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**CHARACTERISTICS AND COMBUSTION OF FUTURE  
HYDROCARBON FUELS**

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## CHARACTERISTICS AND COMBUSTION OF FUTURE HYDROCARBON FUELS

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## SUMMARY

As the world supply of petroleum crude oil is being depleted, the supply of high-quality crude is also dwindling. This dwindling supply is beginning to manifest itself in the form of crude oils containing higher percentages of aromatic compounds, sulphur, nitrogen, and trace constituents. The result of this trend is described and the change in important crude oil characteristics, as related to aircraft fuels, is discussed. As available petroleum is further depleted, the use of synthetic crude oils (i.e., those derived from coal and oil shale) may be required. The principal properties of these "syncrudes" and the fuels that can be derived from them are described and discussed. In addition to the changes in the supply of crude oil, increasing competition for middle-distillate fuels may require that specifications be "broadened" in future fuels. The impact that the resultant potential changes in fuel properties may have on combustion and thermal stability characteristics is illustrated and discussed in terms of ignition, soot formation, carbon deposition, flame radiation, and emissions.

## INTRODUCTION

This paper describes some of the changes in fuel properties that may be expected in future hydrocarbon fuels for aircraft and discusses the effect that these property changes may have on selected combustion and thermal stability characteristics relevant to aircraft jet engines. Many studies are currently under way within the United States to predict the future availability and characteristics of crude oils (1-4). Included in many of these studies is an analysis of the processing required to upgrade low-quality feedstocks, such as crude oils derived from oil shale and coal, to the current specifications for jet aircraft fuels. Severe economic and energy consumption penalties will likely occur if these low-quality crudes must be refined to current specifications. Similarly, converting high-boiling petroleum fractions to current-specification jet fuel, which may be necessary because of a shortened supply of middle distillates, requires energy-intensive hydroprocessing (5). An alternative would be to relax fuel specifications and thereby minimize the economic and energy consumption penalties. However, the relaxed-fuel-specification approach would require the development of a new level of engine and aircraft fuel-system technology (6).

An assessment of the main advantages and disadvantages of these two approaches is shown in Figure 1. The continued production of current-specification jet fuel certainly is the best approach from the aircraft airframe and engine manufacturers' point of view. But, as already mentioned, it may be prohibitive from an economic and refining-energy-consumption point of view. Relaxing the current jet-fuel specifications would obviously minimize the energy consumption and economic penalties but may be prohibitive because it may require more complex component technology and may adversely affect engine life.

The solution to projected fuel availability problems will most likely be to relax the fuel specifications to a point governed by a trade-off between the fuel cost and refinery energy consumption and the cost and development difficulty of new technology for engines and aircraft fuel systems. Developing the data base needed to make this trade-off is the primary objective of the Fuels Technology Program being conducted by the National Aeronautics and Space Administration (NASA). Much of the information presented in this paper is derived from this program. Other U.S. Government and aircraft-industry-sponsored programs also provided information to this paper.

Illustrations are used to describe the changes in jet aircraft fuel properties that will most probably occur if fuel specifications are relaxed. The effect of these properties on certain combustion characteristics is also illustrated, and possible variations in fuel thermal stability are described. This is the first part of a two-part lecture on the characteristics of possible alternative hydrocarbon fuels and their effects on future jet aircraft. Reference 7 is the second part of the lecture.

## CHARACTERISTICS OF JET-FUEL FEEDSTOCKS

## Petroleum Crude Oil

The compositions of some typical petroleum crude oils from various sources are shown in Table I (taken from ref. 8). Selected data are included in Table I for both the total crude and several middle-distillate fractions from which jet and diesel fuels are produced. The sulfur content of petroleum obtained from different sources varies considerably. The variability of the hydrogen content is significant in that many of the currently important sources of petroleum, such as the Alaskan crude from Prudhoe Bay, tend to have a relatively high aromatic content. The nitrogen content of petroleum is gen-

erally quite low. The higher-boiling range fractions contain relatively more sulfur and nitrogen and less hydrogen (a lower hydrogen-carbon ratio, thus a higher aromatic content) than the lower-boiling-range fractions.

### Synthetic Crude Oils

A similar set of data for "synthetic" crude oils derived from oil shale and coal are shown in Table II (taken from ref. 8). The sulfur, nitrogen, and hydrogen contents of the shale-derived crude oils are reasonably comparable with one another regardless of the process used to extract the oil from the shale. The sulfur, nitrogen, and hydrogen contents of the coal-derived syncrude produced by the Synthoil process were all lower than those of the shale oils. The higher-boiling-range fractions in the shale oils contain considerably more nitrogen, in the form of organic nitrogen compounds, than do the lower-boiling-range fractions. The hydrogen content for both the shale oils and coal syncrude is reduced significantly as the boiling range is increased. The low hydrogen content of the middle-distillate fractions in the coal syncrude is particularly significant because of the corresponding high aromatic content. (The composition of the Synthoil fractions can vary considerably depending on the properties of the coal feedstock used and the process operating conditions, including the degree of hydrogenation.) In addition, other processes such as H-coal (9) would produce an oil with somewhat different properties from the same Kentucky coal feedstock.

### Comparison of Selected Key Properties

Two of the key crude-oil properties that have an important effect on jet-fuel characteristics are compared in Figures 2 and 3 for various crude-oil feedstocks. Figure 2 compares the hydrogen content by weight percent of petroleum crude, shale oil, and coal syncrudes derived from a variety of sources and processes. The variation in shale-oil hydrogen content is minimal, but the variation in petroleum-crude hydrogen content is rather large, with the lower end nearly at the same level as the shale oil and coal syncrude. This factor is important because the need to upgrade low-quality petroleum crudes to the same extent as the shale oil and coal syncrude may impose an economic penalty on refining current-specification jet fuel long before any of the "synthetic" crude oils are available. As mentioned earlier, the hydrogen content of coal syncrudes may vary considerably beyond that shown in the figure, depending on the amount of hydrogen added to the coal, which has a hydrogen content of about 4 to 5 percent. Figure 3 compares the nitrogen content by weight percent of the various crude-oil feedstocks. For this property, both the variation and the level in petroleum crude are minimal, but both the variation and the level in shale oil are very significant. These characteristics imply that upgrading of the crude to reduce nitrogen content in jet fuels probably will not be needed until shale-oil feedstocks become available.

The importance of the hydrogen and nitrogen levels in fuels is discussed in detail in the section FUEL PROPERTY EFFECTS and THERMAL STABILITY.

### CHARACTERISTICS OF JET FUELS

#### Current-Specification Fuels

Some of the key characteristics of aircraft hydrocarbon jet fuels are shown in Table III, along with their effect or relevance in aircraft propulsion systems. The American Society for Testing Materials (ASTM) specifications for jet fuels, including Jet B, Jet A and Jet A-1, are shown in Table IV. The average properties for a current Jet A fuel are also shown in Table IV for comparison. In general, the average property values for Jet A fuel fall well within the required maximum or minimum specification limits. Many of these characteristics are interrelated and can vary considerably with changing base-point conditions. For example, the variation in heat of combustion with specific gravity is illustrated in Figure 4. A significant decrease in heat of combustion by weight occurs as specific gravity (density) is increased over the range allowable in the specification. This decrease is somewhat compensated for by the increase in the heat of combustion by volume that occurs simultaneously. Since aircraft fuel systems are volume limited and the aircraft themselves are often weight limited, there are no significant range or performance penalties as long as the specific gravity remains within the specified limits.

The boiling range of jet fuels can vary from about 60° C for Jet B to about 270° C for Jet A. The boiling ranges of these fuels and two other petroleum products are shown in Figure 5. The boiling range of Jet B fuel (JP-4) is directly comparable to the boiling range of gasoline (also naphtha for petrochemicals) at the low ends and to the boiling range of Jet A (JP-5), no. 2 diesel oil, and home heating oil at the high end. The boiling range of Jet A fuel is primarily comparable to the high-boiling-range no. 2 diesel and home heating oils. This overlap of boiling ranges can have a significant impact on the specification values if they have to be relaxed to improve jet-fuel availability. Complete distillation curves for some fuels are presented in Figure 6. Jet A and Jet A-1 fuels are less volatile than Jet B and Avgas, as clearly illustrated on this figure by the

much higher initial boiling point (0 percent evaporated).

Another measure of fuel volatility is the vapor pressure characteristics shown in Figure 7. The initial boiling point of jet fuels is determined by the allowable limits for flashpoint (Jet A) or Reid vapor pressure (Jet B) shown in Table IV. The fuel volatility must be low enough to prevent the formation of flammable vapors at ambient conditions. Jet A is currently endorsed for commercial aircraft because of its lower probability of fire during emergency landings (10). Although low volatility is desirable for safety, it adversely affects the ignition and altitude relight capabilities of the fuel.

Another fuel property that is important in determining fuel ignition characteristics is fuel viscosity. The variation of viscosity as a function of fuel temperature is shown in Figure 8. The less volatile fuels are more likely to encounter ignition difficulties because of their higher viscosities. As with vapor pressure, the variation of viscosity with temperature is an exponential effect and becomes much more severe as temperature is reduced.

This discussion does not include all the characteristics of current-specification fuels. It was intended only to point out some selected key fuel characteristics and to describe how they vary within the listed specification limits.

### Projected Changes in Fuel Properties

Perhaps one of the most significant trends in fuel properties over the last 15 years has been the steady increase in the average aromatic content of commercial Jet A fuel. This trend is illustrated in Figure 9, where it is compared with the current ASTM Jet A specification limit. During the emergency period 1973-74, limited quantities of highly aromatic jet fuels were used as illustrated in Figure 9 by the 22-percent aromatic content of Jet A refined from a heavy Arabian crude. An estimate for Jet A refined from Alaskan crude indicates that aromatic content may be as high as 25 percent. Because of these recent trends, a waiver limit of 25-percent aromatic content has been set by the ASTM for Jet A fuel. The higher-aromatic-content petroleum crude sources may require additional hydroprocessing at the refinery to reduce the aromatic content to current specifications. Furthermore, future shortages of middle distillates may necessitate the conversion of higher-boiling-range petroleum cuts to middle-distillate fractions (5). These "cracked" fuels would have higher aromatic content and thus would require additional hydroprocessing to meet current specifications. A very simplified schematic of the type of processing required is shown in Figure 10.

