DOE/PC/30302--1

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Report

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FIRST QUARTERLY TECHNICAL PROGRESS REPORT

on

SYNTHETIC-FUEL AROMATICITY AND STAGED COMBUSTION

to

U. S. DEPARTMENT OF ENERGY
PITTSBURGH ENERGY TECHNOLOGY CENTER

Contract No. DE-AC22-80PC-30302
Battelle No. G-7662

Period Covered: September 23, 1980-
December 31, 1980

January 28, 1981

by

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INTRODUCTION

Synthetic liquid fuels, otherwise referred to as synfuels or coal-derived liquids, are probably best characterized from a combustion-environmental point of view as low in hydrogen, low in sulfur, high in nitrogen, and high in aromatics. As a consequence two of the more critical problems in synfuel combustion are NO_x formation and soot formation (and polycyclic organic matter).(1,2) This program is directed to these two issues.

At first hand the solutions to burning synfuels high in aromatics and fuel-bound nitrogen are diametrically opposed, i.e. high temperature and excess air keep soot levels down, low temperatures and vitiated air keep nitrogen oxide levels down. Staged combustion however offers a logical solution to the above. This program separates and analyzes the synfuel combustion problem via its component parts and then puts them together again phenomenologically via the stage combustion process.

OBJECTIVES

The overall objective of this program is to elucidate the pyrolysis and oxidation behavior of synfuel and to integrate this behavior in staged combustion to determine the effects of staged combustion on the formation of soot and NO_x.

More specifically, this program is divided into five tasks. The title and objective of these tasks are as follows.

Task 1. Characterization of the Aromatics and the Fuel-N Components. The objective is to determine the volatility and to characterize the aromatic and fuel-N compounds present in a typical synfuel.

Task 2. Pyrolysis Studies. The objective is to determine the aromatic and fuel-N characteristics of narrow (50 F) distillation cuts of synfuel as a function of time, temperature and oxygen level.

Task 3. Oxidation of Pyrolysis Products. The objective is to determine the ease of oxidation of the pyrolysis products (the condensible fraction) of Task 2.

Task 4. Staged Combustion Studies. The objective is to define the burning characteristics of synfuel as a function of equivalence ratio, temperature and residence time in two-stage combustion.

Task 5. Modeling. The objective is to apply the results from Tasks 2, 3 and 4 into existing models for soot and NO_x formation in flames.

SUMMARY

In the first quarter Tasks 1 and 2 were initiated and procedures for obtaining middle and heavy distillate samples were initiated.

SRC II Samples

Our initial activity was directed toward obtaining representative samples of SRC II for use in this program. We were also interested in defining suitable safety procedures for storing and handling SRC II in our laboratory.

Arthur Levy and James Longanbach visited Dr. John Haebig at Gulf and Dr. Egon DeZubay at Westinghouse in Pittsburgh to discuss safety procedures and SRC II samples. John Haebig provided safety procedures used at Gulf and showed us their facilities used to transfer SRC II within the laboratory. He also provided the names of people to contact at SRC International to obtain SRC II samples for use in the experimental program. Battelle has a one-year old, 2-barrel sample of a blend of SRC II middle and heavy distillate from Westinghouse. Egon DeZubay and P. Richard Mulik at Westinghouse provided analyses for this material and discussed their safety procedures for handling SRC II.

Arthur Levy and James Longanbach also attended the workshop on Synthetic Fuel Combustion hosted by the Pittsburgh Energy Technology Center on December 12, 1980. At this meeting it was decided that standard SRC II samples would be provided through PETC. Since these will be available too late to fit into the Battelle program schedule, we have contacted Dr. David Schmalzer of the Pittsburgh and Midway Coal Mining Company to request 5-gallon samples of SRC II naphtha, middle distillate, and heavy distillate. The paperwork has been completed and the samples are expected by the end of January.

