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**Low-Temperature Pyrolysis
of Coal to Produce
Diesel-Fuel Blends**

Toby B. Shafer
Orlando J. Jett
Jiann-Shing Wu

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ENGINEERING TECHNOLOGY DIVISION

MASTER

LOW-TEMPERATURE PYROLYSIS OF COAL TO
PRODUCE DIESEL-FUEL BLENDS

Toby B. Shafer
Orlando J. Jett
Jiann-Shing Wu

Consultants: R.L. Graves
J.H. Stewart, Jr.

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Oak Ridge Station
School of Chemical Engineering Practice
Massachusetts Institute of Technology
G.A. Huff, Jr., Director

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830
Operated by
Union Carbide Corporation
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ABSTRACT

Low-temperature (623 to 773 K) coal pyrolysis was investigated in a bench-scale retort. Factorially designed experiments were conducted to determine the effects of temperature, coal-particle size, and nitrogen flow rate on the yield of liquid products. Yield of condensable organic products relative to the proximate coal volatile matter increased by 3.1 and 6.4 wt % after increasing nitrogen purge flow rate from 0.465 to 1.68 L/min and retort temperature from 623 to 723 K, respectively. The liquid product may be suitable for blending with diesel fuel. The viscosity and density of coal liquids produced at 723 K were compared with those of diesel fuel. The coal liquids had a higher carbon-to-hydrogen ratio and a lower aliphatic-to-aromatic ratio than premium quality No. 2 diesel fuel. It was recommended that liquids from coal pyrolysis be blended with diesel fuel to determine stability of the mixture and performance of the blend in internal combustion engines.

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1. SUMMARY

Hydrocarbon liquids produced by low-temperature (623 to 773 K) pyrolysis of coal contain less nitrogen and carcinogenic polyaromatic compounds and have a higher aliphatic content than pyrolysis liquids produced at temperatures greater than 773 K (5). These qualities are expected to make low-temperature pyrolysis liquids compatible for blending with petroleum-based diesel fuels.

The Engineering Technology Division of ORNL is studying the pyrolysis of coal at low temperatures to characterize the liquids produced and to test blends of these liquids with diesel fuel in an internal combustion engine. About 650 g of coal was charged to a bench-scale retort and pyrolyzed in a nitrogen atmosphere. Volatile products were condensed with a chilled-water heat exchanger and collected in a flask. The dependence of volatile yield, hydrocarbon liquid composition (hydrogen-to-carbon and aliphatic-to-aromatic ratios), and the boiling-point range of the liquid product on retort temperature, coal particle size, and flow rate of nitrogen purge gas was investigated with experiments designed by a two-level factorial approach. Experimental conditions were: retort temperatures of 623 and 723 K, coal-particle sizes ranging up to 0.2 cm (-10 + 1 mesh) and 0.06 to 0.48 cm (-4 + 30 mesh), and purge-gas flow rates of 0.465 and 1.68 L/min.

The yield of volatile matter was found to depend on retort temperature and the flow rate of the nitrogen purge gas. Volatile yield increased five-fold after increasing the retort temperature from 623 to 723 K. The volatile yield doubled after changing the purge-gas flow rate from 0.465 to 1.68 L/min.

The composition of the pyrolysis liquids was compared with a sample of diesel fuel. The viscosity and density of the coal liquids produced at 723 K were similar to those of diesel fuel. The aliphatic-to-aromatic ratio of the pyrolysis liquids ranged from 2.33 to 3.27, while that of diesel fuel was 5.28. The carbon-to-hydrogen ratio of the pyrolysis liquids was higher than the diesel fuel. However, analysis of the diesel fuel revealed that it contained fewer aromatics than average No. 2 diesel oil.

The miscibility of coal-pyrolysis liquid and diesel fuel should be determined by observing whether precipitates or emulsions are formed when the two liquids are blended. The coal-pyrolysis liquids for these blending tests should be produced under retort conditions of 723 K and purge-gas flow rates between 0.465 to 1.68 L/min. The maximum retort temperature at which high-quality pyrolysis liquids are produced should be further investigated. Although higher yields were obtained at 723 K, oil quality was similar to that produced at 623 K.

2. INTRODUCTION

2.1 Background

Most coal conversion processes upgrade the hydrogen content of the organic fuel produced. Coal pyrolysis produces a volatile fraction rich in hydrogenated species and a carbon-rich residual char. When coal pyrolysis is conducted at low temperatures, 623 to 773 K, several advantages are realized over higher-temperature processes:

1. Low-temperature pyrolysis is endothermic (11); the total heating value content of the products is greater than that of the untreated coal.

2. At low temperatures, bound nitrogen is seldom evolved as an oxygenated species.

3. Although liquid hydrocarbons are evolved at a slower rate, the aliphatic content is high for pyrolysis temperatures below 773 K. This is indicated graphically in Fig. 1 for a Roland-seam sub-bituminous coal (50-g sample) pyrolyzed at a constant heating rate (3.33 K/min) in an argon-swept, packed-bed retort (5).

These qualities are expected to make the low-temperature pyrolysis liquids compatible with petroleum-based diesel fuels (4). Based on these observations, the Engineering Technology Division of ORNL began an investigation to characterize the pyrolysis liquids from a low-temperature coal retort and to test these liquids blended with diesel fuel in an internal combustion engine.

2.2 Previous Work

Several investigators of low-temperature coal pyrolysis used the Fischer-retort method (6, 15, 17). In a Fischer retort, 20 to 100 g of coal is slowly heated in an aluminum tube to a temperature between 673 to 873 K. The effluent vapors are condensed and collected.

Sass (17) examined the pyrolysis of Kentucky #9, high-volatile grade B, bituminous coal in a Fischer retort at 773 K.. In comparing the Fischer assay with results of entrained-flow pyrolysis at 803 to 923 K, Sass reported much lower volatile yields (approximately 26 wt % of the coal) from the retort procedure. However, there is not a common basis for comparison because of the difference between the temperatures.

A study by Peters and Bertling (15) compared the Fischer-retort method with a stirred-bed pyrolysis unit charged with a Furst-Leopold type of coal. Both pyrolysis units were operated at 873 K. Yields of liquid were higher from the stirred-bed unit, whereas the Fischer assay yielded larger

○ C₅ - C₇ Aliphatics

□ Benzene

△ Toluene and Xylene

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SPECIES EVOLUTION DURING COAL PYROLYSIS
RELATIVE TO PEAK OF C₅-C₇ CURVE (5)

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FIG.
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amounts of coke, noncondensable volatiles, and pyrolysis water. The more-rapid pyrolysis conditions of the stirred-bed unit reduced the extent of secondary cracking reactions that convert tar (heavy coal liquids) to gas and char (11). Secondary cracking reactions and carbon deposition in the Fischer retort enhanced formation of light oil and char.

