FUEL PROPERTY EFFECTS IN STIRRED COMBUSTORS

L. A. Ruth and W. S. Blazowski
Exxon Research and Engineering Company

A multi-year effort, funded by the Department of Energy, is being conducted to (a) provide an improved understanding of the effect of fuel properties, such as H and N content, on combustion characteristics and (b) develop analytical models and correlations to predict fuel effects and to assist engine designers in the future development of fuel-flexible systems. The data gathering part of this program, which is the subject of this paper, is being performed by Exxon Research. Analytical modeling is being performed concurrently by Science Applications, Inc.

Our experimental program has focused, thus far, on soot formation in strongly backmixed combustion. Experiments were performed using the jet-stirred combustor (JSC). This device provides a combustion volume in which temperature and combustion are uniform. It simulates the recirculating characteristics of the gas turbine primary zone; it is in this zone where mixture conditions are sufficiently rich to produce soot. Hence, the JSC allows study of soot formation in an aerodynamic situation relevant to gas turbines.

Fuel-rich combustion and soot formation behavior of a number of pure hydrocarbons were investigated. We found that the hydrocarbons tested could be grouped into three categories on the basis of their soot formation characteristics:

Category I	Category II	Category III
(Like ethylene)	(Like toluene)	(Unlike ethylene or toluene)
Hexane	Xylene (o, m, or p)	1-Methyl-naphthalene
Cyclo-hexane	Cumene	
n-Octane	Tetralin	
iso-Octane	Dicyclopentadiene	
1-Octene		
Cyclo-oxtane		
Decalin		

Category I hydrocarbons produced large amounts of exhaust hydrocarbons without sooting. Category II produced measureable soot above the incipient soot limit, defined as the leanest equivalence ratio at which soot was observed. It was at the incipient soot limit, which was about 1.4, that we first detected significant concentrations of exhaust hydrocarbons for Category II fuels. Furthermore, for these fuels, the amount of soot produced as equivalence ratio was increased beyond the incipient soot limit was similar. How-

ever, 1-methyl-naphthalene was significantly different in this respect, producing much higher soot quantities than the second category and having an even lower incipient soot limit. Consequently, this double-ring aromatic represents a third category of soot-forming hydrocarbon.

Blends of iso-octane and toluene were also tested to determine the behavior of a two-component mixture of Category I and II hydrocarbons. Mixtures of 50 or more percent toluene sooted, while a 25-percent toluene blend did not. For mixtures which did soot, increases in the toluene content resulted in increased soot production at all equivalence ratios. It was also determined that, with less toluene in the blend, the concentration of hydrocarbons at the incipient limit tended to increase. These results indicate a combination of Category I and II behaviors, and imply that a combination of the analytical descriptions for iso-octane and toluene might be a reasonable approach for the prediction of sooting characteristics of such fuel blends.

The iso-octane/toluene soot production data was also examined to evaluate the effect of fuel hydrogen content, a parameter often reported as useful in correlating sooting characteristics. At constant equivalence ratios of 1.6 and 1.8, a good correlation implying a linear relationship was obtained. Actual gas turbine combustor testing has also found an approximately linear relationship between fuel hydrogen content and soot production; thus, our results indicate a similarity between sooting in the well-characterized JSC and that in an actual combustor.

Many mechanistic models for soot production have been proposed. A simplified model (following Graham) suggests that aromatic hydrocarbons can produce soot via two mechanisms: (a) condensation of the aromatic rings into a graphite-like structure or (b) breakup to small hydrocarbon fragments which then polymerize to form larger, hydrogen deficient, molecules which eventually nucleate and produce soot. Based on his experiments, Graham concluded that the condensation route is much faster than the fragmentation/polymerization route. Further, since aliphatics can soot via fragmentation/polymerization only, aliphatics should produce much less soot than aromatics.

