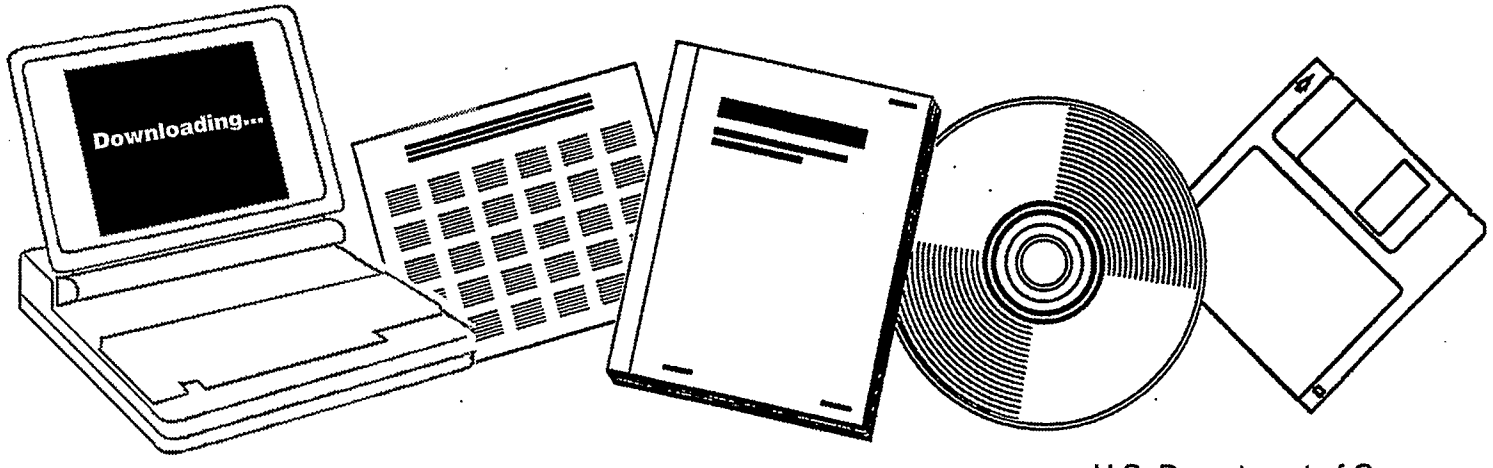
NEW CATALYSTS FOR THE INDIRECT LIQUEFACTION OF COAL. FIRST QUARTERLY TECHNICAL REPORT, AUGUST 1-OCTOBER 31, 1981

VIRGINIA COMMONWEALTH UNIV., RICHMOND.
DEPT. OF CHEMISTRY

1981



NEW CATALYSTS FOR THE INDIRECT LIQUEFACTION OF COAL

First Quarterly Technical Report for Grant No.

DE-FG22-80PC-30228

DOE/PC/30228--T10

DE85 013156

Period Covered: August 1, 1981 - October 31, 1981

Principal Investigator: Gordon A. Melson
Department of Chemistry
Virginia Commonwealth University
Richmond, VA 23284

Abstract

The evaluation of several iron/zeolite catalysts for synthesis gas conversion has been conducted. Effects of % iron loading, pre-treatment and method of preparation have been determined.

New Catalysts for the Indirect Liquefaction of Coal

During the first three months of the second year of support under grant No. DE-FG22-80PC-30228 work has concentrated on the evaluation of the catalytic ability of some iron/zeolite catalysts for synthesis gas conversion. The catalysts were prepared from $Fe_3(CO)_{12}$ and the zeolite support 13X by methods previously reported or from $Fe(NO_3)_3 \cdot 9\ H_2O$ and the support by the incipient wetness technique. All catalysts have been evaluated using a synthesis gas mixture of H_2:CO, 1:1 at 300 psig and at 280° and 300°C with a Chemical Data Systems Series 804 CF-HP microreactor. Effluent gases and liquid products have been analyzed by techniques described in previous reports. Each catalyst was evaluated for a period of 2-3 weeks.

The catalytic data obtained are presented in the Table. Catalysts #1 and #2 were prepared from $Fe_3(CO)_{12}$; #3 was catalyst #2 heated at 500°C in air for 18 hrs and catalyst #4 was prepared from $Fe(NO_3)_3 \cdot 9\ H_2O$. Data at both 280° and 300° are reported and correspond to periods of up to 96 hrs at a particular temperature. All catalysts evaluated produce a liquid product which is low in aromatics although the relative amounts of olefins and saturates vary. The highest % conversion of synthesis gas is noted for catalyst #3. The effect of calcination in air (compare #2 with #3) is to increase the % conversion; this results in a higher % CH_4 in the total hydrocarbon composition and a higher % CO_2, although the % H_2O produced is smaller. Significant quantities of wax are produced for all catalysts except for #1 in which the % Fe loading is low (~7%); % CO and H_2 conversion for this catalyst are comparable with those for the conventionally prepared catalyst (#4) which produces a large % wax. The temperature at which the evaluation is conducted has a significant

effect on the % conversion; at the higher temperature the % conversion is higher with the most significant increase in product being in the % CO_2 obtained. For the liquid product the higher temperature generally results in an increase in the % olefins and a decrease in the % saturates. X-ray diffraction data for the catalysts indicate that calcination results in an increase in particle size of the supported iron oxide. It was also noted that for catalyst #2, the iron component is γ-Fe_2O_3 whereas for #3 (after calcination in air) and #4 (conventionally prepared) α-Fe_2O_3 is present. Further studies are in progress in an attempt to correlate particle size and chemical differences of the iron component with product distributions. These studies will be the subject of a subsequent report.

Table. Catalytic Data for Synthesis Gas Conversion with Fe/13X Catalysts

Catalyst Temp. (°C)	Conversion (%)		Total Effluent Dist. (%)					H/C Composition (%)						Liquid Product (%)		
	CO	H_2	H/C	H_2O	CO_2	CO	H_2	CH_4	C_2	C_3	C_4	C_{5+}	Wax	AR	OL	SAT
#1. 7% Fe/13X																
280°	34	38	9	8	16	64	4	20	14	26	19	20	0	4	37	59
300°	73	65	18	5	51	25	2	25	15	23	14	23	1			
#2. 14% Fe/13X																
280°	49	57	12	9	27	49	3	14	11	17	14	38	8	2	48	50
300°	77	76	19	9	49	21	2	12	7	13	9	40	19	3	60	37
#3. 14% Fe/13X/H500																
280°	96	80	24	4	66	4	1	18	10	16	8	38	11	3	54	44
300°	98	84	25	4	68	2	1	21	9	16	8	34	11	4	60	36
#4. 15% Fe/13X/Conv																
280°	34	45	12	6	17	61	4	10	6	11	10	35	27	4	66	30
300°	55	61	17	7	32	42	3	14	8	13	11	38	17	3	70	27