinghouse combustor section,as typically used in the W-251 or W-501 gas turbine engines, were tested with SRC-I, SRC-II, EDS coal-derived fuels, and shale-derived fuels. Lower hydrogen content fuels showed increased liner temperatures regardless of fuel composition. At low temperature operation, low hydrogen content fuels produced more smoke.

14. Dodds, W.J., Peters, J.E., Colket, M.B. III, and Mellor, A.M., "Preliminary Study of Smoke Formed in the Combustion of Various Jet Fuels," J. Energy, vol. 1, p. 115, 1977.

    A disk-stabilized combustor was used to study fuel effects and sampling techniques on smoke particulate loading. Hydrogen content and total aromatic content of fuels are reported. Smoke emissions are discussed in terms of hydrogen and aromatic content of fuel but few correlations are found.

15. Ferguson, C.R. and Mellor, A.M., "Probing a Premixed/Prevaporized Type of Combustor," AIAA Paper 80-0285, January 1980.

    Unburned hydrocarbons, CO, NO_x, and gas temperatures are reported for a research combustor burning Jet A fuel under a single operating condition. An analysis of the errors introduced by sampling and probe techniques is given.

16. Friswell, N.J., "The Influence of Fuel Composition on Smoke Emission from Gas-Turbine-Type Combustors: Effect of Combustor Design and Operating Conditions," Combust. Sci. Technol., vol. 19, p. 119, 1979.

    A set of fifteen fuels was tested in a research scale flow tube combustor to ascertain the effect of fuel structure on smoke emission levels and flame radiation. Hydrogen content of the fuels gave the best correlation to the measured quantities. At the higher operating pressures, above 10 atm, the measured parameters were insensitive to fuel composition changes.

17. Gleason, C.C. and Bahr, D.W., Experimental Clean Combustor Program. Alternate Fuels Addendum Phase 2, Final Report, General Electric Co., January 1976.

Five fuels were evaluated for CO, unburned hydrocarbon, NO_x, smoke emission levels, and peak liner temperatures in three CF6-50 engines. All five measurements showed increases as fuel hydrogen content was lowered by the use of different fuels. Results are presented in graphic format.

18. Gleason, C.C. and Martone, J.A., "Pollutant Emission Characteristics of Future Aviation Jet Fuels," J. Air Pollut. Control Assoc., vol. 29, p. 1243, 1979.

A synopsis of the test results on a J79 combustor is presented. Engine Smoke Numbers and NO_x levels are correlated with fuel hydrogen content. Few details of the engine operating conditions or the fuel compositions are given.

19. Gleason, C.C., Oller, T.L., Shayeson, M.W., and Kenworthy, M.J., Evaluation of Fuel Character Effects on a J79 Smokeless Combustor, AFWAL-TR-80-2092, Air Force Aero Propulsion Laboratory, November 1980.

The effects of fuel structure on smoke and NO_x emissions,as well as liner temperature and radiation flux,were measured for a J79-17C combustor. Liner temperatures, flame radiation, smoke, and NO_x emission levels increased as fuel hydrogen content was lowered. Fuel compositions are reported as fuel classes.

20. Gleason, C.C., Oller, T.L., Shayeson, M.W., and Bahr, D.W., Evaluation of Fuel Character Effects on F101 Engine Combustion System, AFAPL-TR-79-2018, Air Force Aero Propulsion Laboratory, June 1979.

Fuel structure effects on the performance, emissions, and durability of the GE F101 main combustor are presented. Fuel compositions are given by fuel classes. At high power conditions, lower fuel hydrogen content raised the smoke and NO_x emission levels and also raised the liner temperatures. At lower power conditions, fuel hydrogen content was unimportant.

21. Gleason, C.C., Oller, T.L., Shayeson, M.W., and Bahr, D.W., Evaluation of Fuel Character Effects on J79 Engine Combustion System, AFAPL-TR-79-2015, Air Force Aero Propulsion Laboratory, June 1979.