Hydroprocessing techniques to improve fuel quality in terms of hydrogen and nitrogen content will also be needed if fuels refined from syncrude feedstocks must meet current specifications. The amount of hydrogen that would be consumed to raise a coal-syncrude hydrogen content from 12.5 percent to 13.5 percent would be 100 cubic meters per cubic meter of oil, as illustrated in Figure 11. Also shown in the figure is the amount of hydrogen that would be consumed to reduce the nitrogen content of a shale-oil syncrude. These large amounts of hydrogen would likely cause both economic and energy consumption penalties at the refinery.

The increasing trend toward higher-aromatic-content fuels, regardless of the crude source, will result in straight-distillation fuels with lower hydrogen content. The relation between hydrogen and aromatic contents is shown in Figure 12. At the currently specified aromatic content of 20 percent, the hydrogen content can vary between approximately 13.2 and 14.2 percent by weight. Within the band shown, the decrease in hydrogen content is generally a linear function with increasing aromatic content. An adverse effect of reduced hydrogen content is illustrated in Figure 13, where heat of combustion by weight is plotted as a function of hydrogen content. This effect is related to the effect of specific gravity shown in Figure 4 since reductions in hydrogen content result in proportionate increases in specific gravity. Substantial reductions in the heat of combustion occur with decreasing fuel hydrogen content. As an example, a reduction of approximately 1000 kilojoules per kilogram results when hydrogen content is reduced from 14 to 12 percent by weight.

In Figure 14 it is shown that Jet A fuel has a relatively narrow boiling range, with a final boiling point of approximately 270° C, which is necessary to comply with limits on the freezing point. The relation between freezing point and final boiling point is illustrated in Figure 14. The freezing point of a fuel is generally defined as the temperature at which wax components in the fuel begin to solidify. As shown in Figure 14, the freezing point is quite sensitive to variations in final boiling point.

The foregoing discussion considered only those fuel properties that are most likely to change. Potential increases in petroleum-crude aromatic content will result in decreased fuel hydrogen content unless additional hydrotreating is done at the refinery. Additional hydrotreating will surely be needed to reduce the nitrogen content and to increase the hydrogen content of fuels refined from oil shale and coal syncrudes if they are to meet current jet-fuel specifications. Hydrocracking will also be required to convert higher-boiling-range fractions to the boiling range and composition of current-specification jet fuels. These projected needs for additional hydrotreating will surely increase the cost of future-specification fuels and energy consumption required to refine them. Therefore, some relaxation of the current specifications may be needed to minimize

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Another measure of fuel volatility is the vapor pressure characteristics shown in Figure 7. The initial boiling point of jet fuels is determined by the allowable limits for flashpoint (Jet A) or Reid vapor pressure (Jet B) shown in Table IV. The fuel volatility must be low enough to prevent the formation of flammable vapors at ambient conditions. Jet A is currently endorsed for commercial aircraft because of its lower probability of fire during emergency landings (10). Although low volatility is desirable for safety, it adversely affects the ignition and altitude relight capabilities of the fuel.

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The foregoing discussion considered only those fuel properties that are most likely to change. Potential increases in petroleum-crude aromatic content will result in decreased fuel hydrogen content unless additional hydrotreating is done at the refinery. Additional hydrotreating will surely be needed to reduce the nitrogen content and to increase the hydrogen content of fuels refined from oil shale and coal syncrudes if they are to meet current jet-fuel specifications. Hydrocracking will also be required to convert higher-boiling-range fractions to the boiling range and composition of current-specification jet fuels. These projected needs for additional hydrotreating will surely increase the cost of future-specification fuels and energy consumption required to refine them. Therefore, some relaxation of the current specifications may be needed to minimize

the adverse impact on cost and energy consumption. Several of the major fuel properties that could be affected by such a relaxation are shown in Table V. The values in the table are levels that have been suggested (11), as being reasonable for setting the possible limits of a candidate "broad-specification" fuel.

#### Measurement Techniques

As was pointed out in the preceding discussion, an accurate knowledge of the level of certain critical fuel properties is needed to evaluate the level of other dependent properties. The current methods for measuring several key fuel characteristics are shown in Table VI and are also compared with test methods that may be required for future fuels. It may be necessary to modify or replace current laboratory test methods for fuels with broadened specifications because test results using certain methods may be unacceptable when fuel property values exceed the range of sensitivity of current methods. Since hydrogen content is one of the key fuel properties, a direct measurement of hydrogen content should be made by using a technique such as nuclear magnetic resonance (NMR). Also, the hydrocarbon composition may be needed to determine its effect, if any, on combustion and thermal stability characteristics. Gas chromatography - mass spectrometry (GCMS) is a likely candidate for hydrocarbon analysis. New techniques to measure volatility, fluidity, and thermal stability will also be valuable to more accurately determine the volatility of high-boiling-range fuel, correlations between freeze point and pumpability, and correlations between fuel deposition and engine life. Finally, techniques such as the Kjeldahl method will be needed for measuring the nitrogen content of future syncrude-derived fuels.

#### FUEL PROPERTY EFFECTS

The preceding sections of this paper described and discussed fuel properties that are most likely to change in future broad-specification fuels. In this section, the effect of varying these properties on the combustion and thermal oxidation characteristics of future fuels is considered.

#### Flame Characteristics

The fuel property that has the largest effect on the characteristics of the flame within a gas-turbine combustor is the hydrogen content of the fuel. It affects soot formation, carbon deposition, flame temperature, and total flame radiation. The effect of hydrogen content on soot formation is shown in Figure 15 (taken from ref. 12), where the soot concentration is shown to increase markedly with decreasing hydrogen content. These results were obtained by collecting soot samples from the primary zone of an experimental atmospheric burner at near-stoichiometric conditions for blends of benzene and n-heptane. The tendency to form soot is a function not only of hydrogen content but also of combustor inlet pressure and temperature and primary-zone equivalence ratio. The results shown in Figure 15 were obtained in a very carefully controlled experiment and may not be typical of the actual characteristics that would occur in a gas-turbine combustor. Soot formation rate can also be affected by the atomization quality and vaporization rate of the fuel being injected into the flame zone. Both volatility and viscosity can affect these processes. The calculated effect of fuel viscosity on drop-size distribution of a typical fixed-orifice fuel nozzle is illustrated in Figure 16 (taken from ref. 13).

The effect of hydrogen content on carbon deposition characteristics is illustrated in Figure 17 (taken from ref. 14). Also included in this figure is the effect of volatility. Figure 17(a) shows the effect of hydrogen content (hydrogen-carbon weight ratio) and volatility (volumetric average boiling temperature) on a correlating parameter, the NACA K factor. The effect of NACA K factor on average carbon deposition in a single-can combustor operating for 4 hours at a pressure of about 2 atmospheres, an inlet temperature of 130° C, and a fuel-air ratio of 0.0123 is illustrated in Figure 17(b). Both increases in boiling temperature and decreases in hydrogen content resulted in increases in the NACA K factor (Fig. 17(a)) and, therefore, increases in the average carbon deposition (Fig. 17(b)). The fuel properties were varied by "doping" a MIL specification fuel to get the desired characteristics. The carbon deposition results shown in Figure 17(b) were obtained in a single-can combustor operating at relatively low inlet temperature and pressure and are not necessarily typical of advanced high-pressure-ratio, gas-turbine-engine combustors. Fuel injector characteristics can also affect these relations; hence fuel viscosity is also an important fuel property when evaluating carbon deposition characteristics.

Figure 18 shows the calculated effect of hydrogen content on maximum flame temperature within a combustor at simulated takeoff and cruise conditions (ref. 15). This increasing flame temperature characteristic with decreasing hydrogen content can have several adverse effects within an aircraft engine combustor. Both the rate of oxides-of-nitrogen ( $\text{NO}_x$ ) formation and the total flame radiation energy would increase. A more dramatic impact of hydrogen content on flame radiation is shown in Figure 19 (taken from ref. 16), where total radiant energy is plotted as a function of combustion pressure and fuel hydrogen content. Two distinct characteristics are observable: (1) total radiant energy increases dramatically as the hydrogen content of the fuel is decreased at a con-

stant combustion pressure; and (2) total radiant energy increases significantly as combustion pressure is increased at a constant fuel hydrogen content. Reducing hydrogen content or increasing pressure both increase soot concentrations and thus increase flame luminosity.

### Emission Characteristics

The effect of fuel properties on the formation of pollutants manifests itself in both soot (particulate) and gaseous emissions. The effect of hydrogen content on the smoke emissions of a single-can combustor is shown in Figure 20 (taken from ref. 15). Over the range of hydrogen content tested, a nearly twofold difference in smoke number was measured. The effect of hydrogen content on the  $\text{NO}_x$  emissions of this combustor is shown in Figure 21 (also taken from ref. 15). The increase in  $\text{NO}_x$  emissions noted is attributed to the increase in maximum flame temperature that was illustrated in Figure 18. The combined effect of hydrogen content and fuel volatility on the formation of total unburned hydrocarbon (HC) and carbon monoxide (CO) emissions in a single-can combustor is shown in Figure 22 (taken from ref. 17). The largest effect is at the low-power operating conditions, where low pressure, temperature, and fuel-air ratio are all conducive to poor combustion efficiency and, hence, high CO and HC emission levels. Reducing fuel volatility and hydrogen content (i.e., going from a Jet B (JP-4) to a no. 2 diesel fuel (DF-2)) resulted in a more than twofold increase in HC emissions and a 50-percent increase in CO emissions at the lowest power condition (idle). The increases in the CO and HC emissions are most likely the result of poor fuel atomization and vaporization characteristics.

One other fuel property that affects the formation of pollutant emissions is shown in Figure 23 (taken from ref. 18), where the  $\text{NO}_x$  emissions of a single-can combustor are plotted as a function of fuel-bound-nitrogen content for various simulated engine operating conditions. At all operating conditions, increasing fuel-bound nitrogen resulted in substantial increases in the  $\text{NO}_x$  emissions. These increases are caused by the conversion of fuel-bound nitrogen to nitric oxide. The conversion rate for this process can vary from about 50 percent to 100 percent, depending on combustion geometry and operating conditions.

