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FLASH HYDROLYSIS OF COAL

QUARTERLY REPORT NO. 12

JANUARY 1 - MARCH 31, 1980

MEYER STEINBERG

PETER FALLON

BHARAT L. BHATT

August 1980

DEPARTMENT OF ENERGY AND ENVIRONMENT

BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973

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Master

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(Coal Conversion and Utilization-
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PROCESS SCIENCES DIVISION

DEPARTMENT OF ENERGY AND ENVIRONMENT
BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.

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Summary

A number of experiments were conducted using both Pittsburgh No. 8 and Illinois No. 6 bituminous coals. Diluents of limestone, sand, CaO and K_2CO_3 were used to prevent agglomeration. No significant effect on product yield was observed for the various diluents.

The Pittsburgh No. 8 gave greater yields of gaseous hydrocarbons when used at 1000 psi and 950°C than at the same pressure at 900°C. Similar experiments with New Mexico sub-bituminous coal both treated with Na_2CO_3 and untreated did not produce any increase in yields. The Pittsburgh No. 8 coal also yielded 15% BTX when used at 1000 psi and 820°C.

The Illinois No. 6 coal showed no effect of pressure on yield when hydrogenated at 775°C and increasing pressures of 1000, 1500 and 2000 psi of hydrogen. The yield of gas ranged from 15 to 21% and the liquids from 9 to 14%. A first recycle of Illinois No. 6 char showed some remaining reactivity increasing the gaseous yield from 43% to 51% and the liquid yield from 9% to 10%. A second recycle produced only a 1% increase in the gas yield.

The introduction of 20% steam into the hydrogen at 1000 psi and 900°C using New Mexico sub-bituminous coal increased the liquid yield from 7% to 10% but lowered the gaseous yield from 46% to 42%.

A significantly greater fraction of naphthalene was found in the heavy liquids from the bituminous coals than from the lignite and sub-bituminous coal (72% vs 50%).

Preliminary modelling of the sub-bituminous data indicated good correlation with the experimental results. Thermodynamic equilibrium calculations indicate that the rapid hydrogasification of coal is not equilibrium controlled.

I. OBJECTIVE AND SCOPE OF WORK

The program objective is to develop process chemistry and design information and to investigate methods for improving yields and process conditions for the rapid hydrogasification of coal. The rapid hydrogasification or hydrolysis of coal (1,2) is a fast gas phase, non-catalytic direct coal conversion technique for the formation of gaseous hydrocarbons and significant quantities of aromatic liquid hydrocarbons. The work includes the design, construction, and operation of a 1 lb/hr down-flow entrained tubular reactor system capable of operating at up to 900°C and 4000 psi and incorporating on-line product analysis. The experimental unit is used to study the effect of such process variables as temperature, pressure, feed rate, residence time, coal type and feed gas composition on the yields of liquid and/or gaseous hydrocarbon products. Complete mass balances of feed to product are made, the data are correlated and modelled for determination of rate equations.

II. TUBULAR REACTOR EXPERIMENTAL RESULTS

Work Accomplished

a) Hydrogasification of Bituminous Coal

Continued experimental work was conducted using the two caking bituminous coals Illinois No. 6 and Pittsburgh No. 8, previously reported (3). Diluents of sand or limestone were used to prevent agglomeration. Other experiments were conducted to study the effect of both calcium oxide (CaO) and potassium carbonate (K₂CO₃) diluents on the yields. Some differences were observed between the results obtained using the sand and limestone. Up to 20% weight concentration of Pittsburgh 8 could be fed to the tubular reactor without agglomeration while for Illinois No. 6 up to 40% could be fed.

The Pittsburgh seam coal has a slightly higher free swelling index than the Illinois, (3 vs 2).