Our present results are consistent with this model. We observed that soot formation with aromatics (Category II) commences with the initial presence of hydrocarbons in the exhaust. If it is assumed that these breakthrough hydrocarbons maintain their aromatic character, this observation reflects the fast kinetics of the ring-building or condensation reactions. Further, the results for 2-methyl-naphathalene indicate that a double-ring aromatic provides the most rapid soot formation of the hydrocarbons studied. On the other hand, the aliphatic hydrocarbons produced large concentrations of exhaust hydrocarbons without soot formation. This observation is consistent with the slow process of polymerization of small hydrocarbon fragments.

The following conclusions were drawn from this multi-year experimental study:

1. C_2H_4 and $C_6H_5CH_3$ are distinctly different.
2. Total hydrocarbons are the key factor in consideration of soot limit and production.
3. Other hydrocarbons are like C_2H_4 or like $C_6H_5CH_3$.
4. Fuel blend testing indicates a combination of behaviors.
5. Results are consistent with simple soot formation mechanisms.
6. There is encouragement for quasi-global characterization.

Future experimental work should characterize exhaust hydrocarbons in a variable-pressure stirred reactor; investigate unmixedness/droplet effects; include continuous flow system studies on soot formation, soot oxidation, and FBN chemisty; investigate turbulence/unmixedness coupling; and include small-scale combustor tests.

