APPENDIX D

DESCRIPTION OF CSTR REACTOR SYSTEM AND EXPERIMENTAL PROCEDURE

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1. Description of CSTR Reactor System

A schematic flow diagram of the CSTR reactor system that was operated at the University of Kentucky Center for Applied Energy Research located in Lexington, Kentucky is shown in Figure E-1.

The system consists of 3 mass flow meters, one each for H_2, CO, and Argon. There are two CO purification traps for removing iron carbonyls from the CO feed stream. The reactor is a one liter stirred autocalve with two internal filters. The autoclave temperature is controlled by an external electrical heater with a programmable controller. The reactor pressure is controlled by a manually operated Tesome back-pressure regulator. The off gas and vapor products pass through a hot trap (200°C), a lower temperature hot trap (100°C), and a cold trap (0°C) that is cooled by an external refrigeration unit. The cold trap off gas is vented to a manifold that can direct this gas to the blowdown or to a gas measuring device connected to a gas chromatograph. The gas measuring device was a 500 ml volume bubble column. The gas volume was calculated from the measured rates corrected to standard temperature and pressure.

2. Reactor Charge Procedure

Approximately 16 gm of catalyst was hydrogen reduced in the fluidized column at EI's research lab in Pittsburgh, Pennsylvania. The catalyst was slurried in approximately 150 ml of synfluid and put in a plastic bottle protected under nitrogen. Four bottles of catalyst slurry were transported to Lexington, Kentucky by William Gall. Before charging the reactor, the bottles were shaken by hand to reslurry the catalyst. The autoclave vessel bottom was lowered and pivoted to one side. An argon purge line was placed in the autoclave and the vessel was purged for several minutes. A hand held purge line was placed into the top of the catalyst bottle and held there while the catalyst slurry was poured into the autoclave. The bottle was rinsed with about 100 ml synfluid under N_2 purge. The vessel bottom was pivoted back under the head and bolted shut. The reactor was charged and ready for startup.

3. Reactor Run Procedure

The reactor was brought up to the initial run conditions and held there for several hours. At the end of the initial startup conditions, an off gas rate was taken, an off gas G.C. analysis was done, and all the product collection vessels were drained. The first catalyst tested was run at six sets of reaction conditions, while the three additional catalysts were run at sevel sets of reaction conditions.