2.3 Objective

The objective of this project was to obtain and characterize low-temperature coal-pyrolysis liquids evolved from Kentucky #9 coal. The specific goals were to:

1. Determine the effect of temperature, particle size, and inert-gas flow rate on the yield, hydrogen-to-carbon ratio, boiling points (from simulated distillation curves), and the aliphatic-to-aromatic ratio of coal-pyrolysis liquids.
2. Compare the qualities of coal-pyrolysis liquids with a diesel-fuel standard.
3. Predict critical properties, molecular weight, and specific gravity of coal liquids and diesel fuel with the Wilson correlations.

3. APPARATUS AND PROCEDURE

3.1 Coal Pyrolysis

The coal pyrolysis apparatus is shown in Fig. 2. The reactor consisted of a 9.08-cm (2-in.) ID by 40.6-cm (16-in.) long carbon-steel tube placed in an insulated electric furnace, with a variac to control heating. Volatile materials were swept out of the reactor by a nitrogen purge stream. A needle valve controlled the gas flow rate and a Bourdon-tube gauge measured the system pressure, which was close to atmospheric.

The inlet gas stream was preheated by passing it through a tube wrapped around the outside wall of the vessel and in the inside wall of the insulated furnace. The effluent gas from the outlet of the reactor was condensed by heat exchange with ice water. The condensed products were collected, and the noncondensable vapor was vented into an exhaust hood at less than 311 K (100°F), the lowest recoverable temperature.

Six thermocouples were used to measure the temperature at various points in the apparatus. Two thermocouples measured the reactor-outer-wall temperature, one located 12.7 cm (5 in.) from the bottom of the reactor and the other 7.62 cm (3 in.) from the top of the reactor. The temperature of the center of the vessel was measured with two thermocouples located

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COAL-PYROLYSIS APPARATUS
(Not to Scale)

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across the reactor vessel, as illustrated in Fig. 2. The other two thermocouples measured the temperature of the effluent gas at the outlet of the vessel and the condenser.

About 640 g of Kentucky #9 bituminous or Dean Seam #3 coal was charged to the reactor, which had been opened by a flange at the top before each run. The outlet tube and the space between the furnace wall and outside reactor wall were insulated with glass wool to minimize axial temperature gradients through the reactor and to avoid condensing volatile material inside the tube that connected the condenser and vessel.

After the reactor top was sealed, purge gas was passed through the vessel and furnace heating begun. The rate of temperature increase was about 500°K/h until the reactor approached the desired temperature, after which the heating rate was decreased until all four reactor thermocouples indicated that temperatures were within 11 K (20°F) of the desired temperature. The final temperature was maintained for 3 to 4 h.

The condensed coal liquids were collected in three fractions. The first contained liquids collected while the reactor temperature was increasing; the second consisted of coal liquids produced while the reactor was at the final temperature; and the third fraction included the remaining coal liquids collected while the reactor cooled overnight (about 15 h) to room temperature. For selected runs, the flow rate of noncondensable gas from the pyrolysis unit was measured with a soap-film bubble flowmeter.

The char was removed from the cooled reactor and weighed. The condenser and connecting tubes were flushed with acetone to remove any residue and thus avoid contamination of products from different experiments. Water was removed from the organic liquid with a separatory funnel before the coal liquids were analyzed.

3.2 Coal-Product Analysis

The yield, aliphatic-to-aromatic ratio, boiling-point distribution, and carbon-to-hydrogen ratio of all coal-pyrolysis liquids collected, and the density, viscosity, sulfur, and nitrogen content of selected liquid samples were measured. The composition of the gas leaving the condenser was determined for one run, and the volatile, moisture, and ash contents of the Kentucky #9 coal and three different samples of char were measured to complete a material balance around the reactor.

Yield is defined as the collected weight of coal-pyrolysis liquid relative to the total weight of volatile matter in the coal charged to the reactor as determined by proximate analysis. Nuclear magnetic resonance (NMR) spectroscopy was used by the Analytical Chemistry Division to determine the aliphatic-to-aromatic ratio. With NMR, molecular groups near hydrogen atoms are differentiated by measuring the absorption of

visible light as the hydrogen energy levels change with magnetic-field frequencies (16). The aliphatic-to-aromatic ratio was calculated by dividing the percentage of hydrogen atoms attached to aliphatic groups by the percentage of hydrogen atoms attached to aromatic groups. The disadvantage of NMR is that molecules that contain both aliphatic and aromatic groups are counted twice. These aliphatic and aromatic compounds could not be satisfactorily separated on a gel chromatographic column, as discussed in Appendix 9.1.

The boiling points of the pyrolysis liquids were determined by a simulated distillation technique performed by the Analytical Chemistry Division, with a Shimadzu GCGA gas chromatograph and a Sigma 10 Perkin-Elmer integrating chart recorder. To obtain a smoother curve, the components were assumed to be straight-chain hydrocarbons.

The carbon and hydrogen content of the pyrolysis liquid was determined by oxidizing the liquid sample in a Lindberg carbon + hydrogen analyzer. The hydrogen reacted with oxygen to form water, which was adsorbed and weighed. The carbon reacted with oxygen to form carbon dioxide, which was adsorbed separately and weighed. The percentage of carbon and hydrogen in the sample was calculated by material balance.

If more than 10 cm³ of the coal liquid was collected, the density was measured with a pycnometer, as detailed in Appendix 9.2. The viscosity of the coal-pyrolysis liquid was measured with an Ubbelohde viscometer. The Kjeldhal method was used by Analytical Chemistry (1) to determine the nitrogen content of selected coal liquids, and the sulfur content was determined with a Leco sulfur analyzer.

The gaseous products were separated with a Perkin 3920 gas chromatograph and detected by thermal conductivity at the Analytical Chemistry Division. The volatile, moisture, and ash contents of the coal and char were determined with a Fisher coal analyzer at Analytical Chemistry.

3.3 Experimental Design and Procedure

Experiments to determine the effects of reactor conditions on volatile products were designed by two-level factorial statistics. The three variables (factors) — reactor temperature, coal-particle size, and the volumetric flow rate of purge gas through the reactor — were considered in this design. Each factor was studied at the two levels listed in Table 1.