Task 1. Characterization of Aromatics and Fuel Nitrogen Components

Analytical Methods

The objective of Task 1 is to characterize the volatility and the aromatic and fuel-N compounds present in the synfuels to be used in this research program. The synfuels will be distilled into narrow boiling point range fractions and a variety of analytical tests will be done on each fraction with emphasis on aromatics and fuel-N characterization

In preparation for the SRC II samples which will be used in the experimental program we are defining and testing our analytical procedures on the SRC II blend sample. The analyses provided for this sample by Westinghouse are listed in Table 1.(3)

The analytical scheme needed for this work must provide more detail on nitrogen and aromaticity. The physical and chemical properties and trace metal analyses listed in Table 1 are not of direct interest. However, an attempt is being made to develop correlations using the elemental analyses and distillation data to calculate the physical and chemical properties. The data listed in Reference 3 and similar data from the same source published in an ACS Fuel Division Preprint(4) are being used to develop the correlations. A total of 24 data points are available. The results are not available at this time.

The following analyses will be used to characterize each distillation cut and pyrolysis and oxidation product:

- Elemental, basic nitrogen
- Simulated distillation by GC
- Molecular weight
- H^1 NMR to measure aromatic distribution.

Each of the analytical methods to be used has been tried on the SRC II blend sample and is discussed in detail below. No distillation cuts were made on the SRC II blend sample. The sample was used as received.

Elemental Analyses for C, H, N, S and O

A Perkin Elmer Elemental Analyzer is used for C, H, and N. There are no problems with this method when low-ash liquid samples are used. This should give more accurate values for total nitrogen than the Kjeldahl method which can give low values when pyridine-type compounds are present. Sulfur is measured by X-ray fluorescence and oxygen is calculated by difference. The sample size required is less than 5 ml, almost all of which is used for the sulfur analysis. The SRC II blend sample has been submitted for analyses but no data are available at this time.

TABLE 1. ANALYTICAL DATA FOR BLEND OF SRC II MIDDLE AND HEAVY DISTILLATES(a)(3)

Fuel Type	SRC II Blend (medium)	
Physical and Chemical Properties		
Gravity, API	11.7	
Pour point, F	<-65	
Flash point, F	168	
Gross heat of combustion, Btu/lb	17090	
Kinematic viscosity, cs at 40 C	3.87	
Kinematic viscosity, cs at 100 C	1.19	
Conradson carbon residue, wt %	0.36	
Aromaticity, % C_A	63	
Elemental Analysis, wt %		
Hydrogen	8.70	
Sulfur	0.23	
Nitrogen	0.91	
Oxygen	4.35	
Ash	<0.01	
	ASTM Method	
Distillation, F at	D2887	D86
Initial boiling point	276	220
5	331	382
10	358	404
30	404	433
50	445	459
70	482	491
90	540	578
95	593	640
End point	762	640
Trace Metals, ppm wt		
Titanium	0.5	
Sodium	1.4	
Potassium	1.5	
Calcium	1.6	
Vanadium	0.23	
Lead	0.12	
Iron	13	
Phosphorus	<0.01	

(a) SRC II blend provided by Westinghouse.

Basic Nitrogen

If typical nitrogen compounds are arranged in order of ionization constants in aqueous solutions, those above a certain value are titratable with perchloric acid while those with lower ionization constants are not. The separation point is reported to be about $K_b = 1 \times 10^{-11}$.(5) Examples of basic (titratable) nitrogen compounds include the pyridines, quinolines, piperidines, and anilines. 2-Aminobenzothiazole is right on the separation point. Examples of nonbasic nitrogen compounds include pyrrole, indoles, carbazoles, urea, acetamide and cyanide. Most oxygen and sulfur compounds do not interfere. We expect the basic nitrogen compounds to be more refractory during pyrolysis and thus we expect to see a change in the basic/total nitrogen ratio as a result of pyrolysis.

The titration of basic nitrogen with perchloric acid in acetic acid has been tested successfully. The method(5) consists of diluting an accurately weighed sample of SRC II (∿1.0 gram) with 100 ml of glacial acetic acid and 5 ml of toluene, to improve solubility, and titrating the mixture, while stirring, with 0.1N $HClO_4$ in glacial acetic acid. Water must be excluded from the system and it may be necessary to add 1 ml of acetic anhydride to ensure that the system is dry. This has not been tried as yet. After titration with a pH meter using a combination electrode, MV readings are plotted versus ml of acid added to find the breakpoint on the curve. We have automated this procedure by pumping acid into the stirred sample and continuously recording the MV response. A sample of pure pyridine was used to standardize the perchloric acid titrant. Analysis of the SRC II blend sample gave a value for basic nitrogen of 0.54 g/100 g sample. The total nitrogen content is 0.91 g/100 g (Table 1). Thus, the ratio of basic/total nitrogen is 0.59. Ratios of 0.30 ± 0.05 are typical for crude oils.(6)

