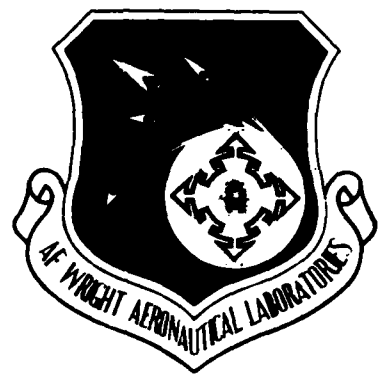


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FUEL PROPERTY EFFECTS ON COMBUSTION

Cynthia A. Obringer
Fuels Branch
Fuels and Lubrication Division

October 1985

Final Report for Period September 1984 - April 1985.

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


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19. ABSTRACT (Continue on reverse if necessary and identify by block number) This report deals with fuel property effects on gas turbine engine combustors. The main subject covered in the report is a statistical analyses of the data from a program conducted by Rosfjord of United Technologies Research Center under a contract with NASA Lewis Research Center. Also discussed is a "hydrogen available for release" theory first introduced by Solomon of Advanced Fuel Research, Inc. A threshold sooting index derived by Calcote and Manos of AeroChem Research Laboratories, Inc. is also discussed.			
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FOREWORD

This Fuel Property Effects on Combustion Report was prepared by the Fuels Branch of the Aero Propulsion Laboratory, Air Force Wright Aeronautical Laboratories, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio. The work was performed under Work Unit 30480536. Ms Cynthia Obringer was the Project Engineer.

The report presents the results of a statistical study on the effects of changing fuel properties on gas turbine engine combustors. The combustor data used for the study was from a study performed by Dr T. J. Rosfjord at United Technologies Research Center under a contract with NASA (NASA Contract Report 168334).

The author wishes to thank 1Lt Richard Striebich for performing the hydrogen by NMR analyses, and Dr T. J. Rosfjord for providing the UTRC data, and thanks to both of them for taking the time to discuss the results. Thanks is also extended to Dr Peter R. Solomon for his many meaningful discussions. I also wish to thank Mr Charles Martel for his helpful suggestions in preparing the text.

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SECTION I

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INTRODUCTION

In order to increase jet fuel availability and decrease cost, the Air Force is investigating alternate feedstocks such as tar sands, shale oils, heavy oils, and coal derived fuels. As these lower quality feedstocks begin to play a major role as sources of military jet fuels, it becomes increasingly important to be able to evaluate the effects of these fuels on engine life and performance. ~~To date,~~ these effects have usually been measured using expensive and time-consuming engine tests.

During the past five years, the USAF has spent over \$7,000,000 on 11 different programs (References 1-11) to study fuel effects on gas turbine engine combustors. Of major concern in each of these programs was the effects of fuel properties and composition on soot formation, and the effects of soot on engine performance and durability. Being able to predict the change in soot formation due to changing fuel properties would be an invaluable tool in future research and development efforts to eliminate soot formation and its deleterious effects on engines. The reduction in exhaust plume, through reduced soot formation, reduces a vehicle's visibility for tracking and targeting purposes, thus increasing its survivability.

There have been several studies performed on the subject of fuel effects on soot formation with many different results. The findings of a recent study by Lefebvre, using the data from several gas turbine engine fuel effect programs (References 6-11), clearly brings into view the present level of understanding. Lefebvre writes, "it is quite possible that not all of the various types of aromatics (1-ring, 2-ring, etc.) are equally effective in producing soot; and thus a better correlation of smoke emission might be achieved by neglecting certain aromatic constituents of the fuel. Also worthy of further investigation is the use of hydrogen content, instead of percentage aromatics, as an indicator of propensity to soot formation" (Reference 2).

In a study by Pratt & Whitney Aircraft, using the same test data as Lefebvre, it was concluded that "smoke and combustion liner radiative heating correlate well with hydrogen content", (Reference 1). The two common results of both the Purdue University (Lefebvre) and Pratt & Whitney program were: that hydrogen content is as

effective as any parameter at predicting soot formation; and the questioning of the validity of the data, and the need for more and better data.