Table 1. Experimental Design Factors and Levels

Factor	Low Level	High Level
Reactor temperature	623 K	723 K
Coal-particle size	0 to 0.2 cm (-10 + 0 mesh)	0.059 to 0.48 cm (-4 + 30 mesh)
Purge-gas flow rate	0.465 L/min	1.68 L/min

The two-level factorial design was appropriate for the exploratory analyses of this pyrolysis study. With the minimum number of runs, the sensitivity to variables was determined, which indicated parameters that should be studied further (3). The factors were examined experimentally at each level in all possible combinations. The matrix on which these experiments were designed is shown in Table 2. The levels are coded in the lower portion so that a minus sign represents the low level and a plus sign the high level of each variable. Experiments were conducted at each of the eight retort conditions described in the matrix. The dependence of volatile yield, final boiling point, aliphatic-to-aromatic ratio, and the carbon-to-hydrogen ratio on retort conditions was determined analytically. The effect of the factors on the various responses was calculated by an algorithm developed by Yates and described in Appendix 9.6. The effect of a factor is defined as the change in the response of that factor when the experimental condition moves from the minus (low) to the plus (high) level.

The symmetry of the factorial design is geometrically illustrated in Fig. 3. Each vertex of the cube denotes one of the retort conditions described in the design matrix, and the numbers correspond to the run conditions listed in Table 2. The temperature T increases from the minus (623 K) to the plus (723 K) level along the ordinate. The coal-particle size M increases from the minus (0 to 0.2 cm) to the plus (0.059 to 0.48 cm) level along the abscissa. The purge-gas flow rate F increases from minus (0.465 L/min) to plus (1.68 L/min) on the axis extending out of the plane of the page.

Experiments were designed by factorial statistics in the following manner. We shall discuss the effect of temperature first. The responses between conditions 1 and 2 in Fig. 3 differ only due to the change in temperature. There are four measures of the change in response caused by temperature. The main effect of temperature is the difference between the average response of the plus levels and the average response of the minus level. In terms of corresponding retort conditions, this is:

$$T' = \frac{y_2 + y_4 + y_6 + y_8}{4} - \frac{y_1 + y_3 + y_5 + y_7}{4} \quad (1)$$

Table 2. Factorial Design Matrix

Experiment No.	Temperature (K)	Coal Particle Size (cm) (mesh) ^a	Purge-Gas Flow Rate (L/min)
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a. Original Units of Variables

1	623	0 to 0.2 (-10 + 0)	0.465
2	723	0 to 0.2 (-10 + 0)	0.465
3	623	0.059 to 0.48 (-4 + 30)	0.465
4	723	0.059 to 0.48 (-4 + 30)	0.465
5	623	0 to 0.2 (-10 + 0)	1.68
6	723	0 to 0.2 (-10 + 0)	1.68
7	623	0.059 to 0.48 (-4 + 30)	1.68
8	723	0.059 to 0.48 (-4 + 30)	1.68

b. Coded Units of Variables

1	-	-	-
2	+	-	-
3	-	+	-
4	+	+	-
5	-	-	+
6	+	-	+
7	-	+	+
8	+	+	+

Temperature (K)		Coal-Particle Size (cm)(mesh)		Purge-Gas Flow Rate (L/min)	
-	+	-	+	-	+
623	723	0 to 0.2 (-10 + 0)	0.059 to 0.48 (-4 + 30)	0.465	1.68

^aSee Appendix 9.2 for particle-size distribution.

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GEOMETRIC REPRESENTATION
OF FACTORIAL DESIGN

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FIG.
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where y_i is the response, such as yield, at the i th experimental condition, and T' denotes the main effect of temperature. The main effect measures the average effect of temperature over all conditions of coal-particle size and purge-gas flow rate.

The main effects of coal-particle size and purge-gas flow rate are determined similarly. M' denotes the main effect of particle size and is expressed as:

$$M' = \frac{y_3 + y_4 + y_7 + y_8}{4} - \frac{y_1 + y_2 + y_5 + y_6}{4} \quad (2)$$

The main effect of purge-gas flow rate F' is:

$$F' = \frac{y_5 + y_6 + y_7 + y_8}{4} - \frac{y_1 + y_2 + y_3 + y_4}{4} \quad (3)$$

The effect of a variable, such as temperature, may be markedly different at the low level of a second variable, such as coal-particle size, than at the high level of that variable. In this case the two variables, temperature and particle size, are said to interact. A measure of this interaction is determined by the difference between the average temperature effect at the high level of particle size and the average temperature effect at the low level of particle size. This temperature-by-particle-size interaction is denoted by the $T' \times M'$ which is expressed as:

$$T' \times M' = \frac{y_1 + y_4 + y_5 + y_8}{4} - \frac{y_2 + y_3 + y_6 + y_7}{4} \quad (4)$$

Two-factor interactions can occur for all three variables. The temperature-by-purge-gas-flow-rate interaction is expressed as:

$$T' \times F' = \frac{y_1 + y_3 + y_6 + y_8}{4} - \frac{y_2 + y_4 + y_5 + y_7}{4} \quad (5)$$

The particle-size-by-purge-gas-flow-rate interaction is expressed as:

$$M' \times F' = \frac{y_1 + y_2 + y_7 + y_8}{4} - \frac{y_3 + y_4 + y_5 + y_6}{4} \quad (6)$$

Three-factor interactions measure the difference between the average effect of two-factor interaction $T' \times M'$ at the high level of purge-gas flow rate and the average $T' \times M'$ interaction at the low level of purge-gas flow rate. If the three-factor interaction is negligible, then the statistical

error is a difference of the averages:

$$T' \times M' \times F' = \frac{y_2 + y_3 + y_5 + y_8}{4} - \frac{y_1 + y_4 + y_6 + y_7}{4} \quad (7)$$

4. RESULTS

The conditions of the eight runs performed to complete the factorial design are listed in Table 2. The effect of temperature, particle size, purge-gas flow rate on yield, maximum boiling point, aliphatic-to-aromatic ratio, and carbon-to-hydrogen ratio is shown in Figs. 4 through 7 and in Table 3. Simulated distillation curves are presented in Appendix 9.4, and the weights of water and coal liquids produced and temperature histories are listed in Appendix 9.5.

Both temperature and flow rate affect the pyrolysis liquids. By increasing the temperature from 623 to 723 K, the yield increased by a factor of 5. By increasing the flow rate from 0.465 to 1.68 L/min, the yield increased by a factor of 2. Flow rate affects the maximum boiling point, whereas neither the temperature nor particle size affect the aliphatic-to-aromatic and carbon-to-hydrogen ratios.