Simulated Distillation by Gas Chromatography

It will be necessary to determine the volatility of the liquid residues collected after pyrolysis and oxidation to determine how much material was lost. This will be one direct way used to measure the temperature experienced by the sample. Simulated distillation by gas chromatography, similar to the method described in ASTM 2887, will be used for this analysis. This technique requires much less sample, time and money compared to even small scale conventional distillation techniques. We have previously set up this procedure and expect to be able to obtain better agreement with conventional distillation results than those shown in Table 1 for the Westinghouse SRC sample.

A comparison of a preliminary result of the Battelle GC simulation method with the results reported for the SRC II blend sample is shown in Table 2. The Battelle results are closer to the ASTM D86 results at all points up to the end point. The end point cannot be determined accurately using conventional distillation techniques because of the residue left in the equipment when the distillation pot is empty.

Aromatic Distribution by H^1 and C^{13} NMR

Brown and Ladner have developed a method of calculating several structural parameters of coal liquids based on the amounts of aromatic protons, aliphatic protons next to an aromatic ring and aliphatic protons not adjacent to an aromatic ring.(7) Several assumptions are made in developing the equations which describe the molecular structures. They assume that aromatic rings are not linked by C-C bonds or by C-O-C bonds. Recent studies suggest that these are reasonably good assumptions in depolymerized coal liquids such as SRC II.(8) We also assume that all of the oxygen present in the SRC II is present as phenolic oxygen and appears under the aromatics in the NMR as found by Schwager, et al.(9) We correct for this using the oxygen concentrations from the elemental analysis provided by Westinghouse (Table 1). The fractions of total hydrogen measured are:

TABLE 2. COMPARISON OF DISTILLATION RESULTS USING WESTINGHOUSE SRC II

Volume Distilled/ F wt %	Method Battelle GC Simulation	ASTM D86	2887
IBP	237	220	276
5	341	382	331
10	362	404	358
30	411	433	404
50	455	459	445
70	486	491	482
90	560	578	540
95	628	640	593
EP	774	640	762

0.36 H_O = Aliphatic not adjacent to aromatic
0.37 H_α = Aliphatic adjacent to aromatic
0.24 H_{aro} = Aromatic
0.03 H_{OH} = Phenolic

Using these fractions, the elemental analyses (Table 1) and a molecular weight of 200 g/mole (discussed in the next section) the following molecular structure parameters were calculated for the Westinghouse SRC II.

f_a = Fraction of total carbon which is aromatic = 0.556
$\frac{H_{aro}}{C_{aro}}$ = Ratio of substitutible edge atoms to total aromatic atoms = 0.998
α = Fraction of edge atoms substituted = 0.474
C_A = Total number of aromatic carbon atoms per molecule = 7.95
R_s = Number of substituted aromatic ring carbons = 3.76
n = Number of carbon atoms per saturated substituent = 1.97
R_n = Number of aromatic rings per molecule = 1.01

The molecular formula was calculated to be $C_{14.3}H_{17.4}N_{0.15}S_{0.01}O_{0.54}$.

These easy calculations should provide sufficient characterization of the structures of the pyrolysis and oxidation products to study the effects of aromaticity. These preliminary results suggest that almost all of the aromatics are single ring structures and that the substituents average two carbon atoms in length. These data will be recalculated when the VPO molecular weight and new elemental analysed become available. In addition a sample has been submitted for C^{13} NMR which gives a measure of the ratio of aliphatic to aromatic carbon directly. This will be used as a check on these calculations. Other workers have found that the Brown-Ladner equations agree very well with the C^{13} results so we anticipate that C^{13} NMR analyses will be unnecessary.(10)

Molecular Weight Determination

Most molecular weight measurements for coal liquids reported in the literature are obtained by Vapor Pressure Osmometry (VPO) in either benzene or THF. A sample of the SRC II blend has been sent out for VPO measurement of molecular weight; results have not been received yet. Since these measurements involve a long lag time it would be preferable to find a method for determining molecular weight in-house. VPO yields a number average molecular weight. Number average molecular weights have been obtained using two methods which can be done in-house: Gel Permeation Chromatography (GPC) and Gas Chromatography (GC).