A study sponsored by the Air Force has been underway at Advanced Fuel Research, Inc. (AFR) to relate vaporization, pyrolysis and soot formation to fuel chemical properties. During Phase I of the contract, a Fourier Transform Infrared Spectroscopy (FT-IR) technique, developed by AFR, was used to identify a "hydrogen available for release" theory as possibly the most important factor affecting soot formation (Reference 12). The Phase I test results suggest that soot formation does not depend upon the total hydrogen content of a fuel but instead upon the hydrogen that is available during pyrolysis. In general, the more aromatic a fuel the lower its total hydrogen content will be. Thus low hydrogen content, or low hydrogen available for release, and high aromaticity go together.

SECTION II

APPROACH

Taking into consideration the need for high quality data, a study sponsored by NASA Lewis Research Center was undertaken by United Technology Research Center (UTRC) to rigorously study fuel chemical property influences on gas turbine engine combustion. The program was conducted using 25 test fuels that were especially chosen to cover a wide range of fuel properties. A full-scale cannular combustor was uniquely designed for this program. Fuel physical property effects were down-played to emphasize fuel chemical properties. This was accomplished by specifically choosing fuel injectors which produced a highly atomized, and thus rapidly vaporized, spray. For further details of the actual combustor and fuels used, see Reference 13.

The extra effort put forth by UTRC to rigorously study fuel chemical properties in combustion appears to have paid off. The excellent regression analyses results reported in Reference 13, Table 19, indicate something more than a random fit of data. It needs to be pointed out that although the results of the UTRC study are very significant, by further studying the data, still more can be learned.

Taking into consideration the quality of the data already available from the UTRC study and the successful completion of the Advanced Fuel Research, Inc. (AFR) Phase I study, the Air Force decided to sponsor a Phase II follow-on study to AFR's Phase I study. The on-going Phase II study at AFR is using the same 25 fuels used in the UTRC study to expand upon the AFR Phase I results. The objective of the program is to study droplets of the 25 test fuels using the FT-IR technique to measure pyrolysis species, and temperature and radiation characteristics. The FT-IR results will then be related to the combustor test and fuel property results from the previous program at UTRC.

Calcote and Manos (Reference 14) found a flaw in a "tendency to smoke" parameter, defined as a constant divided by the smoke point. The parameter did not account for increased flame height encountered with increasing fuel molecular weight. Calcote and Manos modified the parameter, now defined as Threshold Sooting Index (TSI) as

$$TSI = a(M/h)+b$$

where M is the molecular weight of the fuel, h is the height of the flame when soot is first observed, and a and b are constants that are dependent upon the particular experimental set up. If the TSI is a true indicator of soot formation, then molecular weight divided by smoke point should also be a good correlating parameter for predicting soot formation. Taking this into consideration, it was decided to try to correlate molecular weight/smoke point with the combustion test results from the UTRC study.

The molecular weights used for the molecular weight/smoke point correlations were calculated using a method outlined in "Petroleum Refinery Engineering" (Reference 15). This method of estimating molecular weights requires the volumetric boiling point, API Gravity, and ASTM slope degree/percent vaporized. The volumetric boiling point is the average of the 10%, 50%, and 90% distillation temperatures. The ASTM slope degree/percent vaporized is the ratio of the 70% to the 10% distillation temperatures divided by the 60% distillation temperature. The fuel distillation and specific gravity data required for these calculations can be found in the NASA report (Reference 13, Table 5).

Lefebvre (Reference 2), along with several others, has stated that there tends to be an increase in soot formation with a decrease in the hydrogen content of the fuel. This, along with AFR's "hydrogen available for release" theory, exemplifies the need to be able to accurately measure and/or calculate the hydrogen content of fuels. Taking this into consideration, hydrogen content was calculated using ASTM D3343-74, Standard Method for Estimation of Hydrogen Content of Aviation Fuels. The hydrogen content was also determined at Wright-Patterson Air Force Base, using ASTM D3701-81, Standard Test Method for Hydrogen Content of Aviation Turbine Fuels by Low Resolution Nuclear Magnetic Resonance Spectrometry. The hydrogen content of the same fuels had previously been determined by Southwest Research Institute (SRI) as part of the NASA study (Reference 13, Table 5). The method used at SRI was ASTM D3178-73, Standard Test Method for Carbon and Hydrogen in the Analysis Sample of Coal and Coke.