Finally, it should be noted that the results reported here were obtained in a very well-mixed system with vapor fuel. In real systems, liquid droplets will be present which will complicate the situation with turbulence/unmixedness/mass transfer effects. Further experiments in this program will consider the inhomogeneity present during spray combustion.
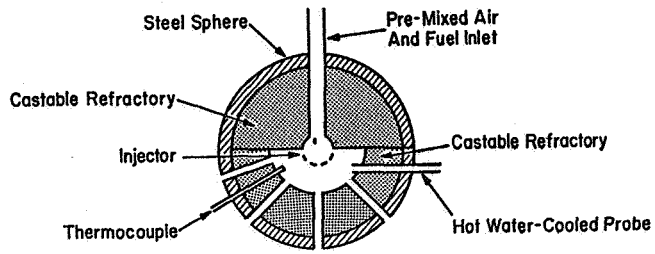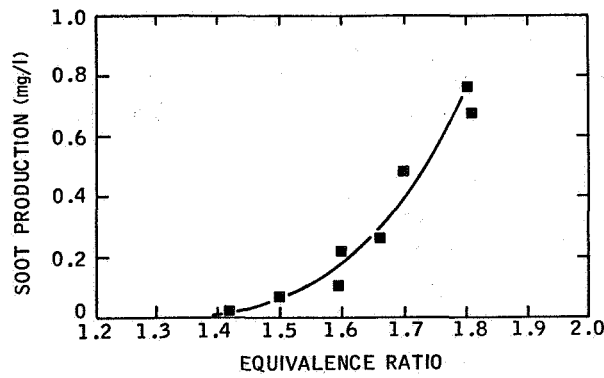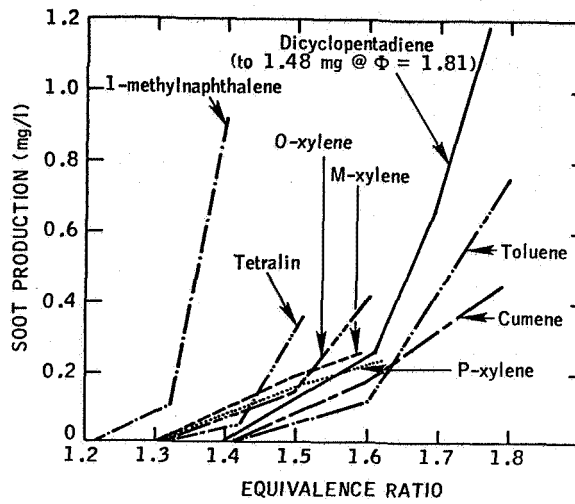
JET-STIRRED COMBUSTOR
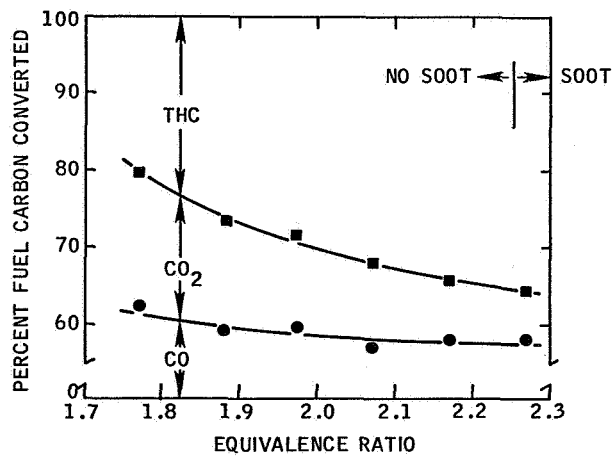
PERCENTAGE OF FUEL CARBON CONVERTED TO EXHAUST PRODUCTS-
ETHYLENE/AIR COMBUSTION
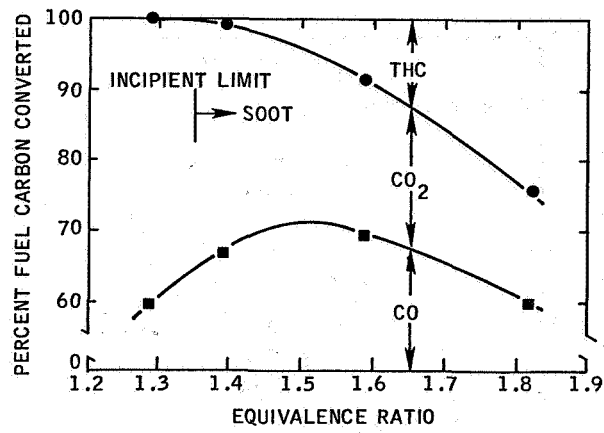
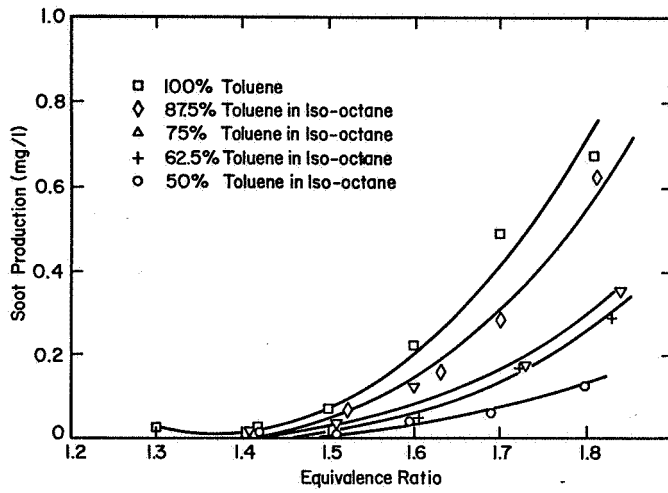PERCENTAGE OF FUEL CARBON CONVERTED TO EXHAUST PRODUCTS-
TOLUENE/AIR COMBUSTION