### Ignition Characteristics

Two fuel properties that have a significant effect on the ignition characteristics of a fuel are volatility and viscosity. Viscosity plays an important role in determining the effectiveness of a fuel injector in atomizing the fuel into small, easily ignitable droplets. (Fig. 16.) The ignition limits of several fuels are plotted as a function of combustor primary-zone equivalence ratio in Figure 24 (taken from ref. 17). Significantly higher primary-zone equivalence ratios (higher injector fuel flows) were needed to successfully ignite the higher-boiling-range fuels than to ignite the lower-boiling-range, more volatile JP-4 fuel. For the operating conditions chosen for these tests, no. 2 diesel fuel (DF-2) could not be ignited without adding a blending fuel (10-percent pentane). One other characteristic shown in this figure is also worth mentioning: For any given fuel, the time to start can be dramatically affected by the flow rate through the injector, as indicated by variations in primary-zone equivalence ratio. The injector spray pattern can be severely distorted at low fuel flow rates (low nozzle pressure drop) especially for the more viscous fuels.

Throughout the foregoing discussion, the effects of selected fuel properties on combustion and emission characteristics were described. It was pointed out that several fuel properties may combine to produce a particular adverse effect and that it is not always clear which property is the predominant factor. Nonetheless, certain trends can be attributed to particular fuel properties and, therefore, changes in these properties in future fuels will cause results similar to those that were illustrated. Therefore, if fuel properties change in accordance with the proposed broad-specification fuel described in the preceding section of this paper, we can expect to be faced with the need to evolve advanced technology to minimize the adverse impacts on combustion, emission, and ignition that have been discussed.

### THERMAL STABILITY

Aircraft jet fuels must be stable at the temperatures that they will encounter in the fuel system. No gums or deposits should occur on heated surfaces such as heat-exchanger tubes and no cracking or particulate formation should occur that could clog small passages such as those in fuel nozzles. Laboratory tests that have been developed to check on this particular fuel behavior subject the fuel to a thermal stress in a test rig such as that shown schematically in Figure 25. A small tube is heated electrically to the test temperature. The fuel flows up through an annulus surrounding this heated surface and out through a test filter. During this procedure, any tendency of the fuel to form particulates large enough to block the test filter can be noted by a buildup of pressure drop across the filter. At the same time, deposits may also form on the heated tube. Any chemical changes bringing about the fuel instabilities should occur at an increased rate



as the fuel temperature is increased. In general, either the pressure drop across this test filter increases at a faster rate or the indicated deposits on the tube build up at a faster rate, as the test temperature is increased. Thus, one way of comparing the thermal stabilities of fuels is to determine the maximum temperature of the heated tube before the test exceeds certain specified limits of pressure drop or tube deposit buildup. This temperature is then referred to as the "breakpoint temperature."

Breakpoint temperatures for a number of oil-shale- and coal-derived fuels were determined by using the test apparatus shown in Figure 25 (taken from ref. 19). The results are shown in Figures 26 and 27, where the breakpoint temperatures were determined from tube deposit buildup, which turned out to be the limiting factor. Figure 26 shows the effect of fuel-bound-nitrogen content on breakpoint temperature for several oil-shale-derived fuels. The variation in fuel-bound-nitrogen content was controlled by hydrotreating the fuels to different degrees of severity. The effect of the fuel-bound-nitrogen content is significant, and these data indicate that nitrogen content in excess of 0.01 percent by weight would reduce the breakpoint temperature to levels below the minimum allowable for current Jet A fuel. Therefore, crude oils with high fuel-bound-nitrogen content would have to be hydrotreated to meet current fuel specifications. Although it is known that fuel-bound nitrogen is a factor contributing to the instability of fuels, it is not possible to determine if it is solely responsible for the stability difference shown in Figure 26.

Figure 27 shows the breakpoint temperature for some coal-derived fuels as a function of the weight percentage of hydrogen. The fuel-bound nitrogen in all the fuels was 6 ppm or less. In this case, a general trend was to higher breakpoint temperatures as the hydrogen content was increased: A 260° C breakpoint generally required at 1st 13-percent hydrogen content. Typical Jet A, which has a hydrogen content of about 13.5 to 14 percent, must have a breakpoint temperature greater than 260° C.

Another factor that affects breakpoint temperature is the final boiling point of jet fuels. Figure 28 shows the decreasing trend that breakpoint temperature follows for fuels from two different syncrudes as the final boiling point of the fuels is increased. The difference in level between the two curves is most likely caused by differences in hydrogen and fuel-bound-nitrogen content. Figures 26 to 28 present some of the early stability data available on turbine fuels from synthetic sources and indicate the general severity of the refining processing that would be required to produce synthetic fuels with stabilities comparable to those of current jet fuels.

#### CONCLUDING REMARKS

The available sources of petroleum crude oil that are used to produce aircraft engine jet fuel have been slowly undergoing changes in several critical properties. Foremost among these changes is the slow average increase in the content of aromatic compounds and several rather large increases in these compounds that have recently occurred or are projected to occur (e.g., in Alaskan crude oil). These large increases in aromatic content have led to considerable concern regarding the hydrogen content in jet fuels derived from these crude-oil sources. Making up for future shortages of middle-distillate fractions by "cracking" higher-boiling-range petroleum fractions would also result in higher-aromatic-content jet fuels unless hydroprocessing were used to upgrade these fuels to current-specifications. In addition, initial evaluations of the characteristics of jet fuels that could be refined from syncrudes obtained from oil shale and coal have shown that considerable hydrotreating will be needed to upgrade the hydrogen content of these fuels to satisfy current specifications. Along with these concerns about hydrogen content, indications are that variations in fuel-bound-nitrogen content, boiling range, freezing point, and trace constituents may all be encountered in future fuels, especially in those derived from syncrudes. In this paper, the effect of varying all the aforementioned fuel properties on the combustion and thermal stability characteristics of a fuel were described and discussed. A knowledge of how severe the effects of variations in hydrogen content, fuel-bound-nitrogen content, and boiling range are on such combustion phenomena as soot and carbon formation, emissions, and ignition, is going to be needed. The severity of these related effects will be an important consideration in determining the tradeoff between the cost and energy consumption needed at the refinery to produce current-specification fuel and the cost of developing new engine combustion chambers that can use broaden-specification fuel.

To provide a common basis for obtaining the data needed for this tradeoff, a specification for a reference-type fuel was developed at a workshop conducted at the NASA Lewis Research Center (11). The proposed specifications for this experimental referee broad specification (ERBS) aviation turbine fuel are presented in Table VII. Both the proposed specification levels and the measurement techniques for determining these levels are shown. The principal properties that have been "broadened" are those that have been discussed in this paper: composition (hydrogen content), volatility (boiling range), fluidity (freezing point and viscosity), and thermal stability (breakpoint temperature). The use of this common broad-specification fuel in experiments conducted by many investigators should provide a basis for maximizing the usefulness of basic studies as well as a basis for comparing the ability of future aircraft-engine combustors to successfully operate with a broad-specification fuel. Future experimental studies should not and will not be confined to the ERBS fuel. Continued effort is still needed to parametrically evaluate the impact that large variations in properties, as discussed in this paper, has on the combustion and thermal stability characteristics of future fuels.

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TABLE I. - COMPOSITION OF PETROLEUM CRUDE OILS

Crude source	Con-stituents	Total crude	Middle-distillate fractions		
			Boiling point, °C		
			120 - 205	205 - 275	275 - 345
			Content, wt%		
Nigeria (light)	Sulfur Nitrogen Hydrogen	0.14 .12 13.0	0.02 .001 13.4	0.09 .001 13.1	0.17 .012 12.8
Aga-Jari, Iran	Sulfur Nitrogen Hydrogen	1.34 .13 13.0	0.04 .001 14.3	0.40 .004 13.6	0.95 .010 13.1
Kuwait	Sulfur Nitrogen Hydrogen	2.53 .13 12.7	0.10 .001 14.2	0.45 .092 13.8	1.52 .10 13.1
Alaska (Prudhoe Bay)	Sulfur Nitrogen Hydrogen	1.04 .23 12.3	0.05 .001 13.8	0.23 .009 13.0	0.60 .028 12.7

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TABLE II. - COMPOSITION OF "SYNTHETIC" CRUDE OILS

Crude source (process)	Constituents	Total crude	Middle-distillate fractions		
			Boiling point, °C		
			120 - 205	205 - 275	275 - 345
Content, wt%					
Shale oil (Paraho)	Sulfur	0.71	0.90	0.66	0.69
	Nitrogen	2.0	.001	1.01	1.9
	Hydrogen	11.5	12.5	12.2	11.5
Shale oil (Tosco)	Sulfur	0.67	0.85	0.82	0.75
	Nitrogen	1.85	1.0	1.45	1.86
	Hydrogen	11.6	13.1	12.3	11.5
Shale oil (Garrett-Insitu)	Sulfur	0.64	0.65	0.55	0.60
	Nitrogen	1.30	.001	.46	1.03
	hydrogen	11.8	12.6	12.5	12.0
Coal syncrude <sup>a</sup> (Synthoil)	Sulfur	0.22	0.10	0.092	0.14
	Nitrogen	.79	.30	.29	.32
	Hydrogen	9.2	11.0	10.8	10.4

<sup>a</sup> Kentucky coal.

TABLE III. - CHARACTERISTICS OF AVIATION TURBINE FUEL

Characteristic	Effect or relevance
Heat of combustion	Specific fuel consumption; takeoff gross weight
Specific gravity	Heat of combustion (by weight, by volume)
Volatility	Ignition; altitude reight; idle emissions; evaporation loss; carbon formation
Viscosity	Fuel atomization; ignition; pumpability
Aromatics (H/C)	Smoke; flame radiation; heat of combustion; carbon formation; thermal stability
Flashpoint	Fire safety
Freezing point	Pumpability on high-altitude, long-range missions
Sulfur	Corrosion; emissions
Olefins	Gum formation (thermal stability)
Thermal stability	Maximum fuel temperature; fuel deposition

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TABLE IV. - SPECIFICATIONS FOR AVIATION TURBINE FUEL

	ASTM D1655-77 standard specification for aviation turbine fuel		Average properties of Jet A (1976 EPLA)
	Jet B	Jet A, Jet A-1 <sup>b</sup>	
Composition: maximum content of -			
Aromatics, vol%	20	20	17.0
Sulfur (total), wt%	0.3	0.3	0.06
Naphthalenes, wt%	-----	a <sub>3</sub>	1.70
Olefins, vol%	-----	a <sub>1</sub>	1.10
Volatility:			
Distillation temperature (max.), °C:			
Initial boiling point	-----	-----	171
10% recovered	-----	204	188
20% recovered	143	-----	195
50% recovered	188	a <sub>2</sub> 32	213
90% recovered	243	Report	246
Final boiling point	-----	300	267
Flashpoint (min.), °C	-----	37.8	53.7
Reid vapor pressure (max.), kPa	20.7	-----	
Specific gravity (15° C/15° C)	0.751 - 0.802	0.775 - 0.840	
Fluidity:			
Freezing point (max.), °C	-50	b <sub>1</sub> -40	-46
Viscosity at -34° C (max.), m <sup>2</sup> /s (cS)	-----	c <sub>1</sub> 15x10 <sup>-6</sup>	9.3x10 <sup>-6</sup>
Net heat of combustion (min.), kJ/kg	42 800	42 800	43 280
Thermal stability (JFTOT breakpoint temperature, °C)	260	260	-----

<sup>a</sup> Value is from earlier specifications; current specifications omit this.