SECTION III

RESULTS TO DATE

1. MOLECULAR WEIGHT ESTIMATES

The chart used in the molecular weight determinations (Reference 15) was originally prepared for petroleum fractions. As a result, the accuracy of the molecular weights estimated for the experimental fuels used in this study is questionable. However, a check of the pure hydrocarbons used, i.e., decalin and tetralin, shows agreement within 95% of the actual molecular weights of these compounds. The calculated and actual molecular weights of the pure hydrocarbons are given in Table 1.

TABLE 1
MOLECULAR WEIGHTS OF DECALIN AND TETRALIN

	Decalin	Tetralin
Calculated	132	130
Actual	138	132

2. HYDROGEN CONTENT

A measure of the accuracy of the three different hydrogen content analyses can be obtained by comparing the known values of the two pure hydrocarbons, tetralin and decalin, with the test results. The calculated method (ASTM D3343) was within 93% and 97% of the actual values for decalin and tetralin, respectively. The results of both of the experimental determinations were within 99% of the actual values for both decalin and tetralin. Figure 1 is a plot of the hydrogen content determined by NMR (ASTM D3701) compared to hydrogen content determined by combustion (ASTM D3178). The known, calculated, and experimental results for decalin and tetralin appear in Table 2 below.

TABLE 2
HYDROGEN CONTENT OF DECALIN AND TETRALIN

	Decalin	Tetralin
Known	13.15	9.17
NMR	13.11	9.08
Combustion	13.10	9.14
Calculated	12.85	9.82