GPC uses size exclusion of the adsorbed SRC II molecules dissolved in a solvent as they pass through a column containing a material with a known pore size distribution. Large molecules which cannot be adsorbed in the pores are eluted first. A polystyrene standard of known molecular weight distribution is tested and used as an external standard to calibrate the molecular size distribution curve. Two problems occur. The results are based on molecular shape rather than weight and the polystyrene standard may have a different molecular size/weight ratio than the SRC II. Second, the SRC II must be totally soluble and must not be permanently adsorbed on the column. Both problems appeared to occur when the Westinghouse SRC II sample was analyzed using GPC. The number average molecular weight was found to be only 53 g/mole. This is clearly too low. Some of the SRC II was not eluted from the column and apparently the polystyrene polymer was not a good standard for SRC II as well.

GC was tried using the same column used for simulated distillation. This column elutes the compounds in order of their boiling point. The flame ionization detector (FID) used measures the mass of sample passing through the flame. Standards of straight chain aliphatics of known boiling point and molecular weight were used to calibrate the results. The aliphatics mixture is not a good model for aromatics because aliphatics boil at much higher temperatures for the same molecular weight compared to aromatics and phenols, as shown in Figure 1. However, the addition of aliphatic side chains to aromatics increases their boiling points, moving them into closer agreement with the n-aliphatic standards. Thus, there is some reason to think that the n-aliphatics may be usable calibration standards. This must be examined more closely.