Table 3. Effect of Run Conditions on Yield, Maximum Boiling Point, and Aliphatic-to-Aromatic Ratio

	Coal Liquid Yield (%)	Maximum Boiling Point (K)	Aliphatic-to-Aromatic Ratio
Average	4.66	676	5.87
T'	+6.40	+13.5	-0.56
M'	+0.07	+ 8.5	-0.01
T'xM'	-1.09	+11.5	-0.28
F'	+3.09	+105	+0.17
T'x F'	+2.20	0	+0.30
M'x F'	-0.32	+ 17	-0.05
T'xM'x F'	-0.80	+ 36	-0.43
T' = temperature effect			
M' = particle-size effect			
F' = flow-rate effect			
+ = positive deviation from average			
- = negative deviation from average

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EFFECT OF RUN CONDITIONS ON YIELD

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FIG.
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EFFECT OF RUN CONDITIONS ON
ALIPHATIC-TO-AROMATIC RATIO

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EFFECT OF RUN CONDITIONS ON
CARBON-TO-HYDROGEN RATIO

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A comparison of the properties of coal-pyrolysis liquids, commercial diesel fuel (CITGO), and diesel fuel reported in the literature (2, 13) is shown in Table 4. The density of coal-pyrolysis liquids is about 12% higher, the carbon-to-hydrogen ratio is 20% higher, and the aliphatic-to-aromatic ratio of the pyrolysis liquids is almost 50% lower than those of diesel fuel. The nitrogen content, maximum boiling point, and viscosity of coal-pyrolysis liquids are within the range reported for diesel fuel. The sulfur content is about three times greater than the allowable level for diesel fuel. The difference between the final and initial boiling points is 570 K (535°F) for diesel fuel and 625 K (634°F) for coal-pyrolysis liquids.

Table 4. Comparison of Coal-Pyrolysis Liquids and Diesel Fuel

	Coal-Pyrolysis Liquid (723 K)	Diesel Fuel	
		Commercial	Literature (2, 13)
Density (g/ml)	0.9 to 1.0	0.85	0.82 to 0.95
Aliphatic/aromatic ratio	2.33 to 3.27	5.28	-
Viscosity, Pa·s (cp)	3.46×10^{-3} (3.46) ^a	2.98×10^{-3} (2.98)	2×10^{-3} to 4.3×10^{-3} (2 to 4.3)
Carbon/hydrogen (wt basis)	8.41 to 8.90	6.90	5.67 to 8.8
Final boiling point, K	606 to 628 or 714 to 730 ^b	662	603
Boiling-point range, K	557 to 561 or 608 to 657 ^b	570	393
Sulfur (wt %)	1.35 ^a	933 ppm	< 0.5%
Nitrogen (wt %)	0.04	0.04	-

^aOne measurement taken.

^bF = 0.465 or 1.68 L/min, respectively.

A mass balance for coal-pyrolysis run 4 (high temperature, low flow rate, large particle size) is presented in Table 5. Half (49 wt %) of the volatiles in the coal charged are removed. A mass balance on the char and effluent product accounts for 95 wt % of coal charged to the reactor but only 74 wt % of the volatiles. Moisture represents adsorbed water on the coal surface, whereas volatile water is that chemically released during pyrolysis. The composition of the gas stream on a volume basis leaving the condenser was: 77% air and nitrogen, 15% hydrogen, 1.1% carbon monoxide, 7.3% methane, 0.72% carbon dioxide, 0.03% ethylene, 0.24% ethane, and 1% propane.

Table 5. Mass Balance for Run 4

	Reactor Contents (g)		Effluent Product (g)		
	Coal Charged	Final Char	Water	Coal Liquid	Gas
Moisture	22.3	2.4	19.9	-	-
Ash	81.3	57.2			
Volatile	245.0	120.8	28.4	12.9	18.8
Residue	<u>291.4</u>	<u>344.8</u>	—	—	—
Total	640	525.2	48.3	12.9	18.8

temperature = 723 K

particle diameter = 0.059 to 0.48 cm (-4 + 30 mesh)

flow = 0.465 L/min

The coal-pyrolysis liquid produced during reactor heat-up was analyzed and compared with the liquid produced after the reactor had reached a final temperature of 723 K (842°F). As shown in Table 6, only the aliphatic-to-aromatic ratio differed.

Table 6. Comparison of Coal Liquids Produced Before and After Reactor Reached 723 K

	<u>≤ 723 K</u>	<u>723 K</u>
Carbon-to-hydrogen ratio (wt basis)	8.6	8.7
Aliphatic-to-aromatic ratio	3.60	2.51
Boiling-point range (K)	335 to 733	379 to 714

flow rate = 1.68 L/min

particle size = 0.059 to 0.48 cm (-4 + 30 mesh)

The aliphatic-to-aromatic ratio is higher in the pyrolysis liquid produced before the reactor reaches temperature than after; as exemplified by run condition 8. Since a higher aliphatic-to-aromatic ratio is desirable, the pyrolysis liquids produced before and after the reactor reaches temperature should not be collected separately for industrial operation. No analysis was performed on the mixed liquids.

The instability of pyrolysis liquids when exposed to ultraviolet light was of concern. A sample of coal liquid produced from run 2 was exposed to sunlight for five days. The analysis of the sample is shown in Table 7. The aliphatic-to-aromatic ratio and maximum boiling point of the liquid increased 5.8 and 40.8%, respectively after exposure because the coal liquid had begun to polymerize (19).

Table 7. Effect of Ultraviolet Light on Coal-Pyrolysis Liquid

	No Exposure to Sun	Exposure to Sun for 5 Days
Carbon-to-hydrogen ratio (wt basis)	8.41	8.90
Aliphatic-to-aromatic ratio	2.33	3.28
Boiling-point range (K)	344 to 606	338 to 749
temperature = 723 K		
flow rate = 0.465 L/min		
particle size = 0 to 0.2 cm (-10 + 0 mesh)		

Coal-pyrolysis liquid was also produced from Dean Seam Coal #3 mined at Graves' Gap in New River, Anderson County, Tennessee. A comparison between this pyrolysis liquid and that produced from Kentucky #9 coal is shown in Table 8. The yield was 28% higher with the Dean Seam coal, and the carbon-to-hydrogen and aliphatic-to-aromatic ratios were 27 and 12% lower, respectively.

