MASTER

SOOT FORMATION IN SYNTHETIC-
FUEL DROPLETS

Second Quarterly
Technical Progress Report

G. England
J. Kramlich
R. Payne

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Energy and Environmental Research Corporation
8001 Irvine Boulevard
Santa Ana, California 92705

April 1981

Prepared for Pittsburgh Energy Technology Center
Department of Energy

Under Contract No. DE-AC22-80PC30298

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

TABLE OF CONTENTS

<u>Section</u>		<u>Page</u>
1.0	INTRODUCTION AND SCOPE	1
2.0	TASK 1 - FUEL SCREENING STUDIES	2
3.0	TASK 2 - FLAME STUDIES	11

1.0 INTRODUCTION AND SCOPE

The main objective of this program is to provide detailed information on methods of minimizing soot formation during synthetic liquid fuel combustion under conditions which minimize the formation of nitric oxides. The program comprises two main tasks, Fuel Screening Studies, and Flame Studies. The purpose of the first task is to investigate the impact of fuel properties on particulate production, to establish the importance of droplet size and examine atomizer effects, and to develop techniques for surrogate fuels production. In the second task, fundamental details of soot formation from syn-fuel droplet combustion will be investigated in variable slip velocity configurations.

This present report describes technical progress during the second three-month period of program effort (January-March 1981). During this period attention has continued to be focussed on the design, construction and commissioning of experimental systems. The Task 1 tunnel furnace modification has been completed and made operational and some preliminary fuel screening studies have been carried out. Similarly, construction of the controlled flow droplet reactor has been completed and efforts directed towards the design and testing of diagnostic systems. Details of this work are discussed in the following sections.

2.0 TASK 1 - FUEL SCREENING STUDIES

The investigations of fuel and droplet effects within this task are carried out in a small (7.0×10^4 Btu/hr) vertically-fired refractory tunnel furnace, under conditions of both normal excess air and staged heat release. During this present reporting period, all modifications to the original tunnel furnace were completed and both furnace and sampling system are operational. Experimental effort has been initiated and has concentrated on a determination of fuel effects on particulate and NO_x emissions from synthetic fuels selected from those currently available at EER. Baseline emissions have also been established with a petroleum-derived diesel fuel and residual oil. Further progress on the Fuel Screening Studies was halted pending selection and delivery of the remaining fuels by DOE.

Five liquid fuels (three petroleum-derived oils, a shale-derived fuel and two coal-derived fuels) have been tested in the 7.0×10^4 Btu/hr tunnel furnace. The synthetic fuels included a shale-derived DFM, SRC-II (5.75/1 middle/heavy distillate blend) and an SRC-II blend with donor solvent. The petroleum-derived fuels included an Indo/Malaysian #6 oil and an Alaskan diesel fuel. Analyses of these fuels are presented in Table 1.

The combustion characteristics of each fuel were determined under comparable combustion and atomization conditions. The parameters which have been studied to date include atomizing air pressure, excess air level, and heat extraction along the axis of the tunnel furnace. The atomizer used for all tests was a SONICORE 052H with the resonator cap removed. A water-cooled oil gun was used and the combustion air was preheated to $400 \pm 25^\circ\text{F}$. Exhaust gas species concentrations (CO_2 , CO , O_2 , NO , and NO_x) were monitored with continuous analyzers; Bacharach smoke number and total particulate loading were determined for each operating condition. NO_x and total particulate emissions under normal excess air combustion from the five fuels which were tested can be compared in Figure 1. NO_x emissions appear to rise with increasing fuel nitrogen content as anticipated from previous studies. The shale-derived diesel fuel marine (DFM) produced significantly higher NO_x levels than the conventional residual oil of the same nitrogen content. This is also consistent with previous data. This may be due to more rapid fuel vaporization/mixing and higher local combustion temperatures resulting from the lower viscosity (hence smaller droplets) and greater volatility