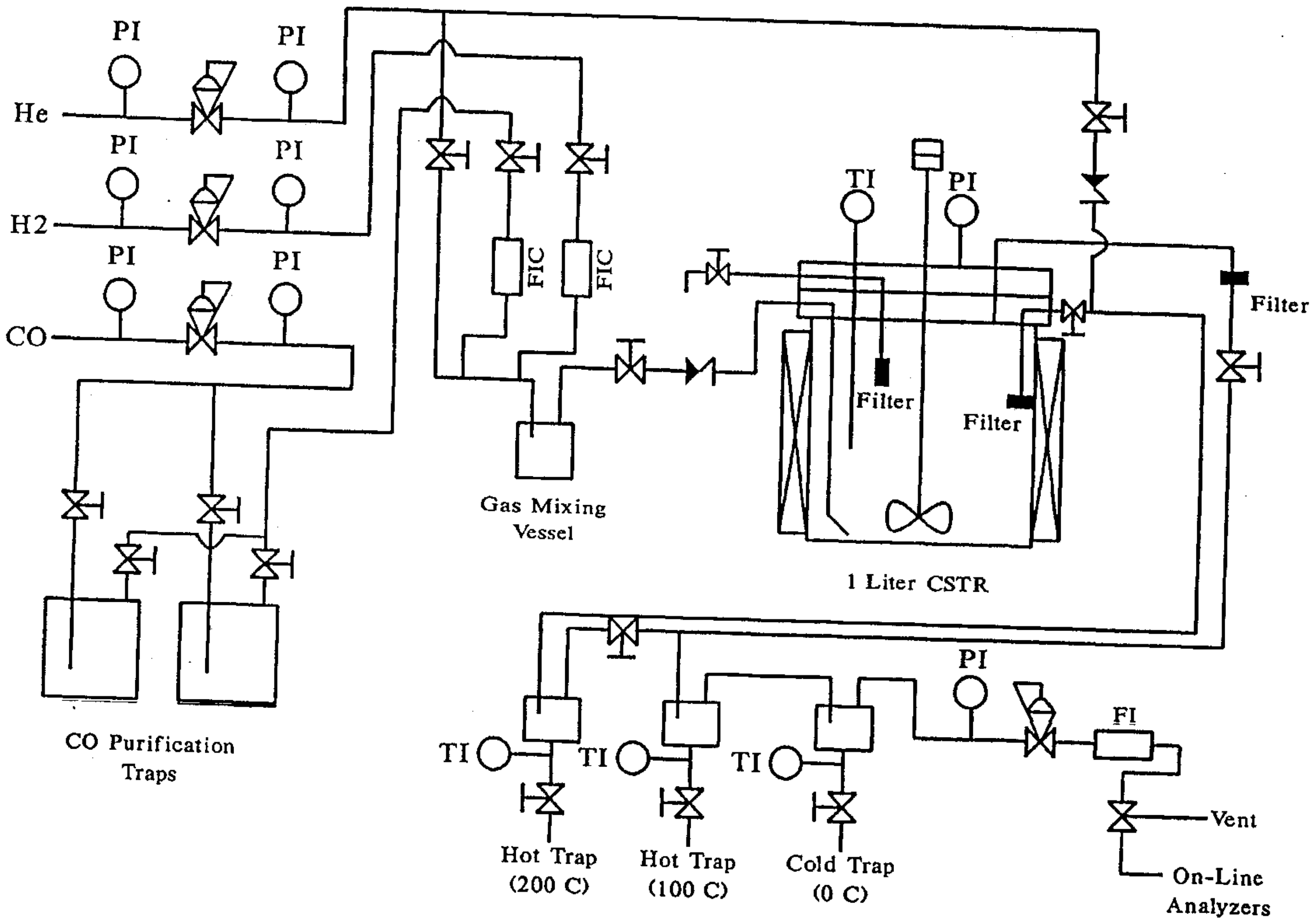
Liquid samples were removed only after the first, fourth, and last run periods. Each run lasted approximately 3 days. The following parameters were studied: reaction temperature, total gas feed rate and inert gas concentration. The reaction pressure was held at 450 psi and the H_2/CO ratio at 2.0.

4. Data Calculations

Mass balance data was obtained from the mass flow meter rates, off-gas rate, and off-gas G.C. analysis. These data were entered into a PC computer, and the gas conversions, reaction rates, and product selectivities were calculated. Some of the liquid products were analyzed by a liquid G.C. to determine the product distribution (alpha) value.

Figure E-1

FTS CSTR Reactor System



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August 24, 1995

William Gall
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135 William Pitt Way
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Bill,

Here are the selectivity and rate data for the four runs we conducted. After looking at the data closely, it is clear that there is an analytical problem which makes calculating the rates and selectivities difficult. GC's taken at the conditions with high flow rates and high argon composition add up to greater than 100% with some as high as 120%. We do not encounter this problem with our runs which do not use argon and are conducted at much lower flow rates; in fact, the problem seems to disappear with the low flow rates used at the end of your runs. Possible causes for this problem that we can think of include:

1. Our standard gas used for calibrations contains only 2% argon whereas the argon composition of the exit stream is >60%.
2. Flow rates about 5X higher than we normally use might have entrained oil from the traps which would affect the GC detector.

We are confident that our mass flow controllers performed correctly because we calibrated them before and after each run. This makes it possible to calculate what the argon composition in the exit stream should be.

$$Ar_{exit}\ (mol\%) = Ar_{in}/(\text{Total flow out})$$

To do the selectivity and rate calculations I assumed the remaining gases comprised 100 - Ar_{exit}, mol%. Each component was then corrected in proportion to the measured value from the GC. This does assume that each component was affected in the same ratio. If you have any questions please contact me at (606) 257-0324.