Table 8. Coal Pyrolysis Liquid from Two Coals

	Kentucky #9 Coal	Dean Seam #3 Coal
Density, g/ml	1.03	0.99
Viscosity, Pa·s (cp)	3.46×10^{-3} (3.46)	3.73×10^{-3} (3.73)
Carbon-to-hydrogen ratio (wt basis)	8.9	6.5
Aliphatic-to-aromatic ratio	3.04	2.68
Boiling-point range (K)	338 to 744	338 to 669
% Yield = $\left(\frac{\text{wt of coal liquid}}{\text{weight of volatiles}} \right) (100)$	13.7	17.5
temperature = 723 K		
particle size = 0.059 to 0.48 cm (-4 + 30 mesh)		
flow rate = 0.465 L/min		

5. DISCUSSION OF RESULTS

5.1 Factorial Design

From the results of the factorial experiments, the effect of temperature, particle size, and flow rate on the yield, maximum boiling point, aliphatic-to-aromatic hydrocarbon ratio, and carbon-to-hydrogen ratio was determined. The yield (wt of coal liquid/wt of volatiles)(100%) increases with higher reactor temperature, as observed by Howard (12). Coal should be pyrolyzed at the highest temperature at which the liquid products have the desired properties. Operation at 623 K (662°F) is unfeasible because the yield of coal liquids is less than 3%.

Although Smith (18) observed that the aliphatic-to-aromatic ratio decreases with higher temperature, no effect of temperature on the aliphatic-to-aromatic ratio was observed in the range studied here. There were several problems with the measurement of the aliphatic-to-aromatic ratio. NMR is not an accurate method for measuring the ratio because molecules can be counted as both aromatic and aliphatic. Another method, such as high-pressure liquid chromatography or liquid extraction with dimethyl siloxane, is needed for accurate measurement of the aliphatic-to-aromatic ratio (20).

There is no trend in the carbon-to-hydrogen ratio with temperature, particle size, or flow rate, as seen in Fig. 7. The factorial effects of temperature, particle size, and flow rate were not calculated because of the unusually low carbon-to-hydrogen ratio (0.94) of coal-pyrolysis liquid produced at 623 K (662°F) from 0.059 to 0.48 cm (-4 + 30 mesh) coal with a purge-gas flow rate of 0.465 L/min. The small carbon-to-hydrogen ratio is likely due to water in the sample. Water must be removed from the sample for accurate results. This was difficult to accomplish when less than 5 g of pyrolysis liquid was produced, as was the case for this run with an analyzed carbon-to-hydrogen ratio of 0.94.

5.2 Compatibility of Coal Liquids with Diesel Fuel

The density, viscosity, and nitrogen content of coal liquids are comparable with diesel fuel. The liquids produced contained between 8 to 10 wt % water and oletins while diesel fuel contains 5 wt % olefins, according the NMR analysis. NMR does not distinguish between water and olefins (11). The coal liquids have a 44 to 62% smaller aliphatic-to-aromatic ratio than premium quality No. 2 diesel. The higher aromatic content could cause ignition or sooting problems when used as a substitute for or in a blend with diesel fuel. A higher aromatic content usually lowers the cetane rating. Diesel fuel should have a cetane number of at least 40 to function effectively as a fuel (14). The sulfur content of diesel fuel must be less than 0.5 wt % (8). The sulfur content of one

coal-pyrolysis sample was 1.35 wt %. The sulfur must be removed or the pyrolysis liquid diluted with diesel fuel sufficiently to reduce the sulfur content to 0.5 wt % to be used in diesel fuel blends.

The maximum boiling point of diesel fuel is within the range of coal liquids produced at both low flow rates (0.465 L/min) and high flow rates (1.68 L/min). The reactor should be operated at the highest flow rate because the maximum boiling point of the product is comparable with diesel fuel; yield also increases with faster flow rates.

5.3 Coal-Pyrolysis Material Balance

A material balance accounted for 95% of the starting material and 74% of the volatiles at 723 K (842°F) at a purge-gas flow rate of 0.465 L/min, with 0.059-to-0.48-cm (-4 + 30 mesh) particles. The error was likely in determination of the composition of the residual gas. The gas sample was not analyzed until two days after it had been collected because of equipment problems. Gas could have leaked and been replaced with air. This would increase the concentration of nitrogen in the sample and would result in a lower concentration of generated gas. The flow rate of gas leaving the reactor was measured only halfway through the run and was assumed constant throughout the run. Another possible source of error is the loss by accumulation of condensed material in the condenser and tube that connects the reactor and condenser.

5.4 Properties of Coal-Pyrolysis Liquids Produced from Dean Seam #3 Coal

The yield [(weight of coal liquids/weight of volatiles)(100%)] of Dean Seam #3 coal was 20% higher than Kentucky #9 coal. Coal liquids produced from Dean Seam #3 coal had a density, viscosity, and aliphatic-to-aromatic ratio comparable with coal liquids produced from Kentucky #9 coal, and the carbon-to-hydrogen ratio was closer to that for diesel fuel. For these reasons, Dean Seam #3 coal liquids should be tested in diesel engines.

5.5 Physical-Property Correlations

Simulated distillation curves of the condensed volatile matter from the coal retort were obtained from a Shimadzu GCGA gas chromatograph. The simulated distillation curves were separated into fractions by mathematically dividing the curve at 50-K intervals from tabulated data. Each fraction of similar boiling point was considered a pseudocomponent, i.e., a blend of pure components having similar physical properties. The arithmetic-mean boiling point of each pseudocomponent was used to predict the characterization parameters of coal liquids: specific gravity, critical temperature, and critical pressure.

The API gravity of each pseudocomponent was predicted with the Prudich correlations (8), tabulated in Table 9, from the pseudocomponent average boiling point T_b . The API gravity is related to the specific gravity by (14):

$$\text{API} = \frac{141.5}{\text{Sp. Gr.}} - 131.5 \quad (8)$$

in which Sp. Gr. is the specific gravity at 289 K (60°F). The predicted specific gravity of the pseudocomponents ranged from 0.822 to 1.06. The measured values for the mixture of pseudocomponents ranged from 0.93 to 0.96.

Table 9. Prudich Correlations

$$\text{API grav} = \frac{141.5}{0.56 + 0.00102 T_b} - 131.5 \quad (9)$$

for $200^\circ\text{F} < T_b < 400^\circ\text{F}$ and T_b = average boiling point, °R.

$$\text{API grav} = 14.678 \quad (10)$$

for $400^\circ\text{F} < T_b < 475^\circ\text{F}$

$$\text{API grav} = \frac{141.5}{0.7647 + 0.000428 T_b} - 131.5 \quad (11)$$

for $475^\circ\text{F} < T_b < 900^\circ\text{F}$

The critical properties of the pseudocomponents were based on the Wilson correlations (21), which relate the characterization parameters of coal liquids to boiling point and specific gravity. The Wilson equations are presented in Table 10.

The predicted characterization parameters of the pseudocomponents for coal-pyrolysis liquids obtained at 723 K with 0.059-to-0.48-cm (-4 + 30 mesh) particles and a nitrogen flow rate of 0.465 L/min are tabulated in Table 11. These properties are tabulated in Appendix 9.7 for other coal-liquid samples. The critical properties of the coal liquids were not determined experimentally, hence there is no basis for comparison.