<sup>b</sup> Jet A-1 freezing point is -50° C.

<sup>c</sup> Current viscosity specification is 8x10<sup>-6</sup> m<sup>2</sup>/s (cS) at -4° C.

TABLE V. - MAJOR PROJECTED CHANGES IN  
FUEL PROPERTIES

	Current Jet A	Future broad- spec fuel
Aromatic content, vol%	17 - 25	30 - 35
Hydrogen content, wt%	14 - 13.5	13.0 - 12.5
Final boiling point, °C	260 - 280	290 - 330
Freezing point, °C	-46 - -40	-34 - -29
Thermal stability (JFTOT breakpoint temp, °C)	≥260	≥240

TABLE VI. - CURRENT AND FUTURE FUEL-CHARACTERIZATION METHODS

Fuel characteristic	ASTM method (current specification)	Test method for future fuel (broad specification)
Composition:		
Aromatic content, vol%	Fluorescent indicator absorption (ASTM D1319-77)	Direct determination of hydrogen weight percent, i.e., by nuclear magnetic resonance, for higher aromatics
Naphthalene content, vol%	Ultraviolet spectrography (ASTM D1840-64)	Hydrocarbon compositional analysis, i.e., gas chromatography - mass spectroscopy, for synfuels
Nitrogen, ppm	None	Kjeldahl or equivalent approach, for nitrogen-containing fluids
Volatility	ASTM distillation (D86-77) or other methods	Simulated distillation by gas chromatography, for high-boiling-point fuels
Fluidity	Freezing point determination (ASTM D2386-67)	Pumpability test for high-freezing-point fuels or correlation of freezing point with pumpability
Thermal stability	CRC coker (ASTM D1660-72) or jet-fuel thermal oxidation test (ASTM D3241-77)	Improved correlation with engine deposition and life; improved test methods

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TABLE VII. - PROPOSED SPECIFICATIONS FOR EXPERIMENTAL REFEREE BROAD-SPECIFICATION (ERBS) AVIATION TURBINE FUEL

Specification.	ERBS jet fuel	Proposed test method
Composition:		
Hydrogen content, wt%	12.8±0.2	Nuclear magnetic resonance
Aromatic content, vol%	Report	ASTM D1319
Sulfur content (mercaptan), wt%	0.003 (max.)	ASTM D1219
Sulfur content (total), wt%	0.3 (max.)	ASTM D1266
Nitrogen content (total), wt%	Report	Kjeldahl
Naphthalene content, vol%	Report	ASTM D1840
Hydrogen compositional analysis	Report	Gas chromatography - mass spectroscopy
Volatility:		
Distillation temperature, °C		
Initial boiling point	Report	ASTM D2892
10% recovered	205 (max.)	
50% recovered	Report	
90% recovered	260 (min.)	
Final boiling point	Report	
Residue, percent	Report	
Loss, percent	Report	
Flashpoint, °C	38 to 49	ASTM D56
Gravity, deg API at 15° C	Report	ASTM D287
Gravity (specific), (15° C/15° C)	Report	ASTM D1298
Fluidity:		
Freezing point, °C	-29 (max.)	ASTM D2386
Viscosity at -23° C, m <sup>2</sup> /s (cS)	12x10 <sup>-6</sup> (max.)	ASTM D445
Net heat of combustion, kJ/kg	Report	ASTM D2382
Thermal stability (JTOT breakpoint temperature, based on TDR = 13 or ΔP = 25 mm, °C)	240 (min.)	ASTM D3241

ACTION	ADVANTAGES	DISADVANTAGES
PRODUCE SPECIFICATION JET FUEL	OPTIMIZED FUEL PROPERTIES AIRCRAFT/ENGINE RETROFIT NOT REQUIRED	INCREASED REFINERY ENERGY CONSUMPTION INCREASED FUEL COST
RELAX JET FUEL SPECIFICATION	CONSERVATION OF ENERGY REDUCED FUEL COST	MORE COMPLEX COMPONENT TECHNOLOGY REQUIRED ADVERSE EFFECT ON ENGINE LIFE

Figure 1. - Assessment of potential actions.

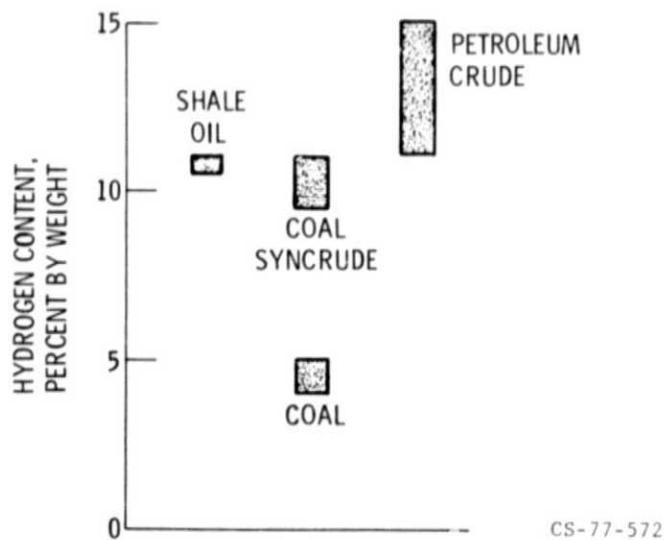


Figure 2. - Hydrogen content of alternative sources of jet fuel.

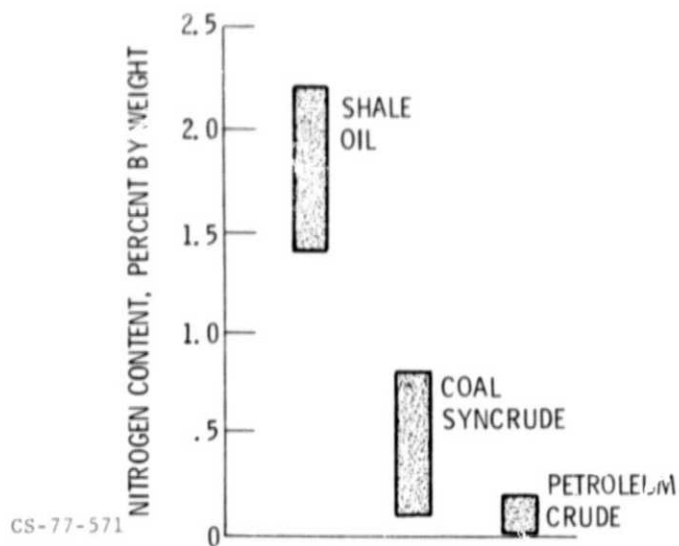


Figure 3. - Nitrogen content of alternative sources of jet fuel.

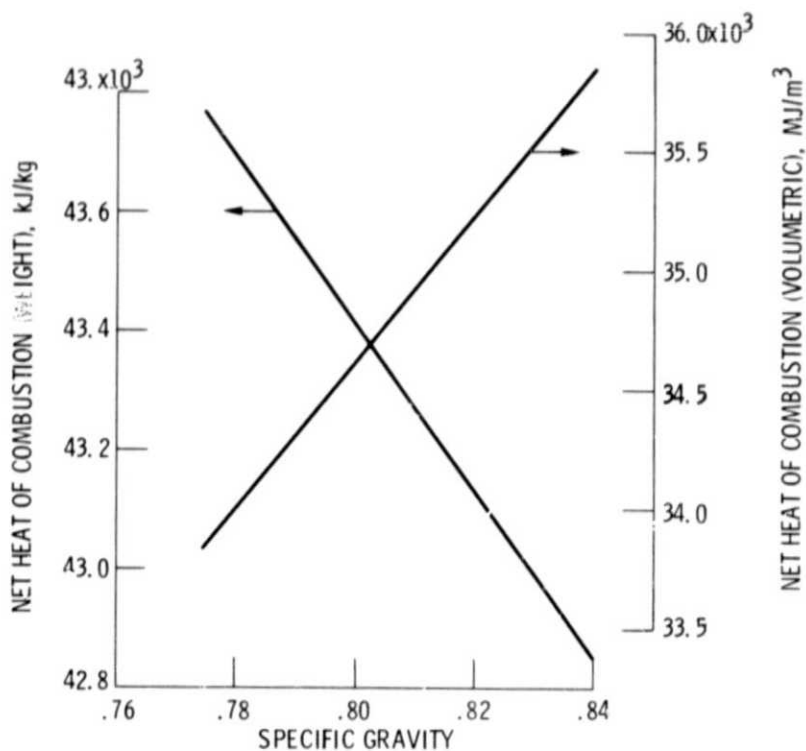


Figure 4. - Effect of specific gravity of jet fuels on heat of combustion by weight and volume.



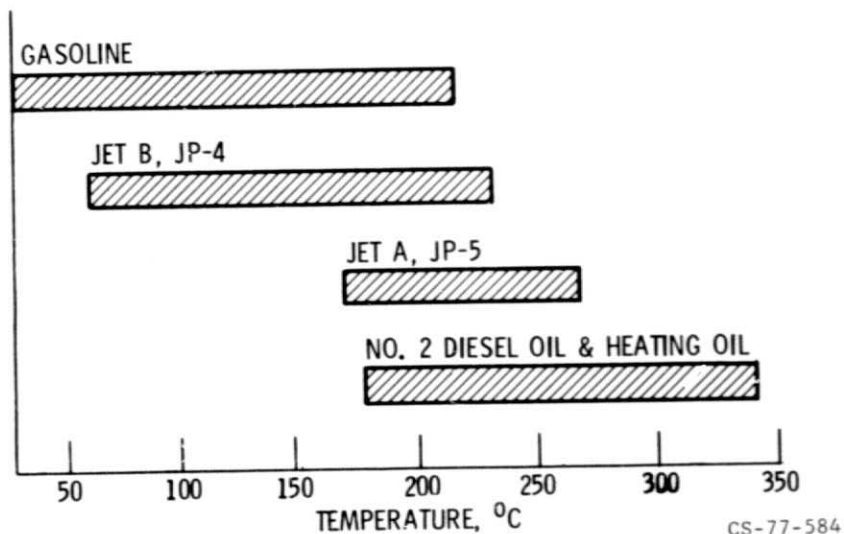


Figure 5. - Boiling range of various petroleum products.