Table 1 shows the results of two experiments conducted using Pittsburgh No. 8 in sand and limestone. In experiment 334, the reactor temperature was raised to 950°C, 50°C above the normal maximum of 900°C used experimentally, to determine if higher temperatures could increase methane yields at 1000 psi hydrogen pressure. The gaseous hydrocarbon yield was 54.5% of the available carbon while for similar experiments conducted at 900°C (runs 318 and 329) approximately 39% gas was produced. However, the BTX yield decreased to 5.6% where previously at 900°C approximately 10% BTX was produced. The other results shown in this table, experiment 333, was conducted while increasing the reactor temperature from 750°C to 925°C to determine the optimum temperature for the production of BTX at 1000 psi. This was found to be 820°C and the maximum BTX yield 15.2%. No heavier liquid hydrocarbons were produced and the gaseous yields were 32.2%. Since only 20% Pittsburgh No. 8 coal can be fed in the various diluents, it was decided to limit work with this coal until some other method of feeding can be developed. The high BTX yield at 1000 psi hydrogen pressure indicates the need for further investigation.

In the next series of experiments, CaO and K₂CO₃ were used as diluents with Illinois No. 6 at 900°C and 1000 psi. Table 2 shows the results of experiments using each of these compounds plus a typical experiment using limestone. The experiment using CaO gave results almost identical to that of the limestone, 46% total hydrocarbons versus 44% except for the much lower oxides of carbon yield for the CaO (1.6% vs

17.1%). The experiment using K_2CO_3 gave a similar total hydrocarbon yield (48.5%) but the gaseous yield was slightly greater than the limestone (43.5% vs 36%) and the BTX slightly lower (5% vs 8%). The oxides of each were much lower than when using limestone since the reactor temperature ($900^{\circ}C$) was above the decomposition temperature of the limestone ($825^{\circ}C$) but not that of the K_2CO_3 ($>900^{\circ}C$).

An experiment was conducted using Illinois No. 6 at 1000 psi while increasing the reactor temperature from 700° to $825^{\circ}C$ in order to determine the optimum temperature for the production of BTX. Although the experiment was not completely successful due to mechanical problems, it did show the temperature to be approximately $775^{\circ}C$. A number of experiments were then conducted using the same coal plus limestone and sand at various hydrogen pressures. The results are given in Table 3. Although the data was very scattered and no trends can be seen, the yields of gaseous and liquid hydrocarbons does not appear to be greatly influenced by hydrogen pressure. The gaseous yields averaged approximately 25% while the liquid yields varied between 9 and 14%.

Other experiments were conducted at $775^{\circ}C$, $800^{\circ}C$ and $850^{\circ}C$ using Illinois No. 6 as shown in Table 4. The hydrogen pressure was 1000 psi and the coal was used with limestone. The gaseous hydrocarbons are seen to be more than double from 16.7% at $775^{\circ}C$ to 35.8% at $850^{\circ}C$. The BTX yields remain almost constant at 7 to 8% and the heavier liquids never exceed 3%. The production of CO increases considerably as the decomposition temperature of the limestone is exceeded.

In order to determine if any reactivity remained in the char from experiments using Illinois No. 6 coal, the char from an experiment using 50% coal and 50% limestone was recycled through the reactor system twice. The results are shown in Figure 1. The first experiment using the fresh coal (5 sec. residence time) produced a maximum of 43% gaseous hydrocarbons and 9% liquids. The first recycle (cumulative to 10 sec. residence time) produced an additional 8% gases and 1% liquids. The second recycle (cumulative to 15 sec. residence time) produced only 1% additional gases and no liquids. It appears that after 10 seconds residence time all the reactivity of this coal is spent and any further reaction is between elemental carbon in the char and hydrogen.

Previous experiments with Illinois No. 6 and limestone has shown the mixture of char and limestone, at the end of an experiment, to retain as much as 90% of the sulfur in the feed coal. The limestone used was ground to approximately the same size as the coal, less than 150 μ (-100 mesh).