An investigation of fuel property effects on performance, emissions, and durability of a J79-17A combustor. Liner temperature, radiation, smoke, and NO_x levels were dependent on fuel hydrogen content at high power conditions but not under low power conditions. Fuel composition is reported by fuel classes.

22. Grobman, J. and Reck, G.M., The Impact of Fuels on Aircraft Technology Through the Year 2000, NASA TM-81492, 1980.

This report reviews the effects of broadened fuel specification, such as lowering fuel hydrogen content on engine performance. results are abstracted from 19-21 above. Fuel hydrogen content and aromatic content of broadened specification fuels are discussed in terms of their effect on smoke emissions, combustor lifetime, and liner temperatures.

23. Horling, J.E., Effect of Smokeless Combustors on Particulates from J52 and TF30 Engines, NAPTC-PE-48, January 1975.

The J52 and TF30 engines were tested with and without smokeless combustor sections. The J52 engine fitted with a smokeless combustor showed reduced particulate emissions as compared to a J52 standard engine. The TF30 engine, however, showed an increase in particulate emissions when fitted with a smokeless combustor.

24. Jackson, T.A., "The Evaluation of Fuel Property Effects on Air Force Gas Turbine Engines - Program Genesis," ASME Paper 81-GT-1, March 1981.

The results of engine testing programs on the J79 and F101 combustion systems are reviewed. The data from 19-21 are abstracted to show the relationship of fuel hydrogen content to engine Smoke Numbers, combustor lifetimes, and liner temperatures. Aromatic content was determined not to be an important fuel property.

25. Jackson, T.A. and Blazowski, W.S., Fuel Hydrogen Content as an Indicator of Radiative Heat Transfer in an Aircraft Gas Turbine Combustor, AFAPL-TR-79-2014, Air Force Aero Propulsion Laboratory, February 1979.

A T56 combustor was tested, using fuels blended with various amounts of single and double ring aromatics. Liner temperatures and radiation levels correlated well with fuel hydrogen content. Fuel structure effects are reported as minor.

26. Johansen, K.M. and Kumm, E.L., Determination of Aircraft Turbine Engine Particulates, EPA/650/2-75/055, Airesearch Mfg. Co. of Arizona, May 1975.

The results of a 12-month program aimed at the development of reliable measurements of particulate emissions from jet aircraft are described. The correlation of particulate mass concentrations with Smoke Number is satisfactory for a single engine at one operating condition. However, if the operating condition of this engine is changed, the correlation changes.

27. Khamidullin, F.A., Strogonov, O.V., and Talantov, A.V., "Comparative Analysis of the Basic Combustion Characteristics of Some Heavy Hydrocarbon Fuels in Application to Aircraft Gas Turbine Engines," Soviet Aeronautics, vol. 22, p. 51, 1979.

The combustion characteristics of city gas, diesel, and jet fuels burned in a gas turbine engine were found to be very similar in terms of flame propagation, velocity, and temperatures.

28. Linden, L.H. and Heywood, J.B., "Smoke Emission from Jet Engines," *Combust. Sci. Technol.*, vol. 2, p. 401, 1971.

This review discusses controlling smoke emissions by methods which are founded on the results of jet engine testing programs. Hydrogen content is suggested to be the major fuel property to adjust in order to achieve lower smoke emissions.

29. Liu, T.M. and Washam, R.M., "Smoke Characteristics of Distillate and Residual Fuel Burning in Gas Turbine Combustors," *ASME Paper 80-GT-13*, March 1980.

A two-stage (rich-lean, low NO_x) combustor was tested with distillate and residual fuel oils. Smoke emissions were measured at different levels of water injection, inlet air temperatures, and vanadium content of fuels. Increased levels of vanadium (≈ 100-300 ppm) caused a dramatic increase in smoke emissions.

30. Lohmann, R.P., "NASA Broad Specifications Fuel Combustion Technology Program," *AIAA Paper 82-1088*, 1982.

Engine modifications required to burn fuels of lower hydrogen content and yet maintain low smoke emission levels are reviewed. Engine tests on a JT90-7F are presented. Flame radiation levels, NO_x, CO, unburned hydrocarbons, and smoke emissions were measured with two fuels and several operating conditions.