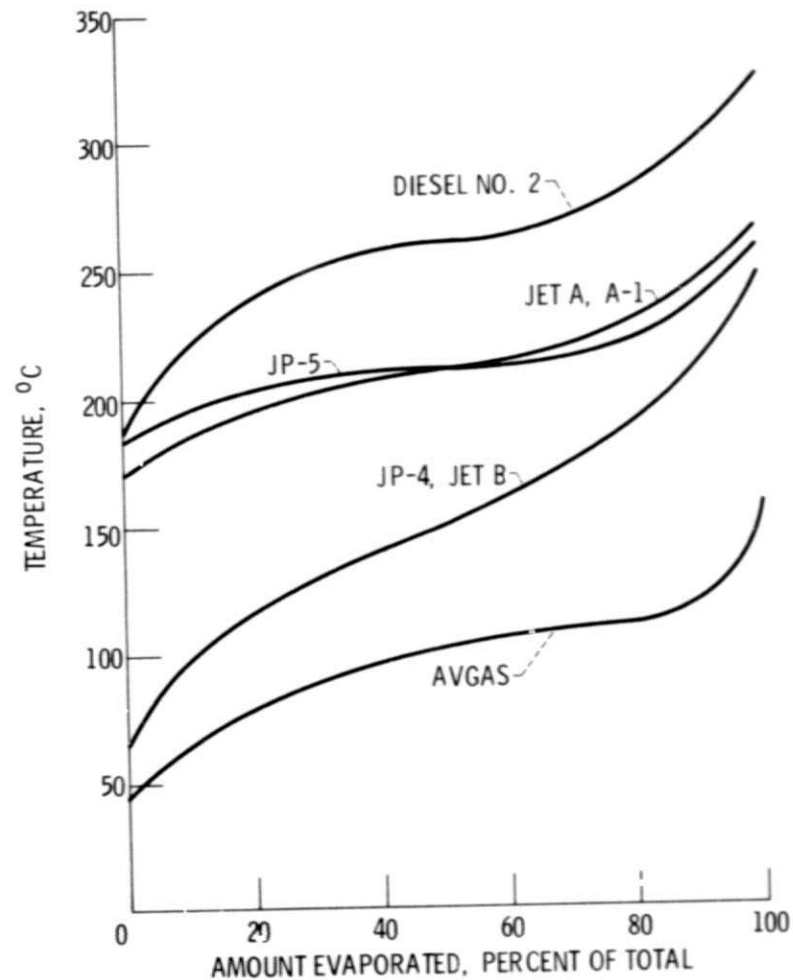


Figure 6. - ASTM D-86 distillation curves for various fuels. (Source, U. S. Bureau of Mines.)

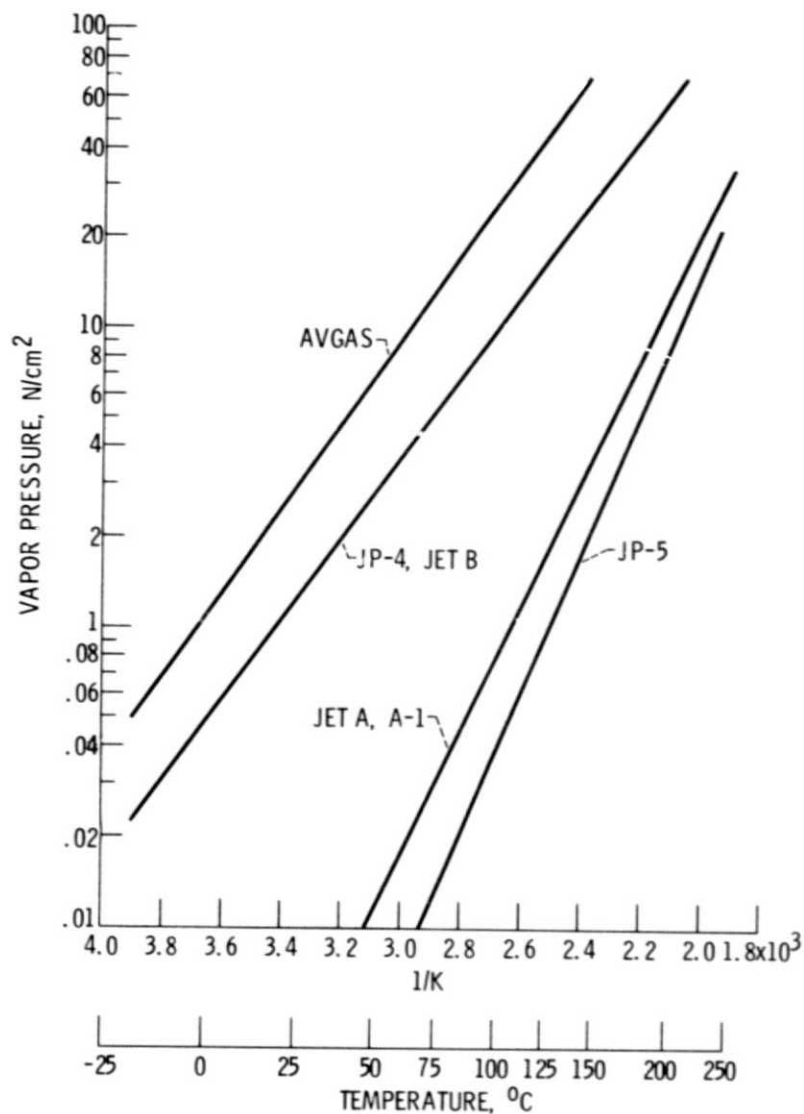


Figure 7. - Effect of temperature on true vapor pressure of aviation fuels. (From ref. 20.)

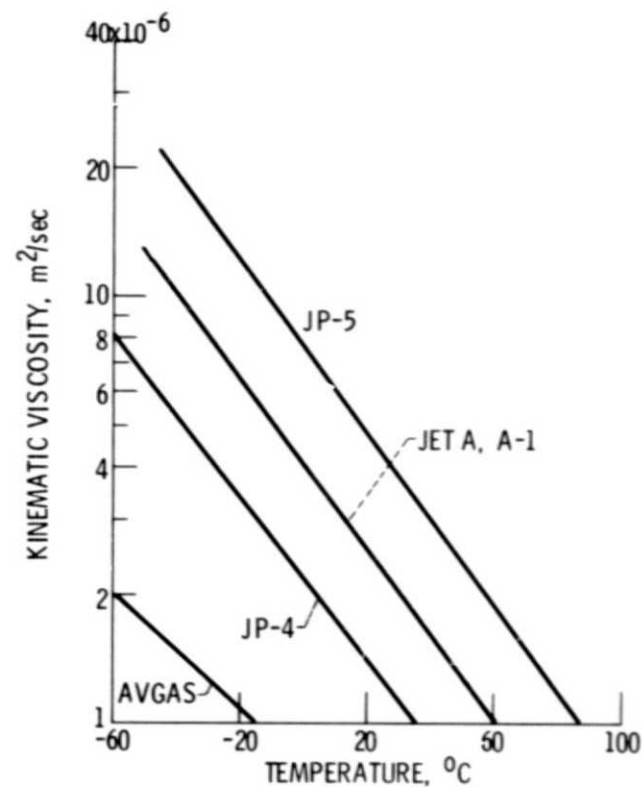


Figure 8. - Effect of temperature on fuel viscosity. (From ref. 20.)

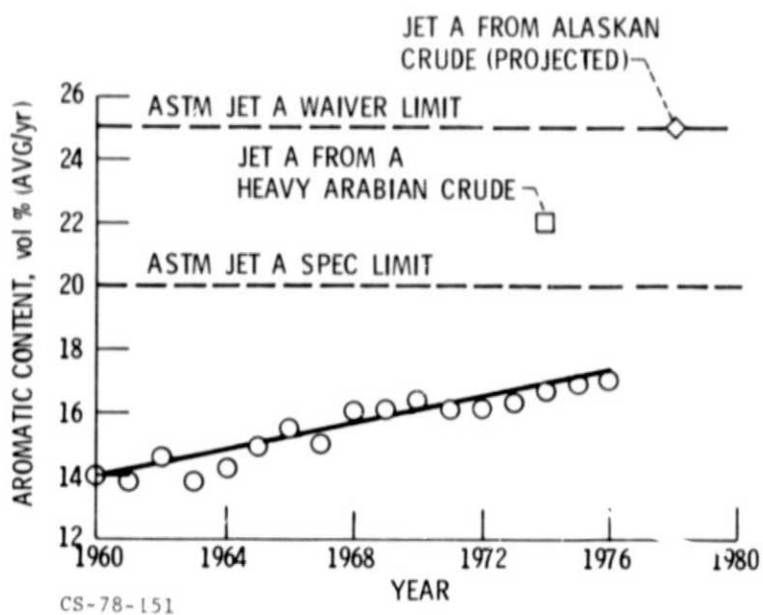


Figure 9. - Trend in aromatic content of commercial Jet A fuel.

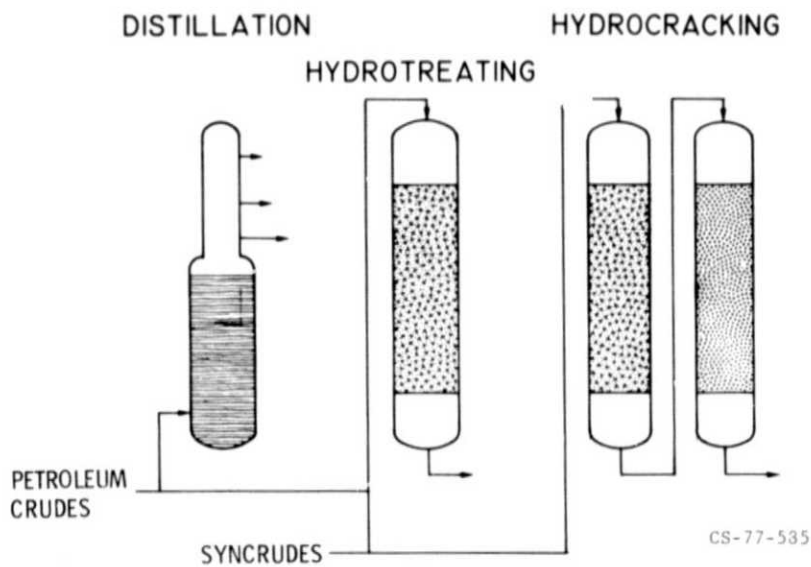


Figure 10. - Simplified refining sequence.