In order to separate the char and limestone to determine the sulfur retention of each, limestone particles of sizes larger than the largest coal particle were tried. First limestone from 250 to 800 μ were tried with 40% Illinois No. 6 and the reactor plugged. Next limestone from 150 to 250 μ in 40% coal was tried and again the reactor plugged. The same particle size was then unsuccessfully tried with 20% coal. This series of experiments was then discontinued. It appeared that the critical parameter is the surface area available on which the coal can wet when the temperature of the coal reaches the plastic state.

b) The Hydrogasification of New Mexico Sub-Bituminous Coal

Aside from six experiments found to be needed to complete the parametric study of this coal, three exploratory experiments were also conducted. Two of these were at 950°C and 1000 psi, one with coal treated with Na_2CO_3 and the other an untreated coal. The third experiment was conducted at 900°C and 1000 psi while introducing approximately 20% steam to determine the effect steam would have on the reaction. The reason for operating at 950°C was to determine if the methane yield continued to increase as sharply above 900°C as it did approaching 900°C.

In Table 5, the results of the experiments conducted at 950°C are compared to similar experiments conducted at 900°C. Although only a few experiments are available, there appears to be no increase in gaseous yields above 900°C and possibly a slight decrease. The liquid yields definitely did decrease due to decomposition at the higher temperature.

Table 6 shows a comparison of the yields from two experiments conducted at 900°C and 1000 psi, one using hydrogen alone and the other hydrogen continuing 20% steam. The major difference in the results observed is a slight increase in the BTX yield (10% vs 7%) at a corresponding decrease in the gaseous yield (43% vs 47%) for the experiment using steam.

Work Forecast

The program is being redirected to investigate the hydrogenation reaction at residence times shorter than presently being studied and at hydrogen to coal ratios less than 0.5. The first series of experiments will be made using Montana Rosebud sub-bituminous coal at temperatures up to 1040°C and 1200 psi hydrogen pressure.

III. PRODUCT ANALYSES AND MATERIAL BALANCES

Work Accomplished

The yields from the bituminous coals did not seem to improve with increased hydrogen pressure as observed with the two coals previously studied. This was particularly true for the liquid yields. One noticeable difference in the liquids produced from the bituminous coals was the high percentage of naphthalene in the heavier liquids ($\geq C_9$) as compared to that produced from lignite and sub-bituminous coal. The naphthalene yield from the bituminous coal averaged approximately 72% of the heavier liquid while the lignite and sub-bituminous coals averaged approximately 50%. Thus, the heavier liquids from bituminous coal is much lower in asphaltenes than liquids from the other coals.

Work Forecast

The shorter residence times at reactor conditions which are to be studied is expected to produce much heavier liquid hydrocarbons which may be higher in sulfur content than previously encountered. This will necessitate some experimentation with analytical techniques in order to best characterize these liquids.

IV. REACTION MODELLING AND DATA CORRELATION

Work Accomplished

A report entitled "Reaction Modelling and Data Correlation for Flash Hydropyrolysis of Lignite"⁽⁴⁾ was published and will be presented at the 15th Intersociety Energy Conversion Engineering Conference, Seattle, Washington. The report contains development of a model and correlation of data obtained from North Dakota lignite experiments for a hydrogen to coal feed weight ratio of approximately 1. Design curves were developed using

the rate expressions and the estimated values of activation energies and pre-exponential factors for the range of the experimental conditions, were presented. The conversion data obtained from hydrogenation experiments using New Mexico sub-bituminous coal is being correlated using similar techniques. Preliminary results from the computer show an overall correlation coefficient of about 0.70 with excellent correlation for CH_4 yields and poor correlation for Oil ($>\text{C}_9$) yields.