Table 10. Wilson Correlations

Watson characterization parameter:

$$K_w = (T_b)^{1/3} / \text{Sp. Gr.} \quad (12)$$

T_b = average boiling point, °R

Molecular weight MW:

$$\ln(\text{MW}) = -10.9419 + 2.3333 \ln T_b - \ln \text{Sp. Gr.} \quad (13)$$

Critical pressure P_c :

$$\log(P_c) = 2.22066 - 0.05445 K_w + 3.12579 \left(1 - \frac{T_b}{T_c}\right) \quad (14)$$

P_c is in psia.

Critical temperature T_c :

$$\log(T_c) = 1.1569 + 0.38882 \log(\text{Sp. Gr.}) + 0.66709 \log(T_b) \quad (15)$$

Acentric factor ω :

$$\omega = \left[\ln\left(\frac{14.7}{P_c}\right) - f_0 \right] / f_1 \quad (16)$$

$$f_0 = 5.92714 - \frac{6.09648}{T_R} - 1.28862 \ln T_R + 0.169347(T_R)^6 \quad (17)$$

$$f_1 = 15.2518 - \frac{15.6875}{T_R} - 13.4721 \ln T_R + 0.43577(T_R)^6 \quad (18)$$

Critical compressibility Z_c :

$$Z_c = \frac{1}{1.28\omega + 3.41} \quad (19)$$

Critical volume V_c :

$$V_c = \frac{Z_c T_c}{P_c} \frac{670.14}{\text{cm}^3/\text{mol}} \quad (20)$$

Heat capacity C_p (Btu/lb-°F):

$$\text{constants for } C_p = a + bT \quad (21)$$

$$a = (0.465 + 0.0436 K_w)(0.4949 - 0.02479 \text{ Sp. Gr.}) \quad (22)$$

$$b = (0.465 + 0.0436 K_w)(0.8117 - 0.3672 \text{ Sp. Gr.}) \times 10^{-3} \quad (23)$$

Table 11. Pseudocomponent Properties for Kentucky #9 Coal

Retort Conditions: Temperature = 723 K
Particle size = 0.059 to 0.48 cm (-4 + 30 mesh)
Flow rate = 1.68 L/min

Pseudocomponent Boiling-Point Range (K)	Accumulated Volume (%)	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
323 - 373	0.33				
373 - 423	7.15	593	3.11	0.82	99
423 - 473	38.73	669	3.43	0.91	117
473 - 523	58.10	734	3.32	0.97	142
523 - 573	75.07	789	2.93	0.99	173
573 - 623	88.53	849	2.76	1.03	204
623 - 673	100.00	909	2.60	1.06	238

6. CONCLUSIONS

1. Coal-liquid yield increased with higher pyrolysis temperature, over the range studied of 623 to 723 K.
2. Greater yields of coal liquids were collected as purge-gas flow rate was increased from 0.465 to 1.68 L/min.
3. The viscosity and density of coal-pyrolysis liquids produced at 723 K, and the maximum boiling point of coal liquids produced at a nitrogen-purge-gas flow rate of 0.465 L/min, were comparable with those of diesel fuel. At this higher temperature, the aliphatic to-aromatic ratio of coal-pyrolysis liquids was lower and the carbon-to-hydrogen ratio was higher than those of diesel fuel.
4. Exposure to ultraviolet light increased the aliphatic-to-aromatic ratio and widened the final boiling point range of coal-pyrolysis liquids.

7. RECOMMENDATIONS

1. The compatibility of coal-pyrolysis liquid and diesel fuel should be determined by observing whether precipitates or emulsions are found when the two liquids are blended.
2. Blends of diesel fuel and coal-pyrolysis liquids produced from Kentucky #9 and Dean Seam #3 coal at 723 K at a purge-gas flow rate between 0.465 and 1.68 L/min should be tested in diesel engines as a final evaluation of their utility in an unrefined state.
3. The maximum operating temperature of the pyrolysis reactor which maintains coal-liquid quality should be determined.

8. ACKNOWLEDGMENT

We thank Ron Graves and Van Brantley for their instruction on the use of the coal-pyrolysis equipment. We especially thank Joe Stewart, Jr., for the speed in which he provided the chemical analyses, and Jim Attrill and C. Ho for their valuable aid in helping with the chemical analyses essential to this work.

9. APPENDIX

9.1 Methods of Determining Aliphatic-to-Aromatic Ratio

Since NMR does not give an accurate measurement of the aliphatic-to-aromatic ratio, column chromatography was tried. The column was made from Sephadex LH-20 gel in isopropanol. The coal-pyrolysis liquid was added to the top of the column and washed with isopropanol. Radioactive ^{14}C beta-emitting hexadecane was added to trace the aliphatics. An additional 300 ml of isopropanol was added, and the effluent was collected in 100-, 50-, 2-to-25-, and 5-to-10-ml fractions. The samples were counted for beta emission to determine which fractions were aliphatic, after which about 500 ml of benzene was added to the column to remove aromatics. The aliphatic fractions were combined, and the isopropanol evaporated with a rotoevaporator. Solvent was evaporated from the aromatic fractions similarly. The solvent-free samples were weighed to determine the fractions of aliphatics and aromatics in the pyrolysis liquids. Only 85 wt % of the coal liquid was recovered because of losses by evaporation. The aliphatic-to-aromatic ratio of the aliphatic and aromatic fractions was determined with NMR to check the separation. The aliphatic-to-aromatic ratio of the coal liquid was 2.8; that of the aliphatic fraction was 4.8. Column chromatography is therefore not suitable for determining the aliphatic-to-aromatic ratio of pyrolysis liquids (10).

9.2 Calibration of Pycnometer

The densities of water, methanol, and acetone from our experimental measurements and literature values (9) are listed in Table 12.

Table 12. Pycnometer Calibration

<u>Liquid</u>	<u>Experimentally Determined Density (g/ml)</u>	<u>Literature (9) Density (g/ml)</u>	<u>Ratio of Experimental to Literature Density</u>
Acetone	0.700 (24.6°C)	0.759 (25°C)	0.922
Methanol	0.703 (23.8°C)	0.786 (24°C)	0.894
Water	0.902 (26.4°C)	0.997 (26.4°C)	0.905

The average ratio of experimental density to the density reported in the literature was 0.907 ± 0.015 . Therefore, all density measurements were divided by 0.907 to obtain the true density.

9.3 Particle-Size Distribution

The particle-size distribution of the coal was measured by placing between 150 and 250 g of coal on top of a stack of sieve pans. The stack was electrically shaken for 4 min, and the amount of material retained on each sieve tray was weighed. The particle-size distribution is given in Table 13.