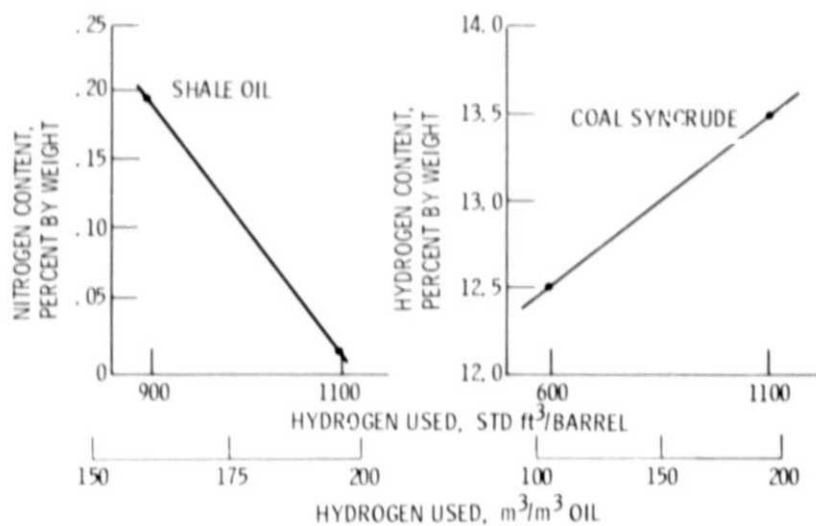


Figure 11. - Hydrogen consumption in processing.

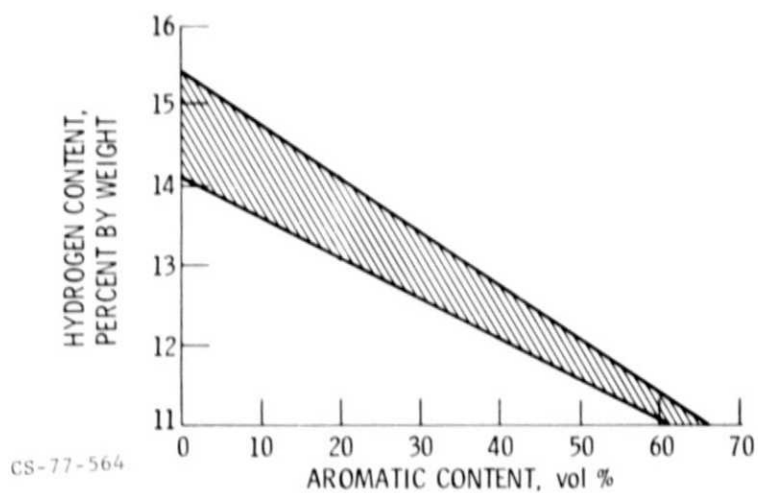


Figure 12. - Relation between aromatic content and hydrogen content.

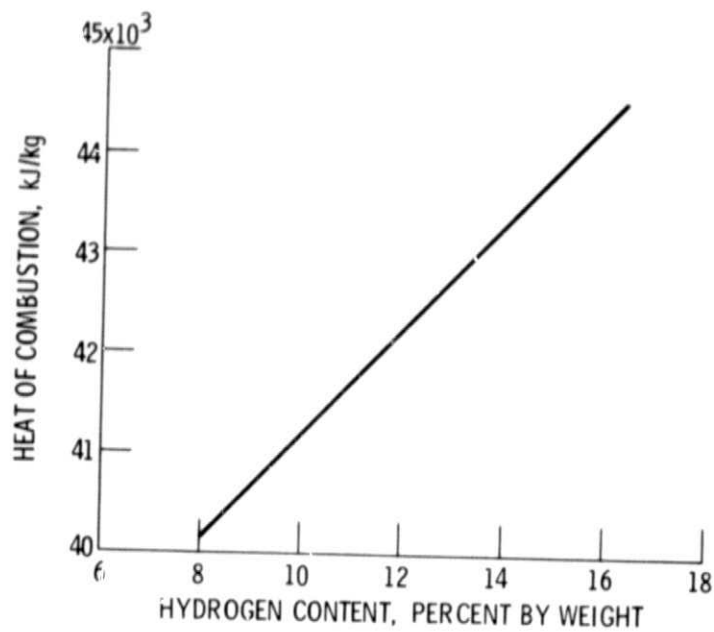


Figure 13. - Effect of fuel hydrogen content on heat of combustion.

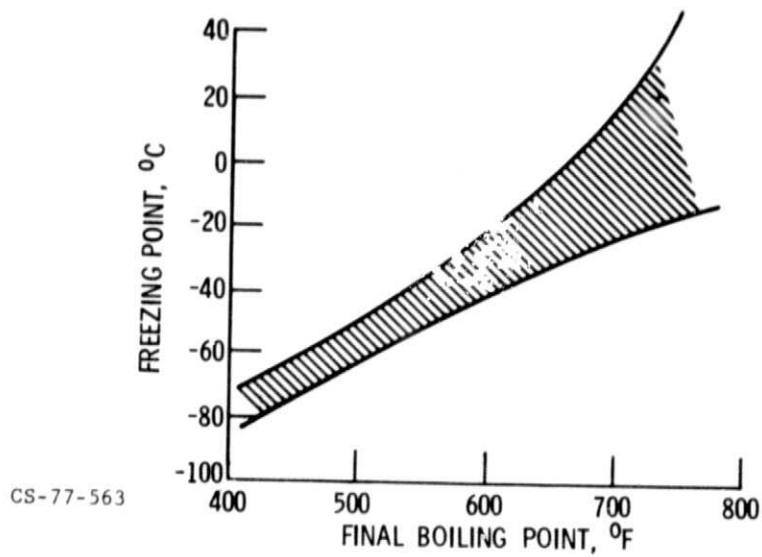


Figure 14. - Typical fuel-blend freezing points.

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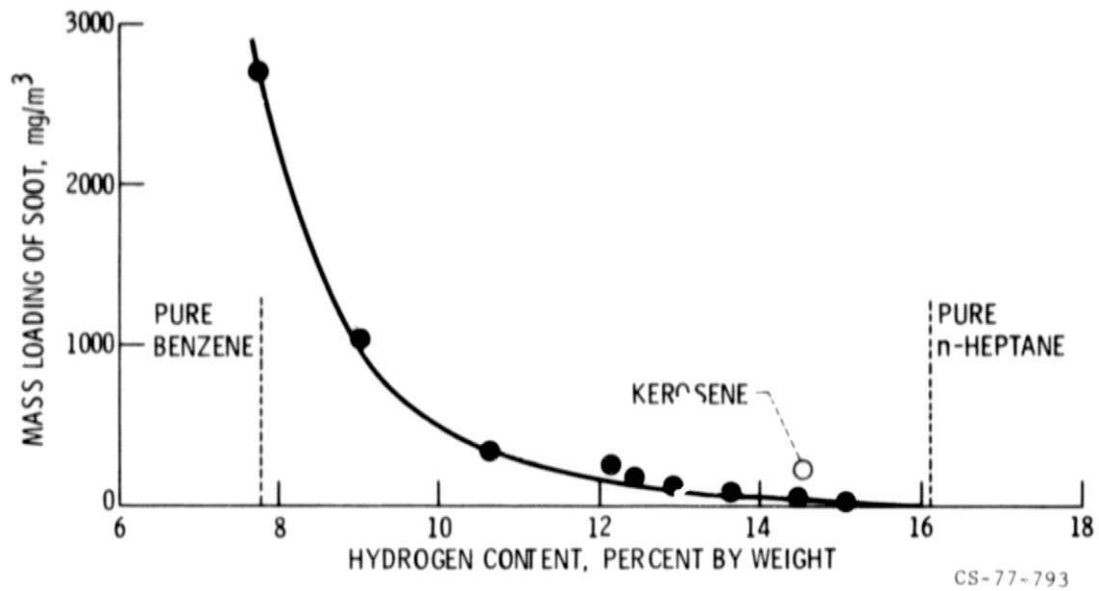


Figure 15. - Effect of fuel hydrogen content on peak soot concentration. (From ref. 12.)

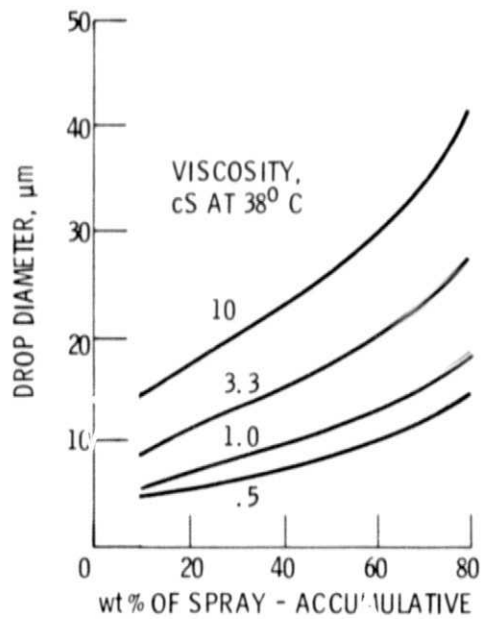
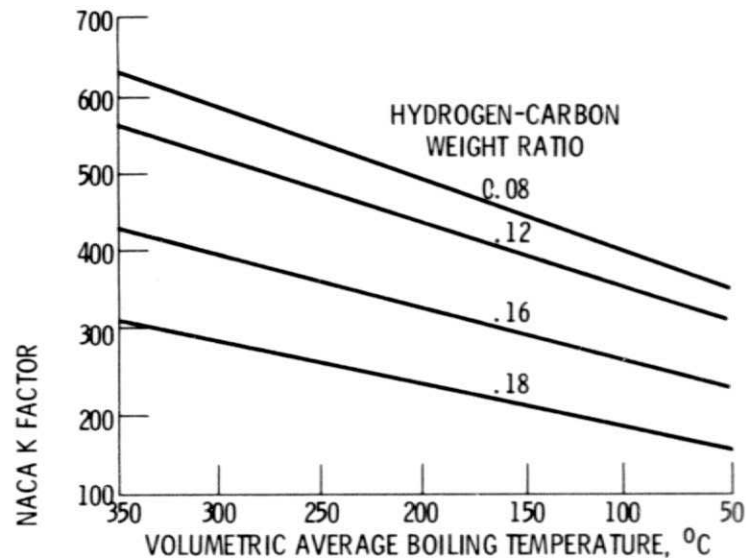
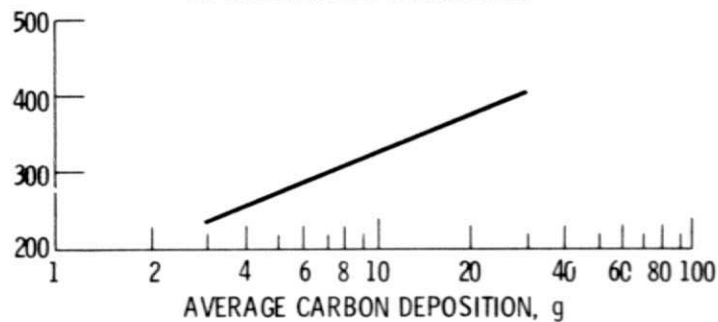


Figure 16. - Calculated effect of fuel viscosity on drop size distribution of sprays. (From ref. 13.)