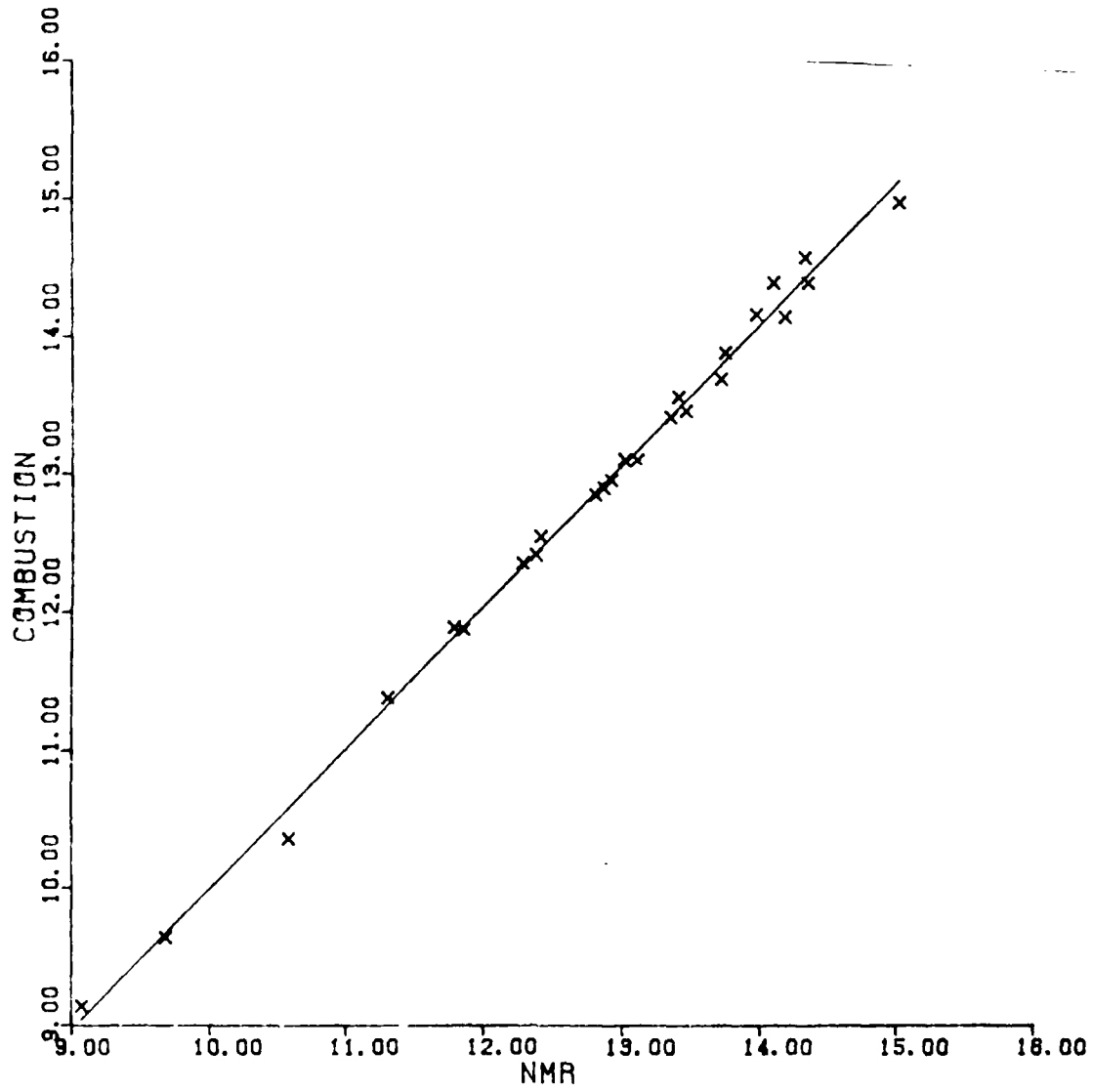


Figure 1. Comparison of Hydrogen Content for Two Analysis Techniques

Table 3 is a list comparing the hydrogen content determinations of the 25 fuels by the three different methods. As can be seen from Figure 1 and Table 3, the NMR and combustion results agreed extremely well.

TABLE 3
HYDROGEN CONTENT OF TEST FUELS

FUEL	NMR	COMBUSTION	CALCULATED
Tetralin	9.08	9.14	9.82
XTB	9.69	9.64	9.68
BLS	10.58	10.36	10.95
ERBLS 3	11.31	11.38	11.75
ERBLS 2	11.79	11.89	12.18
UTRC 2A	11.86	11.87	12.30
ERBLS 1	12.29	12.35	12.54
UTRC 3B	12.38	12.41	12.72
UTRC 7A	12.42	12.54	12.76
UTRC 8A	12.81	12.84	13.14
UTRC 9A	12.87	12.89	12.81
ERBS	12.92	12.95	13.05
UTRC 9B	13.02	13.10	13.11
Decalin	13.11	13.10	12.85
AFAPL 6	13.35	13.41	13.41
AFAPL 2	13.41	13.56	13.39
DF 2	13.47	13.46	13.49
Jet A	13.72	13.69	13.61
JP5	13.75	13.88	13.66
JP4-A	13.98	14.16	13.88
JP4-S	14.10	14.39	14.22
QMSO	14.19	14.14	14.06
JP4	14.33	14.57	14.34
JP7	14.36	14.39	14.29
UTRC 1	15.02	14.97	14.77

3. REGRESSION ANALYSES

Statistical correlations were calculated for fuel hydrogen content, smoke point, and molecular weight/smoke point with the UTRC measured combustor dome radiation, liner temperature and exhaust smoke number data. UTRC had already performed statistical correlations of hydrogen content and smoke point using a logarithmic function. Upon plotting hydrogen content versus dome radiation (Figure 2), it was observed that the data followed a linear fit better than a logarithmic fit. Thus, new regression analyses were calculated by the author for both the real and logarithmic planes and are presented in Table 4.