Thermodynamic equilibrium calculations were made for a carbon-hydrogen-oxygen system at 900°C and 1000 psi. The results giving the equilibrium concentrations were then compared to experimentally determined concentrations at various H_2/coal ratios (Table 7). From this table it is obvious the hydrogen-coal reaction is not equilibrium limited since in one case the experimental results are below equilibrium, in another they are approximately at equilibrium and in the last case, considerably above equilibrium. These results were not unexpected since the hydrogenation of coal involves the fracturing of a complex molecule and reaction at short residence times. The reaction does not occur between elemental carbon, hydrogen and oxygen and the reaction times are probably too short for establishment of equilibrium.

Work Forecast

Different initial guesses and step sizes will be used to obtain a better kinetic model correlation for sub-bituminous data. The results will then be compared with those obtained from lignite.

V. EXPERIMENTAL EQUIPMENT AND MODIFICATIONS

Work Accomplished

A change was made in the experimental equipment to increase the strength of the coal feeder blades to enable it to feed the coal with the large ($\sim 800\mu$) limestone particles.

Work Forecast

Extensive modification of the experimental equipment will be necessary to meet the new operating parameters. Among these, the inside of the reactor will be reduced in diameter by inserting a sleeve, thus decreasing the gas and coal particle residence time. The output of the reactor heaters will be increased in order to reach the higher temperatures.

VI. CONCLUSIONS

The following conclusions can be drawn from this work:

- 1) At 1000 psi hydrogen pressure, increasing the reactor temperature from 900°C to 950°C showed a significant increase in gaseous HC yield (39% vs 54.5%) when using Pittsburgh No. 8 bituminous coal.
- 2) A 15% yield of BTX can be obtained with Pittsburgh No. 8 when operating at 1000 psi and 820°C.
- 3) No significant difference in hydrocarbon yields was observed when CaO and K₂CO₃ was used as diluents in Illinois No. 6 coal at 1000 psi and 900°C as compared to using limestone.
- 4) At 775°C, a temperature at which significant liquid yields were produced using Illinois No. 6 coal, no increase in liquid or gaseous yields was observed as the hydrogen pressure increased from 1000 psi to 2000 psi.

5) Any residual reactivity in the char from an experiment using Illinois No. 6 coal is destroyed after being recycled back through the reactor and any further yield from a second recycle is from the hydrogen reacting with elemental carbon.

6) The percentage of diluent used to avoid agglomeration when using caking coals is not as critical as the particle size or surface area available.

7) Experiments with New Mexico sub-bituminous coal at 1000 psi and 900 to 950°C both treated with Na_2CO_3 or untreated showed no increase in yield at temperatures above 900°C.

8) The introduction of 20% steam into the hydrogen at 900°C and 1000 psi did not show any significant change in product yields.

9) The heavier liquids ($> \text{C}_9$) produced from bituminous coal is much greater in naphthalene than that produced from lignite or sub-bituminous coal (72% vs 50%).

10) Preliminary modelling of the sub-bituminous data indicate good correlation of the experimental results.

11) The rapid hydrogasification reaction is not equilibrium limited.

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Table 1

HYDROGASIFICATION OF PITTSBURGH NO. 8 BITUMINOUS COAL

Run No.	318	329	333	334
Date	12/5/79	1/10/80	1/18/80	1/22/80
Coal Concentration (wt%)	40	40	20	20
Diluent	Limestone	Sand	Sand	Sand
Reactor Temperature (°C)	900	900	820	950
Reactor Pressure (psi)	1000	1000	1000	1000
H ₂ Feed Rate (lb/hr)	0.86	1.11	0.88	0.78
Coal Feed Rate (lb/hr)	0.86	0.49	0.58	0.41
H ₂ /Coal Weight Ratio	1.0	2.26	1.5	1.9
Residence Time (sec.)	1.7	4.5	5.1	5.2

Product Yields (% Carbon Converted)

CH ₄	33.4	38.4	24.0	54.5
C ₂ H ₆	5.8	1.0	8.2	0.0
Total Gaseous H.C.	39.2	39.4	32.2	54.5
BTX	9.9	9.8	15.2	5.6
Total H.C.	49.1	49.2	47.4	60.1
CO	0.4	1.4	1.9	2.1
CO ₂	1.5	0	0	0
Total CO _x	1.9	1.4	1.9	2.1
Total	51.0	50.6	49.3	62.2