(a) CORRELATING PARAMETER.



(b) CARBON DEPOSITION.

Figure 17. - Effect of fuel hydrogen content and volatility on carbon deposition. (From ref. 14.)

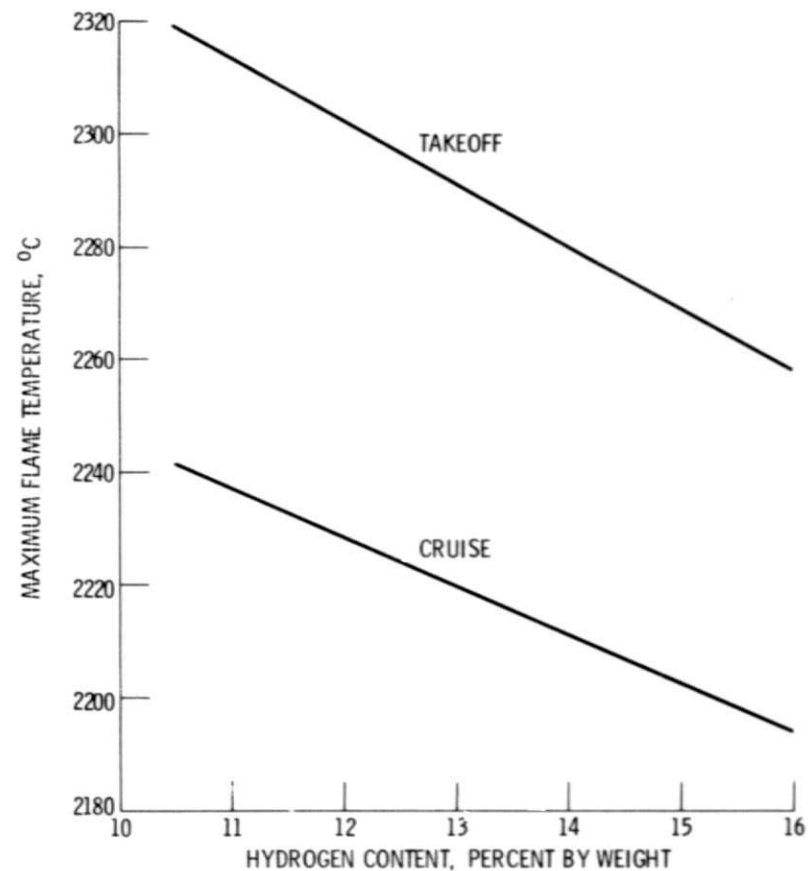


Figure 18. - Effect of fuel hydrogen content on maximum flame temperature.

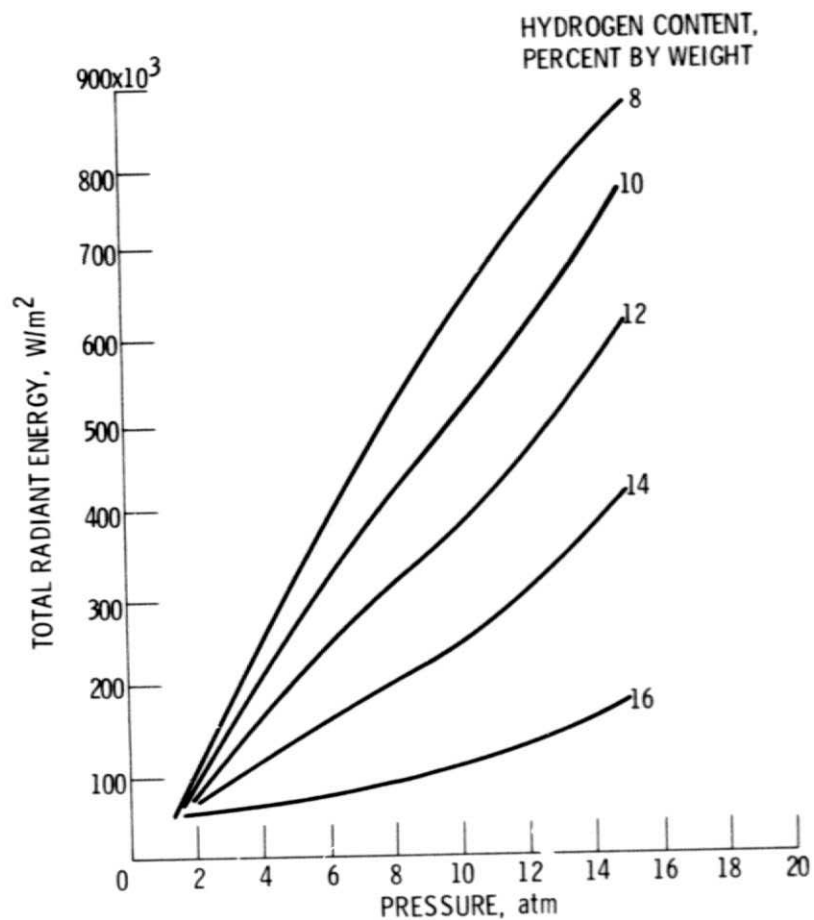


Figure 19. - Effect of fuel hydrogen content and pressure on flame radiation. Inlet-air temperature, 430° C. (From ref. 16.)

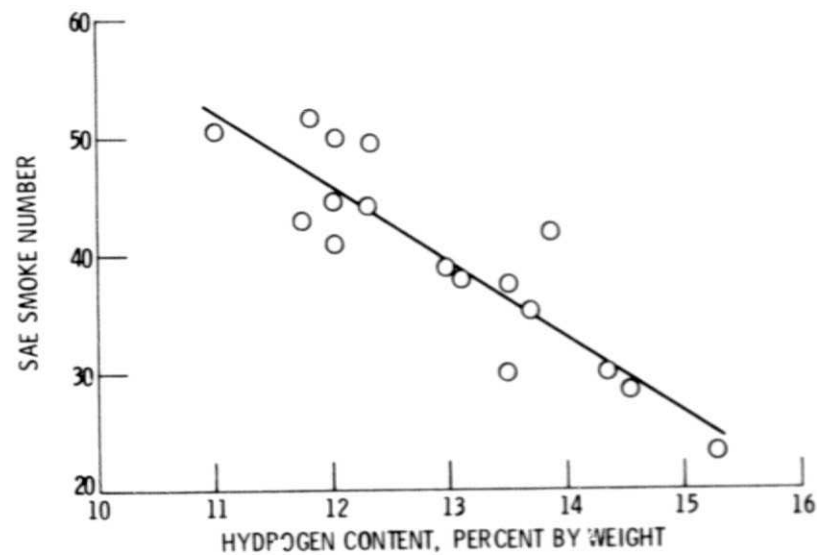


Figure 20. - Effect of fuel hydrogen content on smoke number at takeoff condition. (From ref. 15.)



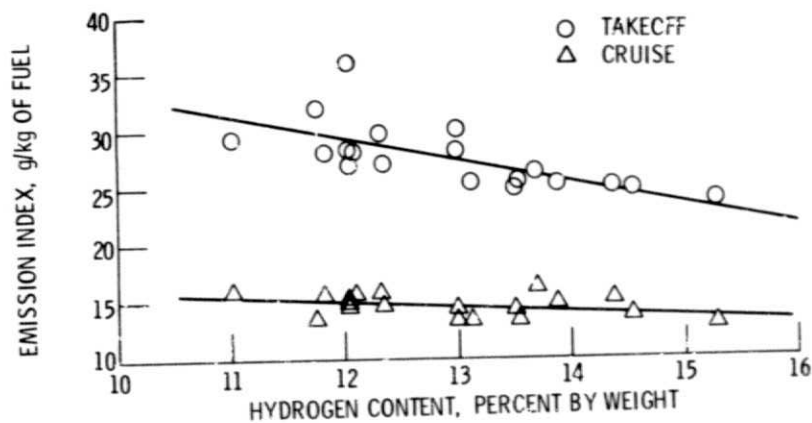


Figure 21. - Effect of fuel hydrogen content on oxides-of-nitrogen emissions at takeoff and cruise conditions. (Taken from ref. 15.)