Table 1. Analyses of Fuels Tested

	Alaskan Diesel	Indo/ Malaysian	Shale- Derived DFM	SRC-II Blend	SRC-II 5.75/1Mih
Ultimate Analysis:					
Carbon, %	86.99	86.53	86.18	89.91	85.91
Hydrogen, %	12.07	11.93	13.00	9.27	8.74
Nitrogen, %	0.008	0.24	0.24	0.45	(0.96)
Sulfur, %	0.31	0.22	0.51	0.065	0.30
Ash, %	<.001	0.036	0.003	0.004	0.04
Oxygen, %	0.62	1.04	1.07	0.30	4.08
Conradson Carbon Residue, %		3.98	4.1	6.18	0.51
Asphaltene, %		0.74	0.036	4.10	
Flash Point, °F		210	182	70	1.73
Pour Point, °F		61	40	<-72	-55
API Gravity at 60°F	33.1	21.8	33.1	10.0	
Viscosity, SSU, at 140°F	33.1	276	38.3	44.5	34.5
at 210°F	29.9	83	32.4	34.7	30.3
Heat of Combustion:					
Gross Btu/lb		19,070	19,430	17,980	17,100
Net Btu/lb		17,980	18,240	17,130	
Calcium, ppm		14	0.13	0.33	
Iron, ppm		16	6.3	3.9	
Manganese, ppm		0.13	0.06	<0.5	
Magnesium, ppm		3.6		0.17	
Nickel, ppm		19	0.43	<0.5	
Sodium, ppm		15	0.09	0.31	
Vanadium, ppm		101	<.1	<1.0

Figure 1. Fuel Screening Studies - Comparison of Emissions From Alternative and Petroleum Fuels.

of the DFM. The emission of particulates was much higher for the residual oil than for any of the other fuels tested. This appears to be largely due to differences in fuel viscosity. The No. 6 oil has the highest viscosity (~200 SSU at 155°F--see Figure 2), the SRC-II blend has the next highest (~100 SSU at 70°F), and the other fuels have less than 60 SSU viscosity at operating temperature. This suggests that spray characteristics may dominate particulate formation under excess air conditions. Further tests will be conducted to match fuel viscosity by adjusting fuel temperature.

Particulate emissions did not appear to have a first-order dependence on Conradson carbon residue or asphaltene content. For instance, the DFM has a Conradson carbon residue of 4.1 percent and the SRC-II only 0.51 percent, yet particulate emissions are nearly identical. Figure 3 shows Bacharach smoke number for the same conditions as in Figure 1. In general, smoke number follows the same trend with fuel and excess air as do particulate emissions, although the relative differences are somewhat less pronounced. Heat extraction from the furnace was accomplished by using movable water-cooled coils, removing approximately 65 percent of the total heat input over a length of approximately 4.3 diameters.

The effect of varying the axial location (i.e., time) at which heat is extracted from the furnace is shown in Figure 4. NO_x emissions are seen to increase and particulate emissions decrease as the point of heat extraction is moved further downstream from the fuel injector. This could be a result of cooling in the region early in the flame which may suppress peak flame temperatures, slow droplet vaporization, and quench soot burnout. The trends appeared to be consistent for both fuels, although the particulate emissions from SRC-II blend showed somewhat higher sensitivity to heat extraction than the DFM.

Figure 5 shows the influence of varying atomizing air pressure on NO_x and particulate emissions for the three alternative fuels. Increasing atomization pressure increased NO_x and decreased particulate emissions, presumably because the mean fuel droplet size was decreased, promoting faster (higher NO_x) and better burnout (less particulate). Although total particulate emission decreased with an increase in atomization pressure, for the SRC-II blend at 2 percent excess O_2 (■) the Bacharach smoke number increased. This may be

Figure 2. Viscosity of the Five Fuels Tested.