It can readily be seen that performing the regression analyses in the real plane, instead of the logarithmic plane as done at UTRC, improved all the correlations for hydrogen content. Table 5 presents results from the linear regression analyses of dome radiation, liner temperature and smoke number data with hydrogen content for all three test conditions.

It was expected that dome radiation, liner temperature, and smoke number should all react the same to a change in fuel. If they do indeed react the same to a fuel change, the result of correlating any two of the above parameters should give a perfect correlation coefficient ($R^2=1$). The different variables were correlated in this manner using the data from the UTRC study. The results reported in Table 6, show that dome radiation and liner temperature correlate better than either dome radiation or liner temperature with smoke number. This is expected considering the poor precision of smoke number measurements.

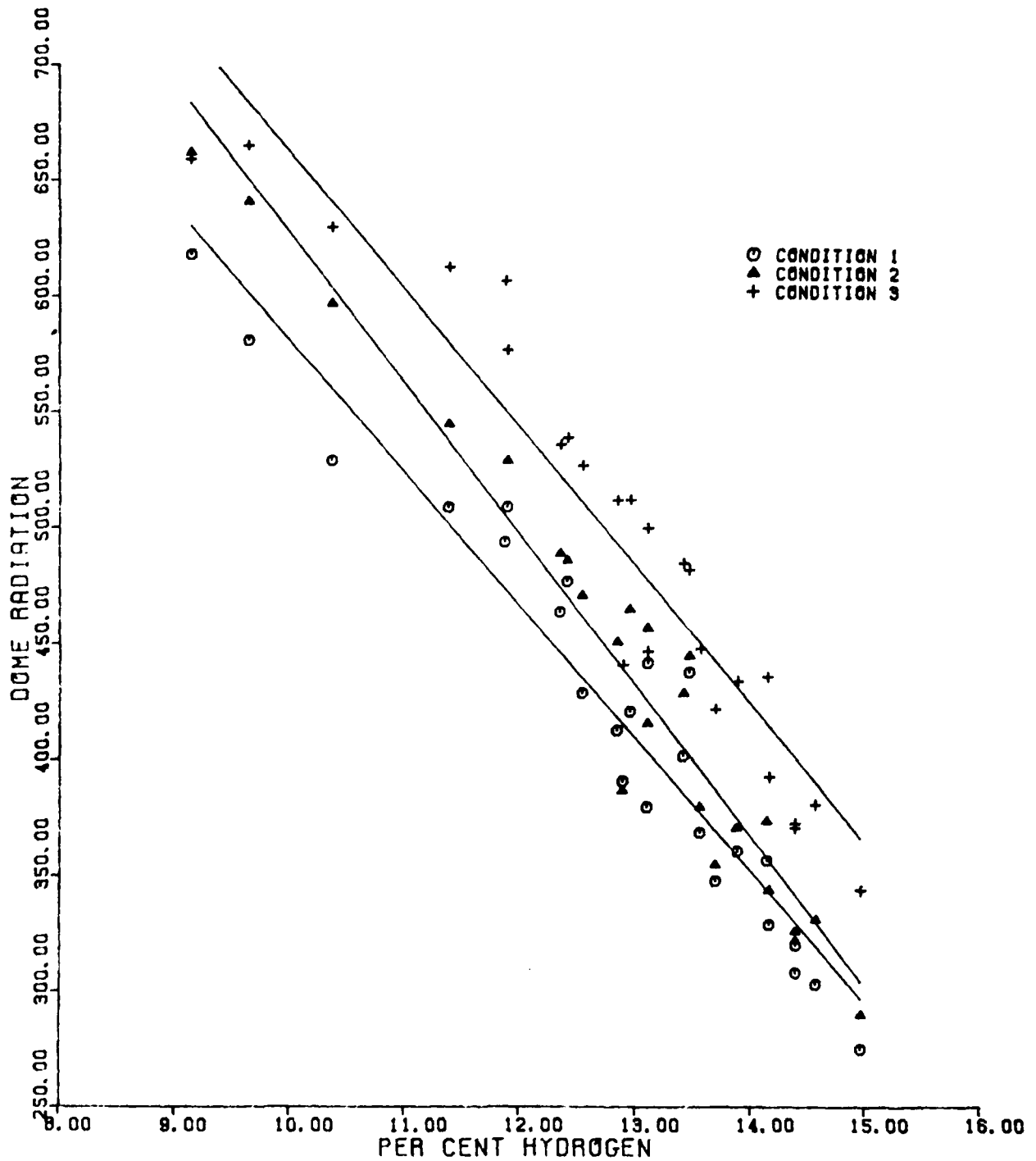


Figure 2. Correlation of Hydrogen Content with Dome Radiation

TABLE 4

REGRESSION ANALYSES RESULTS

Dependent Variable	Independent Variable	Test Condition	R ² Real	R ² Log	
Dome Radiation	Hydrogen Content	1	.93*	.84	
		2	.95*	.87	
		3	.91*	.82	
	Smoke Point	1	.82	.93*	
		2	.78	.91*	
		3	.83	.91*	
		Molecular Weight/Smoke Point	1	.90*	.91*
			2	.87	.87
			3	.86	.88
Liner Temperature	Hydrogen Content	1	.88	.84	
		2	.86	.80	
		3	.73	.66	
	Smoke Point	1	.83	.91*	
		2	.87	.92*	
		3	.90*	.87	
		Molecular Weight/Smoke Point	1	.84	.84
			2	.85	.86
			3	.80	.83
Smoke Number	Hydrogen Content	1	.88	.73	
		2	.88	.72	
		3	.86	.75	
	Smoke Point	1	.81	.83	
		2	.83	.86	
		3	.76	.86	
		Molecular Weight/Smoke Point	1	.87	.88
			2	.88	.90*
			3	.79	.87

* Denotes R² greater than .90

TABLE 5
 LINEAR REGRESSION ANALYSES OF HYDROGEN CONTENT

Dependent Variable	Test Condition	Slope	Intercept
Dome Radiation	1	-57.2	1152
	2	-65.1	1278
	3	-59.6	1259
Liner Temperature	1	-12.8	423
	2	-13.7	459
	3	-11.1	449
Smoke Number	1	-7.16	128
	2	-6.44	112
	3	-4.04	68

TABLE 6