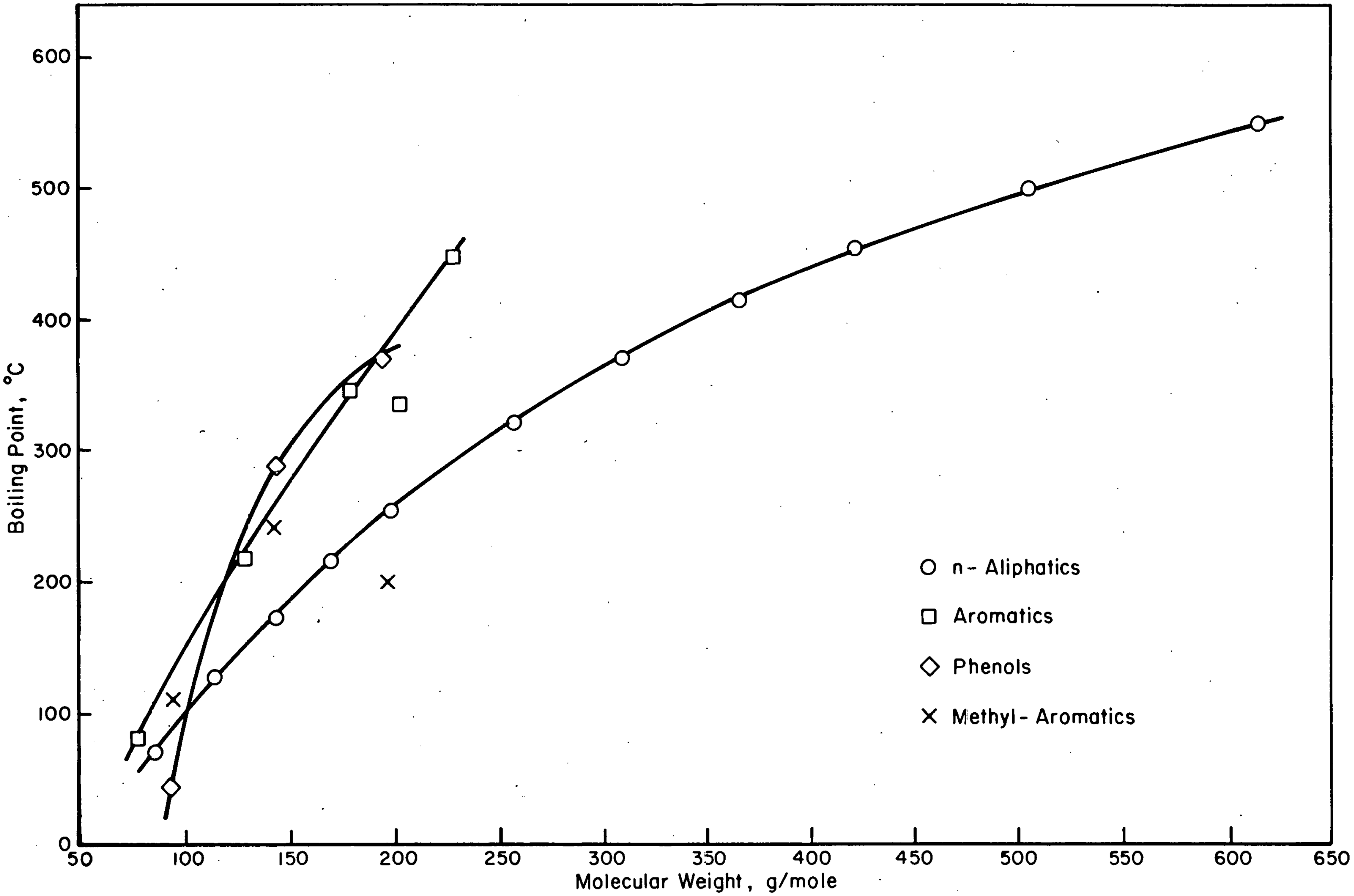

FIGURE 1. BOILING POINT VERSUS MOLECULAR WEIGHT IN VARIOUS TYPES OF AROMATICS AND n-ALIPHATICS

The number average molecular weight obtained by the GC method is 190 g/mole. This also seems low but number average molecular weights are heavily influenced by the concentration of low molecular weight species present so this number may be close. One set of published values for PAMCO SRC molecular weights (by VPO) are propane soluble 307, pentane insolubles-benzene solubles 352, pentane soluble-propane insolubles 563, and carbon disulfide insolubles 600. These seem high considering the other properties of the Westinghouse SRC II such as viscosity (1.19 cs at 100 C) and pour point (-65 F), (see Table 1).

At this time we believe that the standard elemental analyses and GC simulated distillation along with the basic nitrogen and H^1 NMR analyses of aromatics will provide us with sufficient characterization of the individual distillation fractions when combined with a method of molecular weight determination. We anticipate that VPO analysis will be used for molecular weight determinations.

Task 2. Pyrolysis Studies

Objective

The objective of this task is to determine the decomposition and conversion characteristics of the Task 1 distillate fractions as a function of temperature, time and oxygen level. Of particular interest are the distribution of aromatics and fuel-N constituents in the fractions before and after pyrolysis.

Approach

The Task 2 experiments will be conducted in a drop-tube furnace. It was originally planned to conduct these experiments under static, steady state conditions. As a result of discussions with Drs. John Beér and Adel Sarofim(11) it appears more appropriate to carry out the pyrolyses under dynamic, non-steady-state conditions. Preliminary evidence obtained by Beér et. al.(12) show a much higher fuel nitrogen loss per unit mass of the liquid fuel evaporated when 150 μm droplets of a residual petroleum fuel oil was rapidly pyrolyzed (Figure 2), whereas when the fuel oil was vaporized under normal distillation conditions, more nitrogen was retained in the residue (Figure 3). Whether or not this situation will prevail for drops of fuel from narrow (50 F) distillation cuts remains to be seen, but merits consideration in this study. Also of consequence to this study are the fact that the dynamic system provides a better representation of the real combustor, and secondly, independent variables in a flow reactor are more easily controlled.

The drop tube set up has been assembled as shown in the schematic in Figure 4. A two inch diameter quartz tube is positioned vertically and is heated by a two foot long electric furnace. A smaller quartz tube is permanently attached to the top of the reactor, one end of which is sealed with a syrum cap. The liquid flow rate will be maintained constant by means of a syringe pump. Inlet gases are passed into the reactor through a connection on top. The product gases are cooled and separated from the condensables in the collector before passing into the analyzing instruments. The pyrolyzed droplets are collected in one of four sample bottles. In the present apparatus, the residence time of the fuel droplets is controlled solely by varying the drop size.