Load = 7.0×10^4 Btu/hr
Atomizing Air Pressure - 15 psig
Cooling Coils at L/D = 1.7

Figure 3. Fuel Screening Studies - Effect of Fuels on Smoke Number.

Figure 4. Fuel Screening Studies - Influence of Cooling Location (total heat extraction - 65 percent input).

Figure 5. Fuel Screening Studies - Influence of Atomizing Air Pressure on NO_x and Particulate Emissions.

due to a shift in the size of the particulate matter into the visible light scattering size range.

Future experiments will include investigation of these same parameters under two-stage combustion conditions and with different heat extraction profiles to approach combustion conditions for practical systems equipped with low-NO_x combustion equipment. Additional fuels will be investigated as soon as selection and procurement of the test fuels has been finalized.

In order to investigate independently the effects of fuel droplet size and spray characteristics, an atomizer has been designed and constructed which will allow the formation of fuel sprays with variable droplet momentum. This atomizer is based on the SONICORE 052H and incorporates a supplementary primary air screen. Changes of the total air flow to the atomizer and the distribution between atomizing and supplementary air thus allows some measure of control over both atomization quality (droplet size distribution) and fuel spray momentum. A preliminary evaluation of the droplet size distributions produced by this atomizer over its typical operating range has been initiated and will be continued into the next reporting period.

3.0 TASK 2 - FLAME STUDIES

Efforts during the reporting period were directed toward preparation and testing of the various apparatus required for the study. Specific accomplishments include: 1) construction and testing of the droplet studies reactor, 2) design of the probing and sample collection systems for soot, liquid droplets, and gas-phase species, 3) adaptation and upgrading of currently available optical systems for use with the droplet studies reactor, 4) operation of the droplet generator on residual fuel oils, and 5) use of the optical system on burning droplets within the reactor.

The goal of Task 2 is to identify the fuel properties and flow conditions that influence soot production in liquid fuel flames through investigations of droplet combustion under controlled conditions. In order to produce the required controlled environment, a droplet-studies reactor has been designed and constructed in which monosize droplet streams can be injected, under conditions of variable slip velocity, into the stream of combustion products produced by a flat-flame gas burner.

The droplet studies reactor design has been described in the previous quarterly report, and a few further details are presented here, where descriptions are referenced to Figure 6, a view of the burner. The flat flame is supported on a 2.5- x 11.5-inch sintered stainless steel plate. Cooling coils are placed on the upstream face of the plate to remove the heat generated by flame attachment. Optical access to the burning droplets and combustion gases is through the two pairs of Vicor windows shown. The burner situation with respect to the fuel heater and the various traverse mechanisms is shown in Figure 7. The traverse mechanisms allow arbitrary vertical and horizontal burner movement with respect to a stationary optical path. The fuel heater/pressurized-feed system is located directly over the burner. The droplet generator is mounted on the side of the burner and is connected to the fuel heater by a flexible line. A photograph of the burner showing a typical flame structure and soot sheet is given in Figure 8.

The burner has been successfully operated on methane/air over a wide range of stoichiometries and flow rates. Operation has been completely satisfactory with no appearance of burner-associated problems.

Figure 6. Droplet Studies Burner.

Figure 7. Burner and Support Equipment.

Figure 8. Burner Photograph With Droplet Injection, Showing Soot Sheet.

A major objective of this task will be the collection and analysis of soot samples, and a brief examination of the literature reveals that the collection of soot from flame zones is a difficult and uncertain task. Published soot probe designs fall, in general, into three categories: water-spray probes, filtering probes, and porous aspirating probes. Water spray probes use a water jet to quench the sample and are used where soot chemical composition is of prime importance. These probes cannot normally be used for mass loading measurements, however, so their use in the present study was not considered. Filtering probes usually contain a sintered metal filtering element within the probe, normally located near the inlet. These probes must be removed and disassembled after each measurement. Soot mass loading measurements can be reliably obtained with such probes, although their bulky design is a disadvantage in small-scale burners. Also, direct observation of soot structure on the filter is precluded. Thus, this probe design was also rejected.