 DEPENDENT VARIABLE CORRELATIONS

Dependent Variables	Test Condition	R ²
Dome Radiation Smoke Number	1	.92
	2	.89
	3	.83
Dome Radiation Liner Temperature	1	.92
	2	.93
	3	.87
Smoke Number Liner Temperature	1	.89
	2	.90
	3	.75

SECTION IV

CONCLUSIONS

Measuring fuel hydrogen content by both the combustion and NMR methods gives very reliable results if proper experimental care is taken. The NMR method appears to be the preferred method since it is less time-consuming and the sample is conserved for further testing. The calculation method of determining hydrogen content performs well as an estimate and can be very useful when sampling is not possible or practical.

The regression analyses performed in the real plane for hydrogen content give higher correlation coefficients than those performed in the logarithmic plane, as previously reported by UTRC. The best overall correlation is the linear hydrogen content with dome radiation, followed closely by the logarithmic smoke point with dome radiation correlation. The smoke point and molecular weight/smoke point data seemed to follow a logarithmic rather than a linear fit.

Since the smoke point measurement method (ASTM D1322) has a lower precision than the NMR hydrogen content method (ASTM D3701-81) the hydrogen content appears to be the preferred method for predicting fuel effects.

The molecular weight/smoke point correlations did no better, or worse, than the straight smoke point correlations.

Dome radiation and liner temperature show a close dependence upon each other. Smoke number and liner temperature do not show as much dependence upon each other as would be expected. A plausible explanation for this is that some of the soot may actually be consumed downstream of the combustion zone.

SECTION V

RECOMMENDATIONS

Work in the area of fuel effects on gas turbine engine combustion needs to continue to further understand soot production mechanisms and to develop models. The present contract at AFR is a step forward but more work still needs to be performed.

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