Sincerely,

Bob O'Brien

Bob O'Brien

One Liter CSTR Studies at the University of Kentucky CAER

Run No. LGX-185 Catalyst No.- CAL-13 Charge- 16 g

		Flow Rates SLPH					H_2:CO	Reaction Rates (g/kg/hr)						
T (°C)	P (psig)	Ar	H_2	CO	CO Conv	H_2 Conv	Usage	CO	CH_4	C_2	C_3+	THC	CO_2	H_2O
235	440	120	120	60	60.42	61.71	2.04	2831.40	73.36	8.94	1320.04	1402.33	48.92	1781.01
240	450	120	120	60	73.32	73.41	2.00	3436.13	80.06	10.58	1600.63	1691.28	92.51	2134.25
220	450	120	120	60	31.70	31.17	1.97	1485.55	38.56	3.64	698.89	741.09	8.96	948.12
240	450	120	120	60	66.63	68.30	2.04	3131.72	91.55	11.98	1438.05	1541.58	83.69	1945.53
240	450	60	60	30	90.12	85.38	1.89	2111.73	100.99	14.98	861.26	977.23	251.93	1151.94
240	450	0	60	30	99.00	87.29	1.78	2319.67	506.83	49.24	344.02	900.09	820.69	820.05

		Flow Rates SLPH					Selectivity (mol%, based on C converted)						
Temp	Press	Ar	H_2	CO	CO_2	CH_4	C_2	C_3	C_4	C_5	C_2-C_5	C_3+	C_6+
235	440	120	120	60	1.10	4.52	0.59	1.84	2.27	2.31	7.01	94.89	88.47
240	450	120	120	60	1.71	4.07	0.57	1.60	1.96	0.00	4.14	95.36	91.79
220	450	120	120	60	0.38	4.53	0.46	1.74	2.28	0.00	4.48	95.01	90.99
240	450	120	120	60	1.70	5.10	0.71	1.96	2.41	2.73	7.81	94.18	87.09
240	450	60	60	30	7.59	8.35	1.32	2.77	2.97	3.15	10.22	90.33	81.43
240	450	0	60	30	22.52	38.15	3.95	5.33	3.91	2.61	15.80	57.90	46.05

One Liter CSTR Studies at the University of Kentucky CAER

Run No. LGX-186 Catalyst No.- Co.005 Charge- 17 g

		Flow Rates SLPH					H_2:CO	Reaction Rates (g/kg/hr)						
T (°C)	P (psig)	Ar	H_2	CO	CO Conv	H_2 Conv	Usage	CO	CH_4	C_2	C_3+	THC	CO_2	H_2O
235	440	120	120	60	62.98	64.35	2.04	2777.72	62.66	11.69	1311.33	1385.68	16.81	1772.77
240	450	120	120	60	61.08	62.83	2.06	2693.83	102.56	17.54	1214.01	1334.11	46.80	1694.26
220	460	120	120	60	32.65	33.92	2.08	1440.01	39.97	8.37	669.16	717.51	11.38	916.84
240	430	120	120	60	67.27	69.21	2.06	2967.04	78.83	14.48	1384.74	1478.05	24.49	1888.24
240	450	60	60	30	68.14	69.58	2.04	1502.68	114.57	23.58	577.27	715.41	116.43	871.15
240	450	30	60	30	78.26	78.80	2.01	1725.96	81.74	13.34	739.75	834.83	92.58	1034.28
240	450	0	60	30	69.72	70.30	2.02	1537.59	97.48	16.40	616.61	730.49	123.99	867.42

		Flow Rates SLPH					Selectivity (mol%, based on C converted)						
Temp	Press	Ar	H_2	CO	CO_2	CH_4	C_2	C_3	C_4	C_5	C_2-C_5	C_3+	C_6+
235	440	120	120	60	0.39	3.94	0.78	1.32	1.60	1.95	5.66	95.28	90.41
240	450	120	120	60	1.11	6.65	1.21	2.36	2.79	3.29	9.65	92.14	83.70
220	460	120	120	60	0.50	4.85	1.08	1.92	2.32	2.57	7.89	94.07	87.26
240	430	120	120	60	0.53	4.64	0.91	1.65	1.83	2.10	6.49	94.45	88.87
240	450	60	60	30	4.93	13.31	2.82	4.87	6.36	5.66	18.81	83.77	67.88
240	450	30	60	30	3.41	8.27	1.44	3.15	3.29	3.18	11.06	90.29	80.67
240	450	0	60	30	5.13	11.07	1.99	5.16	4.90	3.75	15.79	86.94	73.14

One Liter CSTR Studies at the University of Kentucky CAER
Run No. LGX-187 Catalyst No.- Co.041 Charge- 17 g