Table 2

HYDROGASIFICATION OF ILLINOIS NO. 6 BITUMINOUS COAL
USING VARIOUS DILUENTS

Run No.	285	353	354
Date	8/7/79	3/6/80	3/7/80
Coal Concentration (wt%)	40	40	40
Diluent	Limestone	CaO	K ₂ CO ₃
Reactor Temperature (°C)	900	900	900
Reactor Pressure (psi)	1000	1000	1000
H ₂ Feed Rate (lb/hr)	0.73	0.94	0.76
Coal Feed Rate (lb/hr)	2.06	1.56	0.91
H ₂ /Coal Weight Ratio	0.35	0.60	0.84
Residence Time (sec.)	5.4	4.8	5.3

Product Yields (% Carbon Converted)

CH ₄	36.0	37.2	42.5
C ₂ H ₆	0	0.8	1.0
Total Gaseous H.C.	36.0	38.0	43.5
BTX	8.0	8.0	5.0
Total H.C.	44.0	46.0	48.5
CO	15.2	1.5	2.6
CO ₂	1.9	0.1	0.2
Total CO _x	17.1	1.6	2.8

Table 3

HYDROGASIFICATION OF ILLINOIS NO. 6 BITUMINOUS COAL

Run No.	357	358	365	366	367
Date	3/18/80	3/19/80	4/8/80	4/9/80	4/10/80
Coal Concentration (wt%)	40	40	40	40	40
Diluent	Limestone	Limestone	Sand	Sand	Sand
Reactor Temperature (°C)	775	775	775	775	775
Reactor Pressure (psi)	1000	2000	1000	1500	2000
H ₂ Feed Rate (lb/hr)	1.05	1.00	1.02	1.02	1.06
Coal Feed Rate (lb/hr)	1.53	1.28	0.74	1.11	1.03
H ₂ /Coal Weight Ratio	0.69	0.78	1.38	0.92	1.03
Residence Time (sec.)	4.7	6.5	4.8	3.9	8.6

Product Yields (% Carbon Converted)

CH ₄	14.4	20.8	19.4	15.0	17.6
C ₂ H ₆	<u>6.4</u>	<u>8.3</u>	<u>9.6</u>	<u>7.8</u>	<u>8.2</u>
Total Gaseous H.C.	20.8	29.1	29.0	22.8	25.8
BTX	8.1	6.6	12.6	5.2	11.6
> C ₉	<u>6.2</u>	<u>3.1</u>	<u>1.4</u>	<u>3.5</u>	<u>2.6</u>
Total Liquid H.C.	14.3	9.7	14.0	8.7	14.2
Total H.C.	35.1	38.8	43.0	31.5	40.0
CO	3.9	4.0	3.7	2.4	1.9
CO ₂	<u>0.1</u>	<u>0.1</u>	<u>0.</u>	<u>0.</u>	<u>0.5</u>
Total CO _x	4.0	4.1	4.1	2.5	2.4
Total	39.1	42.9	47.1	34.0	42.4

Table 4

HYDROGASIFICATION OF ILLINOIS NO. 6 BITUMINOUS COAL
AT 1000 PSI AND 775 TO 850°C

Run No.	362	363	364
Date	4/1/80	4/2/80	4/3/80
Coal Concentration (wt%)	40	40	40
Diluent	Limestone	Limestone	Limestone
Reactor Temperature (°C)	775	800	850
Reactor Pressure (psi)	1000	1000	1000
H ₂ Feed Rate (lb/hr)	1.03	1.08	0.95
Coal Feed Rate (lb/hr)	1.22	1.16	1.07
H ₂ /Coal Weight Ratio	0.84	0.93	0.89
Residence Time (sec.)	6.4	6.2	4.9

Product Yields (% Carbon Converted)