31. Longwell, J.P. and Grobman, J., "Alternate Aircraft Fuels," *J. Eng. Power*, vol. 101, p. 155, 1979.

This paper discusses engineering approaches to using broadened specification jet fuels in gas turbine engines. Lowered hydrogen contents of these fuels raised liner temperatures and smoke emissions and thus the engineering solutions to these problems are discussed.

32. Lyon, T.F., Dodds, W.J., and Bahr, D.W., *Determination of Pollutant Emissions Characteristic of General Electric CF6-6 and CF6-50 Model Engines*, Report No. FAA-EE-80-27, Federal Aviation Administration, March 1980.

Higher CO, unburned hydrocarbon, NO_x, and smoke emission levels were found for CF6 engines burning Jet A fuel versus JP-4 fuel under identical operating conditions. No fuel analyses are given.

33. Mellor, A.M., "Soot Studies in Gas Turbine Combustors and Other Turbulent Spray Flames," in *Particulate Carbon: Formation During Combustion*, p. 343, Plenum Press, New York, 1981.

Report reviews engine testing programs aimed at reducing smoke emissions. Effects of increasing inlet air temperature, equivalence ratio, pressure, and hydrogen content of fuel on the level of smoke produced are discussed. Aromatic content of fuel is considered to be the most important fuel property in determining smoke emission levels.

34. Moses, C.A. and Mellor, A.M., "Problems in the Compatibility of Future Fuels with Current Air Breathing Combustion Systems," paper presented at AFOSR Contractors Meeting on Air-Breathing Combustion Dynamics Research, 1982.

Paper reviews work carried out at SWRI (no raw data presented) on the effects of fuel structure on soot formation in gas turbine and research combustors. Although hydrogen content of fuels correlated best with flame radiation in real engine combustors, some engines showed an increased sensitivity to the tetralin and naphthalenes content of the fuel while others did not.

35. Moses, C.A. and Naegeli, D.W., "Fuel Property Effects of Combustor Performance," in Gas Turbine Combustor Design Problems, A.H. Lefebvre, Ed. p. 39, Hemisphere Publ. Corp., New York, 1978.

A research combustor (Phillips 2-inch combustor) and a combustor section of a T63 engine were tested using a set of 19 fuels. Flame radiation, liner temperature, and smoke emissions were measured and related to the hydrogen, total aromatic, and single and double ring aromatic contents of the fuels. Smoke levels were most sensitive to fuel hydrogen content and weakly sensitive to fuel aromatic content.

36. Naegeli, D.W., Dodge, L.G., and Moses, C.A., "The Sooting Tendency of Fuels Containing Polycyclic Aromatics in a Research Combustor," AIAA Paper 82-0299, January 1982.

Jet A and Jet A-1, blended with either aromatics, naphthalenes, tetralin, or indene, were used to determine the sensitivity of flame radiation to fuel structure. A Phillips 2-inch combustor was used for this work. Most of the flame radiation data are well correlated to H/C ratio of the fuels tested. For some operating conditions, the flame radiation data correlate better to fuel tetralin or fuel naphthalenes content.

37. Najjar, Y.S.H. and Goodger, E.M., "Soot Formation in Gas Turbines Using Heavy Fuels. 1.," Fuel, vol. 60, p. 980, 1981.

The experimental results taken on a continuous combustion rig were used to develop a soot formation model. Flame radiation used to calculate flame temperatures, and smoke sampling measurements were compared with the model predictions. Fuel effects were modeled in terms of fuel hydrogen content.

38. Roberts, R., Peduzzi, A., and Vitti, G.E., Experimental Clean Combustor Program. Phase 2, Pratt and Whitney Aircraft, July 1976.