SOOT PRODUCTION vs. EQUIVALENCE RATIO FOR
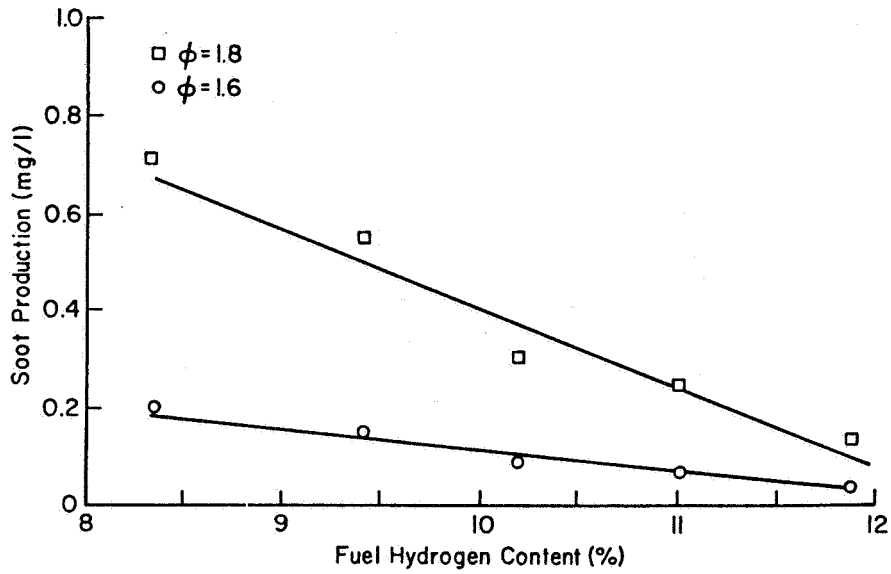TOLUENE/AIR COMBUSTION

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SOOT PRODUCTION vs. EQUIVALENCE RATIO FOR COMBUSTION
OF VARIOUS PURE HYDROCARBONS

SOOTING CHARACTERISTICS OF PURE FUELS

| CATEGORY I	CATEGORY II	CATEGORY III
ETHYLENE	TOLUENE	1-METHYL-NAPHTHALENE
HEXANE	O-XYLENE	
CYCLOHEXANE	M-XYLENE	
N-OCTANE	P-XYLENE	
ISO-OCTANE	CUMENE	
1-OCTENE	TETRALIN	
CYCLO-OCTANE	DICYCLOPENTADIENE	
DECALIN		

SOOT PRODUCTION vs. EQUIVALENCE RATIO FOR
TOLUENE/ISO-OCTANE BLENDS

SOOT PRODUCTION VS. FUEL HYDROGEN CONTENT FOR
TOLUENE ISO-OCTANE BLENDS

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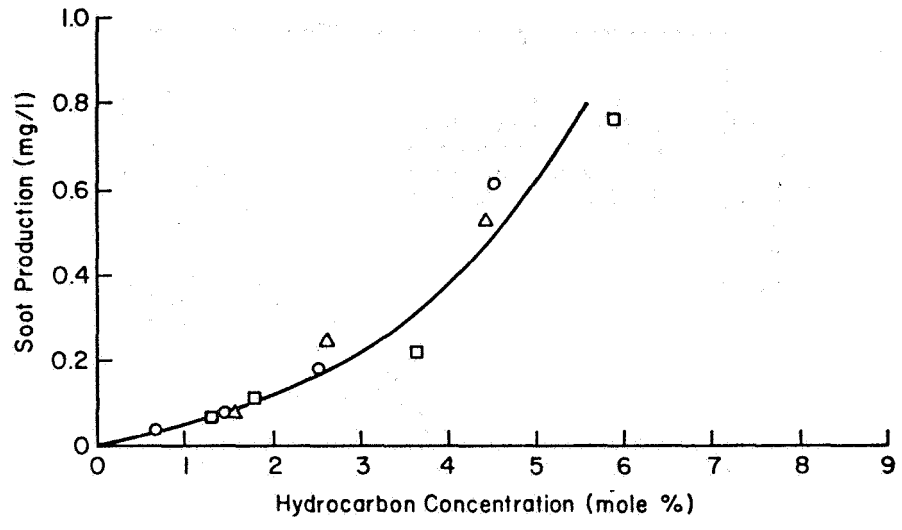
SOOT PRODUCTION VS. EXHAUST HYDROCARBONS CONCENTRATION
FOR TOLUENE AIR COMBUSTION
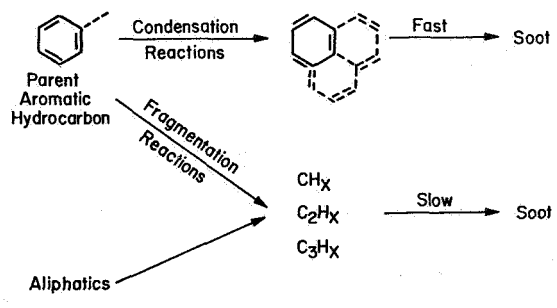
SIMPLIFIED SOOT FORMATION MECHANISM (GRAHAM)

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