CH ₄	12.3	13.8	31.9
C ₂ H ₆	4.4	4.7	3.9
Total Gaseous H.C.	16.7	18.5	35.8
BTX	7.1	7.9	7.5
> C ₉	1.9	2.8	0
Total H.C.	8.0	10.7	7.5
Total H.C.	24.7	29.2	43.3
CO	3.5	4.1	11.6
CO ₂	1.1	0.9	0.8
Total CO _x	4.6	5.0	12.4
Total	29.3	34.2	55.7

Table 5

HYDROGASIFICATION OF NEW MEXICO SUB-BITUMINOUS COAL
BOTH TREATED AND UNTREATED WITH Na_2CO_3

	Untreated		Na_2CO_3 Treated	
Run No.	243	361	297	360
Date	3/29/79	3/27/80	9/26/79	3/25/80
Reactor Temperature ($^{\circ}\text{C}$)	900	950	900	950
Reactor Pressure (psi)	1000	1000	1000	1000
H_2 Feed Rate (lb/hr)	0.98	1.05	0.82	0.93
Coal Feed Rate (lb/hr)	1.02	1.18	3.34	1.04
H_2 /Coal Weight Ratio	0.96	0.89	0.25	0.89
Residence Time (sec.)	3.2	4.6	5.1	4.8

Product Yields (% Carbon Converted)

CH_4	46.5	44.6	47.5	42.1
C_2H_6	0	0.3	0.3	0.4
Total Gaseous H.C.	46.5	44.9	47.8	42.5
BTX	7.0	4.4	6.6	3.4
Total H.C.	53.5	49.3	54.4	45.9
CO	0	3.2	8.4	4.0
CO_2	0	0.1	1.0	0.1
Total CO_x		3.3	9.4	4.1
Total	53.5	52.6	63.8	50.0

Table 6

HYDROGASIFICATION OF NEW MEXICO SUB-BITUMINOUS COAL
THE EFFECT OF STEAM ON PRODUCT YIELD

	No Steam	20% Steam
Run No.	243	351
Date	3/29/79	3/4/80
Reactor Temperature (°C)	900	900
Reactor Pressure (psi)	1000	1000
H ₂ Feed Rate (lb/hr)	0.98	0.91
Coal Feed Rate (lb/hr)	1.02	0.93
H ₂ /Coal Weight Ratio	0.96	0.98
Residence Time (sec)	3.2	4.9
<u>Product Yields (% Carbon Converted)</u>		
CH ₄	46.5	41.7
C ₂ H ₆	0	1.1
Total Gaseous H.C.	46.5	42.8
BTX	7.0	10.1
Total H.C.	53.5	52.9
CO	0	0.1
CO ₂	0	0.5
Total		0.6
Total	53.5	53.5

Table 7

HYDROGASIFICATION OF NEW MEXICO SUB-BITUMINOUS COAL
EXPERIMENTAL PRODUCT CONCENTRATIONS (MOLE %) VS
THERMODYNAMIC EQUILIBRIUM CONCENTRATIONS
AT 900°C AND 1000 PSI

H ₂ Coal Ratio (1b/1b)	0.4		0.14		0.065	
	Exp.	Equil.	Exp.	Equil.	Exp.	Equil.
CH ₄	11.7	40.6	29.0	32.0	42.5	2.0
CO	0.9	1.6	3.1	8.0	4.9	41.0
CO ₂	0.06	0.05	0.4	1.0	1.3	32.0
H ₂	84.0	55.5	56.0	49.0	28.0	12.0
H ₂ O	3.5	2.2	11.0	10.0	23.5	12.0
% C Conv. to CH ₂	48.8		40.5		28.3	
Residence time, sec.	4.9		6.8		7.7	

Figure 1. Hydrogasification of Illinois No. 6 Coal in 50% Limestone Fraction Carbon Converted vs Coal Residence Time at 900°C and 1000 psi

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