Sample experiments have been carried out with the SRC II fuel oil sample (36510-1-10) described earlier. The purpose of these experiments was to determine the collection efficiency, the importance of drop size and the effect of gas flow. The collection efficiency was close to 100 percent when 2.65 mm diameter droplets were passed through the reactor at room temperature. The experiments were also repeated at 800, 1000 and 1200 K under either a constant stream of nitrogen or a no-flow condition. Due to the large drop size used, only a maximum of 6 percent weight loss was recorded at 1200 K. Based on chromatographic analysis the fuel was unchanged in these experiments. The residue collected at 1200 K and under

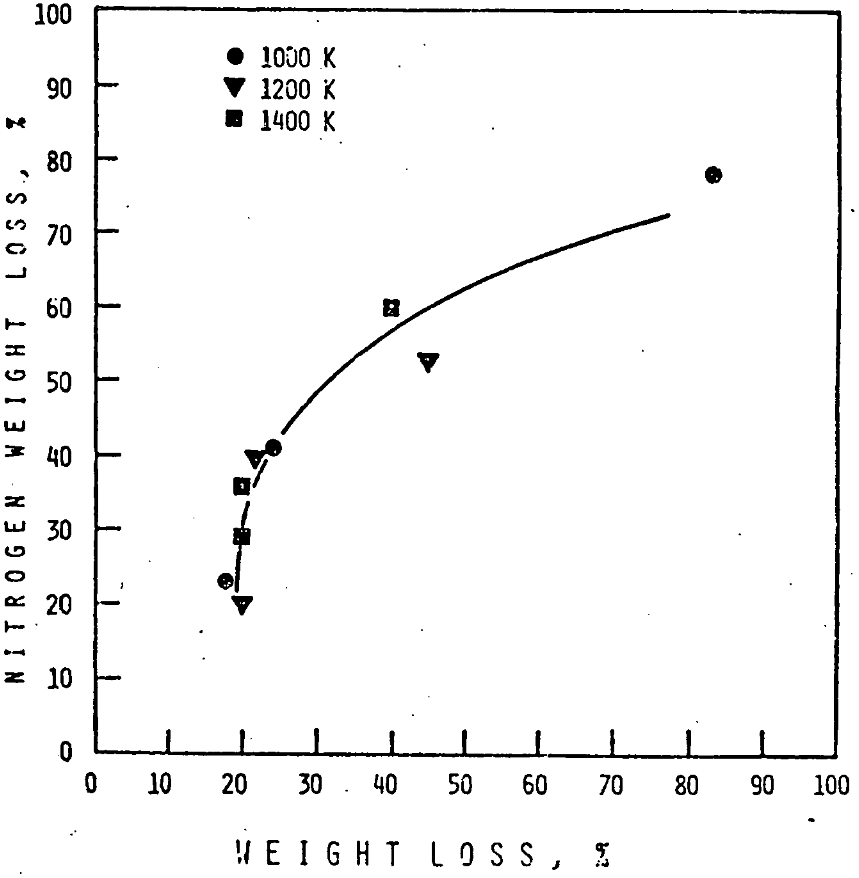

FIGURE 2. NITROGEN EVOLUTION FROM 150 μm DROPLET ARRAY OF INDO-MALAY #6 OIL (12)