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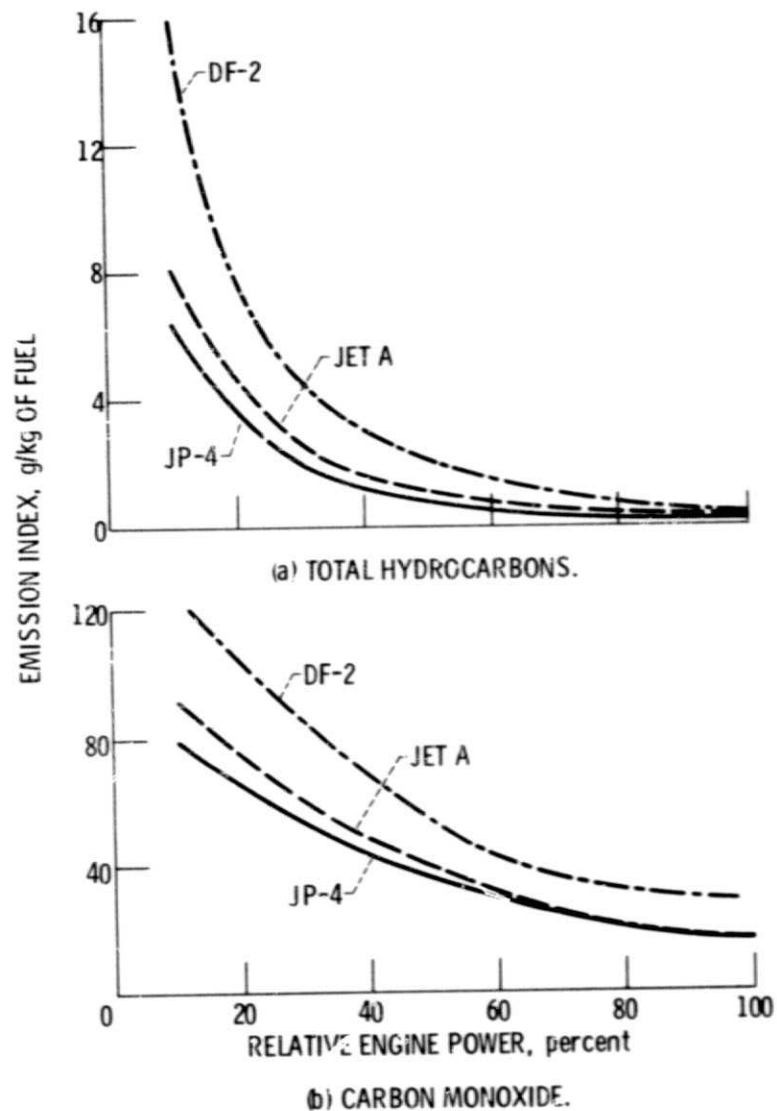


Figure 22. - Effect of fuel type on total hydrocarbon and carbon monoxide emissions. (From ref. 17.)

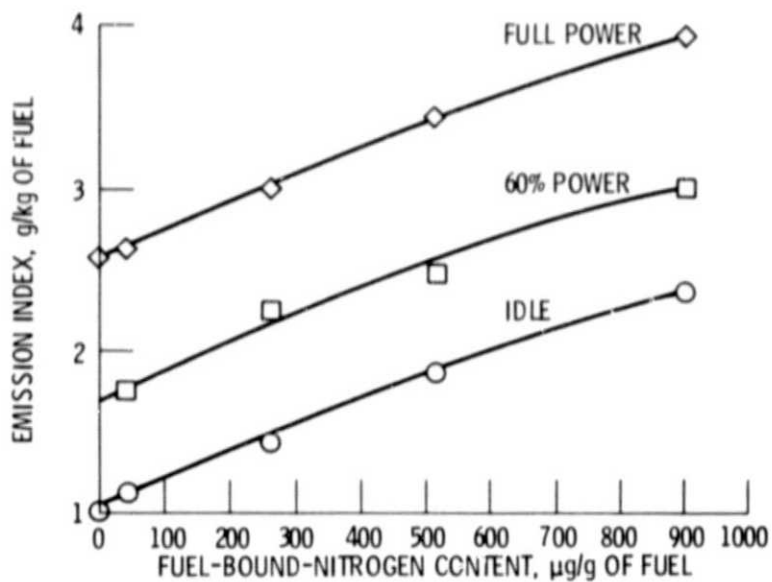


Figure 23. - Effect of fuel-bound-nitrogen content on total emissions of nitrogen oxides. (From ref. 18.)

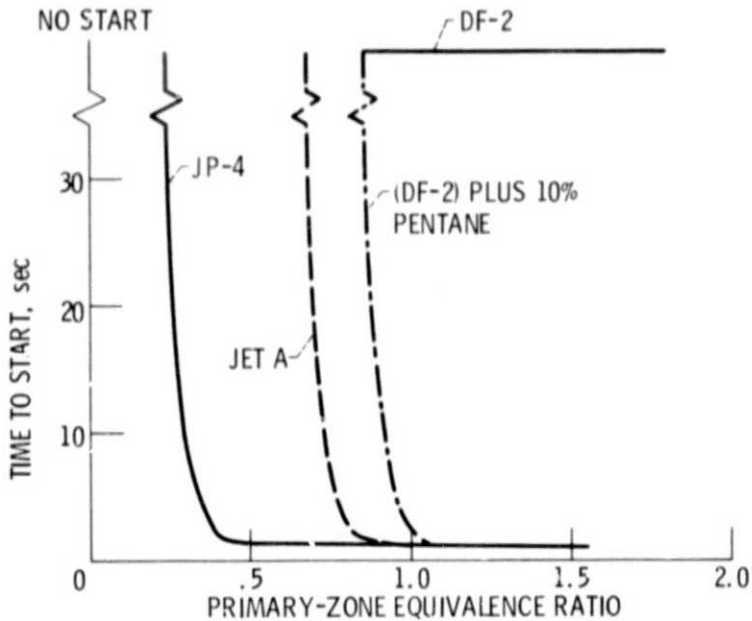


Figure 24. - Combustor ignition characteristics using different fuels. (From ref. 17.)

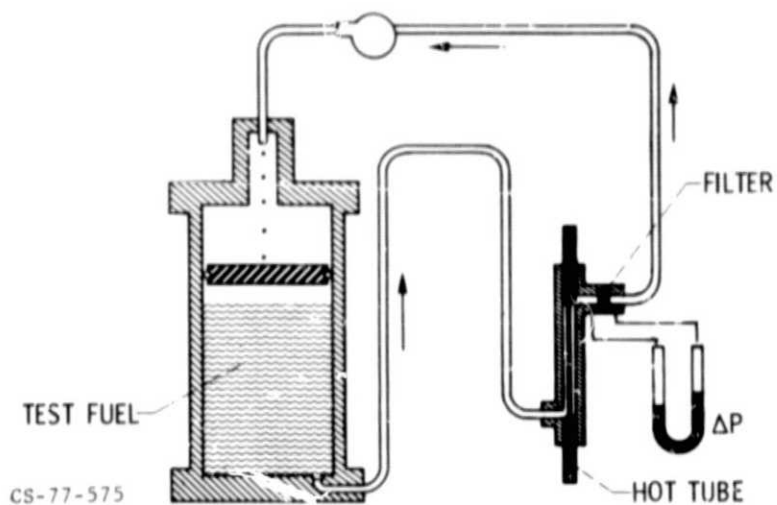


Figure 25. - Schematic of thermal-stability test rig. (From ref. 19.)

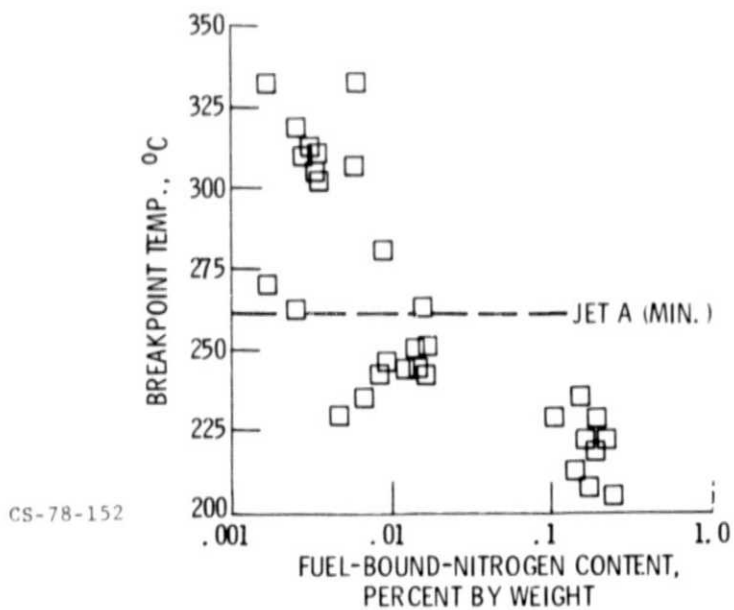


Figure 26. - Effect of nitrogen level in oil shale-derived fuels on breakpoint temperature.

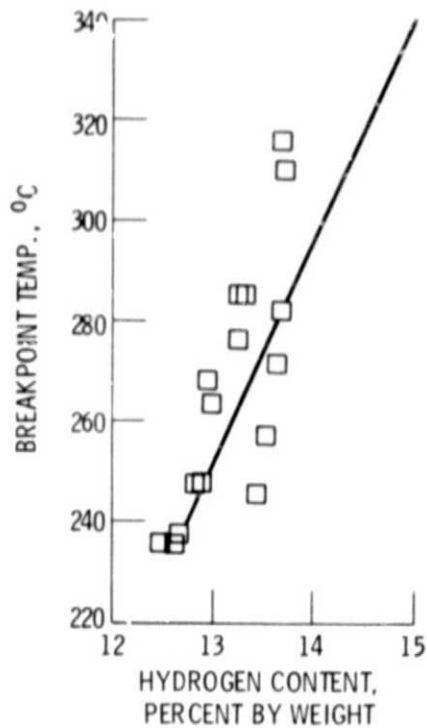


Figure 27. - Effect of hydrogen content in coal-derived fuels on breakpoint temperature.

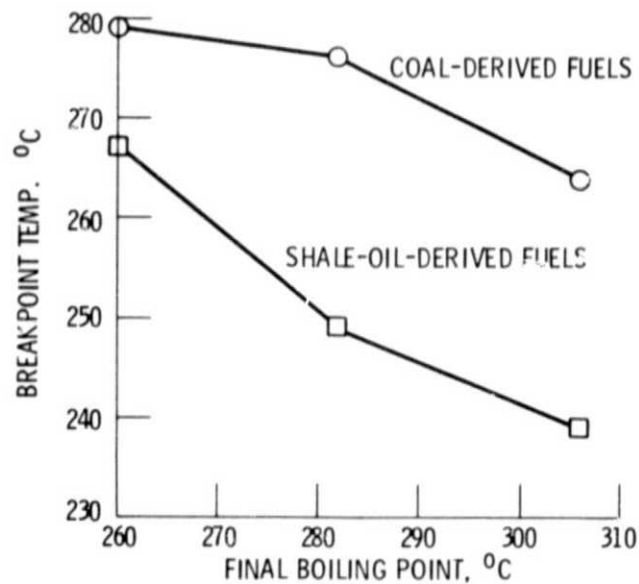


Figure 28. - Effect of final boiling point on fuel thermal stability.

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