		Flow Rates SLPH								Reaction Rates (g/kg/hr)				
T (°C)	P (psig)	Ar	H_2	CO	CO Conv	H_2 Conv	H_2:CO Usage	CO	CH_4	C_2	C_3+	THC	CO_2	H_2O
235	450	120	120	60	71.14	72.44	2.04	3137.50	64.40	13.60	1487.67	1565.68	17.38	2003.70
240	450	120	120	60	59.64	62.28	2.09	2830.36	128.68	25.03	1147.55	1301.26	50.16	1650.68
220	450	120	120	60	20.69	22.86	2.21	912.36	54.76	12.83	387.40	454.98	6.01	581.88
240	440	120	120	60	58.00	60.06	2.07	2568.33	125.37	22.69	1120.45	1268.51	39.75	1612.89
240	450	60	60	30	69.14	71.02	2.05	1524.76	141.12	25.56	553.48	720.15	136.26	869.12
240	450	30	60	30	33.35	37.18	2.23	735.43	182.60	37.48	96.65	316.72	161.80	340.54
240	450	0	60	30	23.09	27.41	2.37	509.25	88.62	12.36	148.18	249.16	18.42	312.46

		Flow Rates SLPH					Selectivity (mol%, based on C converted)						
Temp	Press	Ar	H_2	CO	CO_2	CH_4	C_2	C_3	C_4	C_5	C_2-C_5	C_5+	C_8+
235	450	120	120	60	0.35	3.58	0.81	1.26	1.44	1.58	5.08	95.61	91.34
240	450	120	120	60	1.21	8.54	1.77	2.89	3.20	3.60	11.46	89.69	80.00
220	450	120	120	60	0.42	10.48	2.62	4.56	5.24	5.95	18.37	86.90	71.15
240	440	120	120	60	0.99	8.56	1.65	2.80	3.18	3.47	11.10	89.79	80.35
240	450	60	60	30	5.69	16.16	3.12	5.03	5.48	5.59	19.23	80.72	64.61
240	450	30	60	30	14.00	43.35	9.49	15.07	15.63	15.92	56.12	47.16	0.53
240	450	0	60	30	2.30	30.38	4.52	7.72	7.49	7.31	27.03	65.10	42.59

One Liter CSTR Studies at the University of Kentucky CAER

Run No. LGX-188 Catalyst No.- Co.053 Charge- 17 g

		Flow Rates SLPH					H_2:CO		Reaction Rates (g/kg/hr)					
T (°C)	P (psig)	Ar	H_2	CO	CO Conv	H_2 Conv	Usage	CO	CH_4	C_2	C_3+	THC	CO_2	H_2O
235	450	120	120	60	64.19	66.31	2.07	2831.24	105.42	19.76	1276.11	1401.28	51.95	1778.42
240	450	120	120	60	64.70	66.95	2.07	2853.65	161.15	21.17	1208.57	1390.89	119.77	1737.31
220	450	120	120	60	25.55	27.47	2.15	1126.80	58.76	13.79	488.44	560.99	10.34	716.26
240	450	120	120	60	69.61	71.19	2.05	3070.11	120.80	15.69	1380.07	1516.56	65.58	1920.89
240	450	60	60	30	87.79	87.36	1.99	1935.92	82.03	13.00	838.77	933.80	111.95	1153.46
240	450	30	60	30	87.62	86.14	1.97	1932.33	86.38	13.35	819.74	919.47	151.26	1118.97
240	450	0	60	30	89.22	82.93	1.86	1967.51	135.39	17.99	724.10	877.49	338.27	988.50

		Flow Rates SLPH					Selectivity (mol%, based on C converted)						
Temp	Press	Ar	H_2	CO	CO_2	CH_4	C_2	C_3	C_4	C_5	C_2-C_5	C_3+	C_6+
235	450	120	120	60	1.17	6.50	1.30	2.25	2.69	3.00	9.24	92.20	84.28
240	450	120	120	60	2.67	9.86	1.38	3.26	3.88	4.35	12.88	88.76	77.28
220	450	120	120	60	0.58	9.10	2.28	3.79	4.77	5.85	16.69	88.62	74.21
240	450	120	120	60	1.36	6.87	0.95	2.29	2.64	2.93	8.81	92.18	84.32
240	450	60	60	30	3.68	7.40	1.25	2.24	2.49	2.56	8.54	91.35	84.08
240	450	30	60	30	4.98	7.80	1.29	2.42	2.51	2.35	8.57	90.91	83.63
240	450	0	60	30	10.94	12.01	1.70	3.31	2.85	1.91	9.77	86.28	78.21