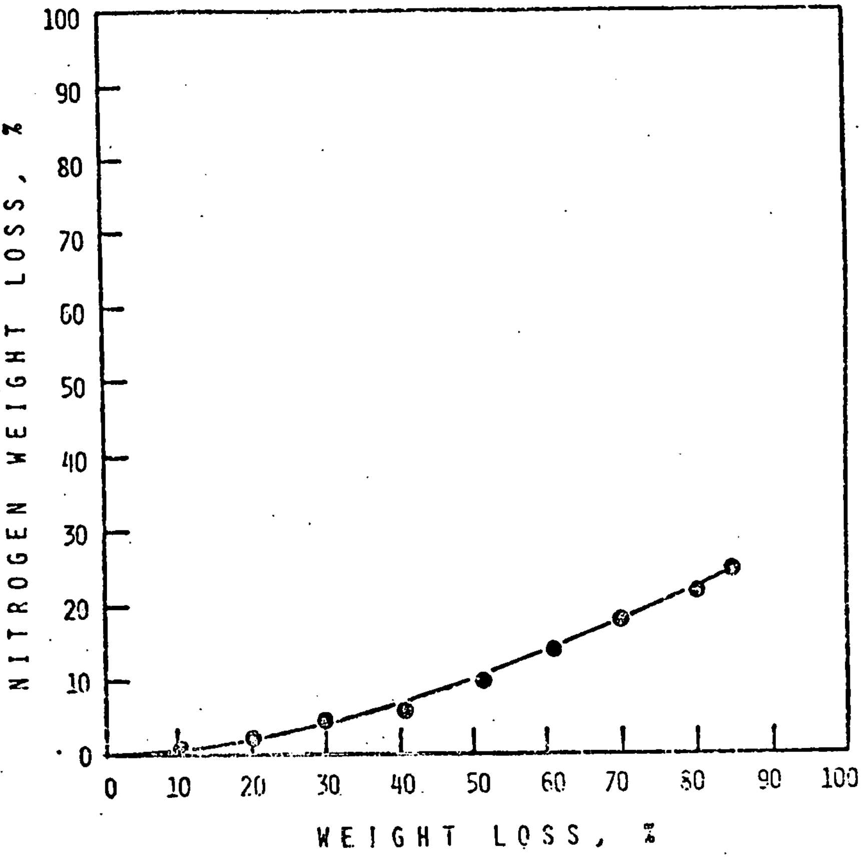

FIGURE 3. NITROGEN EVOLUTION FROM THE EQUILIBRIUM DISTILLATION OF INDO-MALAY #6 OIL AT ATMOSPHERIC PRESSURE (12)