Table 13. Particle-Size Distribution

<u>Sieve Size</u>	<u>Opening (cm)</u>	<u>Cumulative wt % Retained</u>		
		<u>Kentucky #9 Large Size</u>	<u>Kentucky #9 Small Size</u>	<u>Dean Seam #3</u>
6	0.336	62.0		45.0
16	0.119	99.2	54.6	90.6
30	0.059	99.3	98.2	99.1
100	0.015	99.3	99.5	99.4
Pan		100	100	100
<u>Top Size</u>		0.48 cm (4 mesh)	0.2 cm (10 mesh)	0.48 cm (4 mesh)

9.4 Simulated Distillation Curves

The simulated distillation curves constructed for each of the coal liquids and diesel fuel are shown in Figs. 8 through 21.

T = 723 K
M = 0.059 to 0.2 cm
F = 0.465 L/min

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SIMULATED DISTILLATION CURVE
FOR COAL LIQUIDS

DATE 5-17-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 9
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$T = 623 \text{ K}$
 $M = 0.059 \text{ to } 0.48 \text{ cm}$
 $F = 1.68 \text{ L/min}$

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS

DATE
 5-17-82

DRAWN BY
 JSW

FILE NO.
 CEPS-X-355

FIG.
 11

T = 723 K
M = 0.059 to 0.48 cm
F = 0.465 L/min
Sample collected while reactor was heating.

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SIMULATED DISTILLATION CURVE
FOR COAL LIQUIDS

DATE 5-17-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 12
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T = 723 K
M = 0.2 to 0.48 cm
F = 0.465 L/min

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SIMULATED DISTILLATION CURVE
FOR COAL LIQUIDS
(Run 4)

DATE
5-17-82

DRAWN BY
JSW

FILE NO.
CEPS-X-355

FIG.
13

$T = 723 \text{ K}$
 $M = 0.059 \text{ to } 0.48 \text{ cm}$
 $F = 0.465 \text{ L/min}$
 Run to check experimental reproducibility

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS

DATE	DRAWN BY	FILE NO.	FIG.
5-17-82	JSW	CEPS-X-355	14

$T = 623 \text{ K}$
 $M = 0 \text{ to } 0.2 \text{ cm}$
 $F = 1.68 \text{ L/min}$

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS
 (Run 5)

DATE 5-17-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 15
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$T = 723 \text{ K}$
 $M = 0 \text{ to } 0.2 \text{ cm}$
 $F = 1.68 \text{ L/min}$

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS
 (Run 6)

DATE	DRAWN BY	FILE NO.	FIG.
5-17-82	JSW	CEPS-X-355	16

T = 623 K
M = 0.059 to 0.48 cm
F = 1.68 L/min

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SIMULATED DISTILLATION CURVE
FOR COAL LIQUIDS
(Run 7)

DATE 5-17-82	DRAWN BY. JSW	FILE NO. CEPS-X-355	FIG. 17
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$T = 723 \text{ K}$
 $M = 0.059 \text{ to } 0.48 \text{ cm}$
 $F = 1.68 \text{ L/min}$
 Sample collected before reactor reached temperature.

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS

DATE
 5-17-82

DRAWN BY
 JSW

FILE NO.
 CEPS-X-355

FIG.
 18

$T = 723 \text{ K}$
 $M = 0.059 \text{ to } 0.48 \text{ cm}$
 $F = 1.68 \text{ L/min}$

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SIMULATED DISTILLATION CURVE
 FOR COAL LIQUIDS
 (Run 8)

DATE 5-17-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 19
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SIMULATED DISTILLATION CURVE FOR
COMMERCIAL DIESEL FUEL (CITGO)

DATE 5-17-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 20
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T = 723 K
M = 0.059 to 0.48 cm
F = 0.46 L/min

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SIMULATED DISTILLATION CURVE FOR
DEAN-SEAM COAL LIQUIDS

DATE 5-18-82	DRAWN BY JSW	FILE NO. CEPS-X-355	FIG. 21
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9.5 Weight of Coal Liquids and Water Produced

The weight of coal liquid and water, temperature overshoot, and time of temperature overshoot are tabulated in Table 14. The temperature overshoot is the difference between the maximum and the desired temperature, before the reactor assumed steady-state operation.

Table 14. Experimental Conditions

Run	Coal Charged to Reactor (g)	Char (g)	Collected Coal Liquids (g)	Collected Water (g)	Temperature Overshoot (K)	Time of Temperature Overshoot (min)
1	640.0	588.6	1.7	39.0	0	-
2	640.0	541.6	13.0	52.4	17	10
3	640.6	574.6	3.3	43.4	25	50
4	640.0	525.2	12.9	48.3	0	0
5	640.0	581.4	2.75	33.5	0	0
6	640.0	524.0	29.1	37.6	0	0
7	640.0	577.8	6.7	66.1	14	20
8	681.0	564.4	24.6	47.2	14	10

The data from an attempt to reproduce Run 4 were discarded because the temperature overshoot was greater than 28 K (temperature recorder went off scale), and the time of the temperature overshoot was 140 min.

9.6 Yates' Algorithm

Yates' algorithm (1) was used to calculate the main effects and interactions between variables for the factorial experiments. The runs must be arranged in a standard order: the first column of the design matrix must alternate between the two variable levels, the second column must consist of alternating pairs of the two variable levels, and the third column consists of four entries of one variable level followed by four entries of the other level, as listed in Table 15. The yield of each set of run

conditions is given in the fourth column. The first four entries of the fifth, sixth, and seventh columns are obtained by adding successive pairs of the previous columns; and the second four entries are obtained by subtracting the top number from the bottom number of each pair in the previous column, as shown in the table. The eighth column is obtained by dividing all entries in the seventh column, but the first, by 4. The first entry is divided by 8. The effects and interactions between variables are tabulated in column 8.

Table 15. Yates' Algorithm for Calculating Effect on Yield

<u>1</u> <u>T</u>	<u>2</u> <u>M</u>	<u>3</u> <u>F</u>	<u>4</u> <u>Yield</u>	<u>5</u>	<u>6</u>	<u>7</u>	<u>8</u> <u>Effect</u>	
-	-	-	0.68	5.85	12.47	4.66	5.8	average
+	-	-	5.17	6.62	24.83	6.40	8.7	T
-	+	-	1.35	12.66	8.41	0.07	2.4	M
+	+	-	5.27	12.17	17.19	-1.09	1.2	TxM
-	-	+	1.09	4.49	0.77	3.09	0.78	F
+	-	+	11.57	3.92	-0.49	2.20	-0.11	TxF
-	+	+	2.73	10.48	-0.57	-0.32	-2.6	MxF
+	+	+	9.44	6.71	-3.77	-0.80	-3.1	TxMxF

9.7 Pseudocomponent Properties

The physical and chemical properties of the coal pseudocomponents were determined with the Wilson and Prudich correlations. The predicted values for each run are presented in Tables 16 through 23.