The porous probe is a three-wall probe in which the inner wall is made up of a porous metal. Figure 9 illustrates the design of the probe selected for these studies. Inert gas is aspirated continuously through the probe walls into the sample stream. This gas flow serves the dual purpose of quenching the sample and keeping the walls clear of soot. Soot is naturally driven from hot sample to cold walls by thermophoresis. This phenomena is much more active in the early portion of the probe, so an additional, higher velocity quench is added there. Finally, the entire probe is surrounded by a cooling water jacket. Construction of this probe is under way.

In the proposed sampling procedure, soot will be separated from the gas stream by means of a two-stage nucleopore filter. Calculations indicate that isokinetic sampling rates can be accommodated without a large filter pressure drop. These filters are especially attractive because of their low weight (low tare values for gravimetric analysis) and smooth surface (observation of soot structure by optical or scanning electron microscopy). The stream leaving the filter will be available for gas-phase chemical analysis.

The liquid probe will be simply a water-cooled receptical. Most of the time this probe will simply capture liquid during soot collection. However, when liquid samples are required for composition determination, the cleaned probe can be used to obtain grab samples. Quenching of the liquid droplets

Figure 9. Soot Probe Head Design. (Outside Diameter is One Inch).

would rapidly occur by cold-surface contact.

The previously existing optical system was upgraded during the reporting period, and Figure 10 illustrates the optical layout. The alignment laser has recently become available from another experiment. The laser was added both to align the optics and, using a beam expander and spatial filter, provide for precision camera focusing. The spark unit is used for still shadowgraphs and is replaced by a xenon lamp for high-speed motion pictures.

During the reporting period, a large amount of operating experience has been gained with the droplet generation system. This unit has been modified slightly from the design presented previously. The new design is shown in Figure 11. The fuel heater is currently using water as the heating fluid, which limits maximum fuel temperatures to 98°C. With minor modifications, mineral oil can be used to provide 160°C fuel temperatures. At the 98°C temperature, a number of residual fuel oils (kinematic viscosity: 100-150 Saybolt Universal Seconds) have been used with a 35 μm orifice to produce 60 μm diameter droplets. Successful droplet formation depended, firstly, on the even heating of the fuel oil from the reservoir to the orifice; and, secondly, passing the fuel oil through a 2 μm pore size sintered filter element. In particular, the elimination of solid material from the liquid fuel stream was the key to long-term, reliable operation.

A number of tests have been conducted on the burner with liquid fuel injection. Under fuel-lean burner stoichiometry, the soot sheet is relatively bright with sharply-defined boundaries. The sheet collapses into a narrow ribbon after visible radiation ceases. This is probably due to thermophoretic migration to the cooler core of the sooting region. Under fuel-rich conditions, the soot sheet was larger, radiation was less intense, and boundaries were diffuse compared to the fuel-lean case.

Spark shadowgraphs of the burning droplets have not been wholly satisfactory. The soot radiation tends to "wash out" the shadowgraph image. A high-speed shutter is expected to remedy this problem. However, qualitative comparisons between burning and non-burning photographs indicate the following:

- Shortly after injection, there is no observable difference between burning and non-burning droplets.

Figure 10. Top View of Optical Layout.

Figure 11. Fuel Delivery and Droplet Generator Systems.

- At distances far from the point of injection, non-burning droplets show effects of droplet agglomeration, with many large and fine droplets present.
- At distances far from the point of injection, burning droplets show less evidence of agglomeration. Also, the smaller droplets have apparently completely burned out.

The high-speed motion pictures are not expected to suffer from the washout problem because exposure is dominated by the high intensity xenon lamp.

Planned activities for the next quarter include:

- A substantial number of the physical measurements (i.e., photography and burner characterization).
- Completion of the co-flow droplet injection apparatus.
- Construction and testing of the soot and liquid probes.