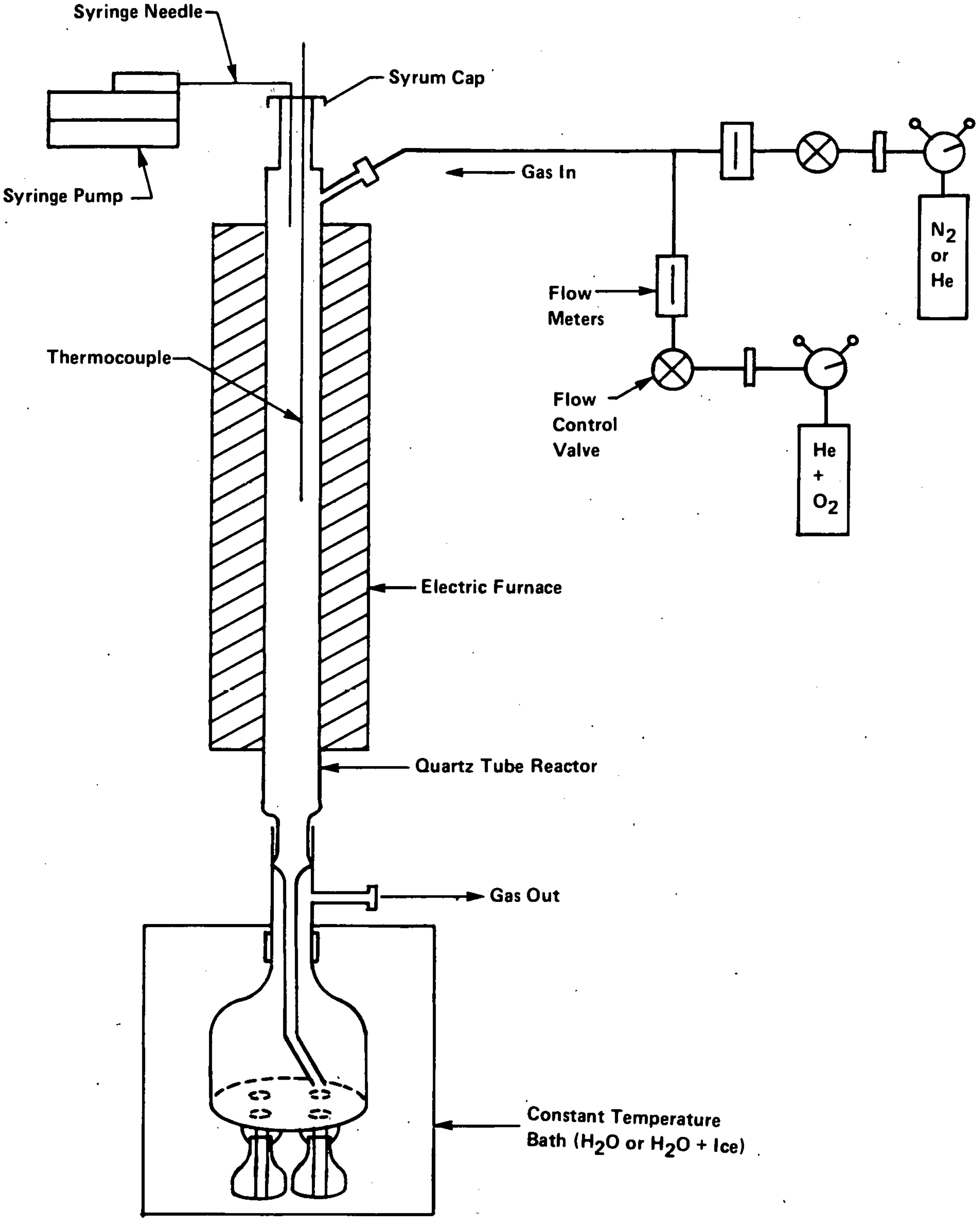

FIGURE 4. A SCHEMATIC DIAGRAM OF THE EXPERIMENTAL SET UP

a stagnant N_2 medium showed the same boiling point distribution, the same concentration of basic nitrogen and the overall composition as those of the original oil. The percent weight loss was the same for the two cases of fuel oil dropping through a 5 liter/min N_2 stream or that through a stagnant medium.

Gas flow, however, may have an effect on soot formation. When the reactor was purged with a constant stream of nitrogen during the pyrolysis experiments, carbon deposition on the reactor walls was not observed. However, under a no-flow condition, a layer of black substance, presumably soot, coated the heated section of the quartz tube. Parts of the substance were hard and parts were flaky. The black residue burned off easily in the presence of oxygen.

Since only one syringe needle size was available at the time, experiments with smaller drop sizes must be postponed until micron size needles are obtained. (These have now arrived). Results of the present experiments, however, did demonstrate the importance of drop size. Calculations assuming a uniform gas(a) and droplet temperature and for the case of a droplet falling through a stagnant medium show that the time required to heat a 2.65 mm diameter liquid fuel drop to within 63 percent of the gas temperature is approximately 40 sec(b). If the drop size is decreased by an order of magnitude, i.e., 265 μm, the heating time would reduce to only 0.4 sec. Significant weight loss will be achieved when smaller drop sizes are used.

Additional computations also indicate that the pyrolysis of the full droplet is controlled by heat transfer from the gas to the droplet. If all the heat convected to the drop were used solely to vaporize the oil, the time necessary to attain 100 percent weight loss in a 2.65 mm diameter droplet is calculated to be 5 and 9 sec for gas temperatures

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a. The assumption of a constant gas temperature throughout the 2 foot long heated section is based on the experimental observation that the gas temperature reading from a thermocouple probe located midway of the hot zone is practically the same as that of the furnace temperature.

b. Properties used in the calculations are those of typical petroleum fuel oils.

of 1200 and 800 K respectively. Similar calculations show a value of approximately 5 sec for the center of the drop to reach 63 percent of the outer surface temperature (assume to be the same as the gas temperature). Both values are significantly smaller than the estimated 40 sec heat transfer time between the gas and the drop.

PLANS FOR SECOND QUARTER

The SRC II samples requested from The Pittsburg & Midway Coal Mining Co. are in shipment and should be available by February 1, 1981.

Task 1. Distillations and analyses will be carried out during the second quarter.

Task 2. A three zone, split tube electric furnace is being purchased for this program. The new furnace is necessary because the present one has an upper limit of only 1200 K, and the oxidation experiments in Task 3 call for a furnace with a higher temperature limit. Pyrolysis experiments will be initiated on the distillate fractions of SRC II provided by Task 1.

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