9.8 Location of Original Data

Copies of the original data and calculation files are located at the MIT School of Chemical Engineering Practice, Bldg. 1505, ORNL. The laboratory book titled Pyrolysis contains coal-pyrolysis data and is located in Room 197, Bldg. 9201-3, Y-12 Plant.

Table 16. Pseudo-component Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 623 K Particle size = 0 to 0.2 cm (-20 + 80 mesh) Flow rate = 0.465 L/min						
Pseudo-component Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	0.110				
100 - 150	125	4.020	593	3.11	0.822	99
150 - 200	175	37.28	669	3.43	0.914	117
200 - 250	225	65.17	734	3.32	0.968	142
250 - 300	275	86.42	789	2.93	0.990	173
300 - 350	325	96.15	849	2.76	1.029	204
350 - 400	375	100.0	909	2.60	1.060	239

Table 17. Pseudocomponent Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 723 K
Particle size = 0 to 0.2 cm (-10 + 0 mesh)
Flow rate = 0.465 L/min

Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	1.26				
100 - 150	125	12.96	593	3.11	0.822	99
150 - 200	175	60.37	669	3.43	0.914	117
200 - 250	225	83.61	734	3.32	0.968	142
250 - 300	275	95.92	789	2.93	0.990	173
300 - 350	325	99.51	849	2.76	1.029	204
350 - 400	375	100.0	909	2.60	1.060	239

Table 18. Pseudocomponent Properties of Kentucky #9 Coal

Report Conditions: Temperature = 623 K
Particle size = 0.06 to 0.48 cm (-4 + 30 mesh)
Flow rate = 0.465 L/min

Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	31.13				
100 - 150	125	42.00	593	3.11	0.822	99
150 - 200	175	81.41	669	3.43	0.914	117
200 - 250	225	97.09	734	3.32	0.968	142
250 - 300	275	99.23	789	2.93	0.990	173
300 - 350	325	100.00	849	2.76	1.029	204

Table 19. Pseudocomponent Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 723 K
 Particle size = 0.06 to 0.48 cm (-4 + 30 mesh)
 Flow rate = 0.465 L/min

<u>Pseudocomponent Boiling-Point Range (°C)</u>	<u>Average Boiling Point (°C)</u>	<u>Accumulated Volume Fraction</u>	<u>Critical Temperature (K)</u>	<u>Critical Pressure (MPa)</u>	<u>Specific Gravity at 289 K (60°F)</u>	<u>Molecular Weight</u>
50 - 100	75	1.12				
100 - 150	125	11.03	593	3.11	0.822	99
150 - 200	175	53.00	669	3.43	0.914	117
200 - 250	225	78.50	734	3.32	0.968	142
250 - 300	275	94.42	789	2.93	0.990	173
300 - 350	325	99.34	849	2.76	1.029	204
350 - 400	375	100.00	909	2.60	1.060	239

Table 20. Pseudocomponent Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 623 K
Particle size = 0 to 0.2 cm (-10 + 0 mesh)
Flow rate = 1.68 L/min

Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	0.19				
100 - 150	125	0.55	593	3.11	0.822	99
150 - 200	175	17.38	669	3.43	0.914	117
200 - 250	225	37.42	734	3.32	0.968	142
250 - 300	275	63.63	789	2.93	0.990	173
300 - 350	325	84.02	849	2.76	1.029	204
350 - 400	375	94.40	909	2.60	1.060	239
400 - 450	425	100.00				

Table 21. Pseudocomponent Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 723 K Particle size = 0 to 0.2 cm (-10 + 0 mesh) Flow rate = 1.68 L/min						
Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	0.91				
100 - 150	125	6.71	593	3.11	0.822	99
150 - 200	175	28.26	669	3.43	0.914	117
200 - 250	225	43.25	734	3.32	0.968	142
250 - 300	275	59.89	789	2.93	0.990	173
300 - 350	325	76.00	849	2.76	1.029	204
350 - 400	375	90.66	909	2.60	1.060	239
400 - 425	425	100.00				

Table 22. Pseudocomponent Properties of Kentucky #9 Coal

Retort Conditions: Temperature = 623 K
Particle size = 0.06 to 0.48 cm (-4 + 30 mesh)
Flow rate = 1.68 L/min

Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	2.00				
100 - 150	125	2.50	593	3.11	0.822	99
150 - 200	175	17.64	669	3.43	0.914	117
200 - 250	225	33.17	734	3.32	0.968	142
250 - 300	275	53.69	789	2.93	0.990	173
300 - 350	325	73.38	849	2.76	1.029	204
350 - 400	375	88.15	909	2.60	1.060	239
400 - 425	425	100.00				

Table 23. Pseudocomponent Properties of Dean Seam #3 Coal

Retort Conditions: Temperature = 723 K
Particle size = 0.06 to 0.48 cm (-4 + 30 mesh)
Flow rate = 0.465 L/min

Pseudocomponent Boiling-Point Range (°C)	Average Boiling Point (°C)	Accumulated Volume Fraction	Critical Temperature (K)	Critical Pressure (MPa)	Specific Gravity at 289 K (60°F)	Molecular Weight
50 - 100	75	0.74				
100 - 150	125	7.44	593	3.11	0.822	99
150 - 200	175	32.88	669	3.43	0.914	117
200 - 250	225	51.03	734	3.32	0.968	142
250 - 300	275	73.22	789	2.93	0.990	173
300 - 350	325	91.11	849	2.76	1.029	204
350 - 400	375	100.00	909	2.60	1.060	239

9.9 Nomenclature

a, b	constants in heat capacity correlation, Eq. (21)
API	American Petroleum Institute specific gravity
C_p	heat capacity, J/kg-K
f_0, f_1	Wilson parameters in Eqs. (17) and (18)
F	purge-gas flow rate, L/min
K_w	Watson characterization parameter
M	particle diameter, cm
MW	molecular weight
P_c	critical pressure, MPa
Sp.Gr.	specific gravity at 289 K (60°F)
T	temperature, K
T_b	boiling point, K
T_c	critical temperature, K
T_r	reduced temperature
V_c	critical volume, cm^3/mol
x	interaction between two factors
y	response at i^{th} retort condition
Z_c	critical compressibility
ω	acentric factor

Superscript

'	main effect in factorial statistical analysis
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