This study was aimed at determining the effects of fuel structure on Hybrid and Vorbix concept, low pollution, combustors. CO and NO_x levels increased for both engine concepts over the unmodified engine. The Vorbix concept combustor showed a strong sensitivity of smoke emissions to fuel aromatic content. Both concepts showed no sensitivity of liner temperature with fuel type.

39. Rosfjord, T.J., Investigation of Soot and Carbon Formation in Small Gas Turbine Combustors, Final Report, NASA-CR-167853, United Technologies Research Center, April 1982.

A 60° sector of the JT15D annular combustor was tested with three fuels: Jet A, ERBS, and diesel fuel oils (No. 2). The smoke emission measurements indicate that smoke levels are increased by poor fuel/air mixing near the fuel injector, poor atomization, and low fuel hydrogen content.

40. Sawyer, R.F., Atmospheric Pollution by Aircraft Engines and Fuels: A Survey, AGARD-AR-40, March 1972.

This report provides a list of references to the early literature on atmospheric pollution caused by jet aircraft. Very little comment is made on fuel effects on smoke emission levels of jet engines.

41. Schirmer, R.M., McReynolds, L.A., and Daley, J.A., "Radiation from Flames in Gas Turbine Combustor," SAE Trans., vol. 68, p. 554, 1960.

Flame radiation is reported to be insensitive to aromatic content or type from the results obtained on both research combustors and a J79 engine single combustor. Flame radiation measurements on a J57 engine single combustor, however, showed that polycyclic aromatic fuel blends burn with higher flame emissivities than do monocyclic aromatic fuel blends.

42. Sonnichsen, T., Baseline Data on Utilization of Low Grade Fuels in Gas Turbine Applications, Volume 3, EPRI-AP-1882, KVB, Inc., June 1981.

A series of tests with a Westinghouse PACE 260 MW gas turbine/heat recovery steam generator was made to determine the effects of afterburner modification, water injection, and operating conditions on CO, NO_x, CO_2, SO_x, and particulate emission levels.

43. Stumpf, S.A. and Blazowski, W.S., "Detailed Investigations of Organic Compound Emission from Aircraft Gas Turbine Engines," IEEE Annals No. 75CH1004-1, pp. 1-12, 1976.

A T56 combustion rig was tested with pure isooctane, ferrocene additives, and JP-4 fuel blends. The CO, NO_x, CO_2, and unburned hydrocarbon emissions were measured but were not correlated to fuel structure. Operating engine conditions strongly affected the unburned hydrocarbon emission levels.

44. Szetela, E.J., Lohmann, R.P., and Smith, A.L., "Impact of Broad Specification Fuels on Aircraft Gas Turbine Combustors," J. Energy, vol. 4, p. 24, 1980.

This analytical paper deals with fuel effects on NO_x, unburned hydrocarbon, CO, and smoke emission levels. Data were taken from the literature on a variety of gas turbine jet engines. It is suggested that both the aromatic type (monocyclic aromatics or polycyclic aromatics) and total aromatic content of fuels are important in affecting smoke emission levels of JT9D engines.

45. Vogel, R.E. and Troth, D.L., "Fuel Character Effects on the TF41 Engine Combustion System," AIAA Paper No. 81-1391, July 1981.

This study on a TF41 engine combustor section shows that fuel properties such as hydrogen content and aromatic content affect smoke emission levels, combustion efficiency, and liner temperatures at high power, but not at lower power engine operating conditions. NO_x, CO, and unburned hydrocarbon emissions are also reported.

46. Vogel, R.E., Troth, D.L., and Verdouw, A.J., Fuel Character Effects on Current, High Pressure Ratio, Can-Type Turbine Combustion Systems, AFAPL-TR-79-2072, Air Force Aero Propulsion Laboratory, April 1980.

This is a detailed study on fuel effects on smoke emissions, liner temperatures, NO_x, and unburned hydrocarbon emissions measured on a TF41 engine. Fuels are analyzed by fuel class contents (single ring aromatics, double ring aromatics, indanes, tetralins, etc.). Both fuel hydrogen content and fuel structure affected engine performance and emission levels.

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