

B. Computerized Run Sheets For Catalyst Screening Studies

SUMMARY FOR RUN # 194-95

CHEM SYSTEMS INC.

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 CATALYST NUMBER : 197-16 DATE : 1/7/80  
 ATOMIC FORMULA : CuCrCoZn<sub>5</sub>K<sub>11</sub>  
 CATALYST SUPPORT : NONE

PREF METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.24 gm/cc REACTOR TYPE: Plug Flow  
 TEST NUMBER 1 2 3 4 5\*

TEST CONDITIONS :

FEED H2/CO RATIO	3.60	3.60	3.60	3.60	3.60
FEED CO2	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	238.0	248.0	259.0	272.0	364.0
HOT SPOT, C	239.0	249.0	261.0	274.0	364.0
PRESSURE, psig	905.0	905.0	900.0	900.0	900.0
VHSV, 1/hr/kcm cat.	3359.0	3449.0	3361.0	3458.0	3398.0
HOURS on STREAM	2.2	3.7	5.0	6.4	6.9
RPM	.0	.0	.0	.0	.0

CONVERSION :

CO to Prods., vol%	6.44	5.88	6.40	15.84	99.50
CO to CO2, vol%	2.26	2.22	3.50	10.16	.00
CO, gm mol/hr/kcm cat.	2.23	2.12	3.04	6.82	25.90
STY of oxogenates <sup>(2)</sup> gm mol/hr/kcm cat.	.57	.46	.69	1.24	.00

STOICHIOM. H2/CO converted 1.96 3.52 3.21 2.66 3.41

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	4.29	7.35	7.51	8.04	.00
C2-C6 ALCOHOLS	24.97	20.63	22.53	20.68	.00
C2-C6 ALD.&ESTERS	5.58	2.29	2.27	1.15	.00
CH4	30.92	40.78	41.38	45.62	91.00
C2-C3 HYDROCARBONS	15.55	17.37	15.31	14.74	6.00
C4+ HYDROCARBONS	16.77	11.66	11.20	9.88	3.00

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 93.2 98.7 112.1 122.6 94.7

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxogenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* Temperature Runaway.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-1

=====  
 CATALYST NUMBER : 197-17  
 ATOMIC FORMULA :  $CuCrCoZn_{.125}K_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 1/14/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.26 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	3.50	3.50
FEED CO <sub>2</sub>	12.00	12.00
AVE. TEMP., C	227.0	239.0
HOT SPOT, C	228.0	240.0
PRESSURE, psig	905.0	905.0
WHSV, 1/hr/k <sub>sm</sub> cat.	3156.0	3154.0
HOURS on STREAM	1.6	2.5
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	9.30	9.60
CO to CO <sub>2</sub> , vol%	.00	.80
CO, gm mol/hr/k <sub>sm</sub> cat.	2.27	2.53
STY of oxysenates <sup>(2)</sup>		
gm mol/hr/k <sub>sm</sub> cat.	.28	.46

STOICHIOM. H<sub>2</sub>/CO converted .93 .78CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.30	2.28
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	3.40	12.68
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	8.60	4.66
CH <sub>4</sub>	25.60	29.47
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	25.50	26.54
C <sub>4</sub> + HYDROCARBONS	22.50	24.38

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 38.1 67.2

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxysenates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-6

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CATALYST NUMBER : 197-20  
 ATOMIC FORMULA :  $Cu_{.18}Co_{.5}Zn_{.49}K_{.09}$   
 CATALYST SUPPORT : NONE

DATE : 1/22/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.42 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER	1	2	3	4	5
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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	3.60	3.60	3.60	3.60	3.60
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	239.0	249.0	261.0	273.0	285.0
HOT SPOT, C	240.0	250.0	262.0	275.0	289.0
PRESSURE, psig	905.0	905.0	905.0	905.0	905.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3060.0	3089.0	3046.0	3056.0	3005.0
HOURS on STREAM	5.8	6.4	7.1	8.2	9.0
RPM	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	2.90	5.30	8.20	11.81	18.23
CO to CO <sub>2</sub> , vol%	.00	.00	.60	2.99	7.77
CO, gm mol/hr/k <sub>sm</sub> cat.	.67	1.22	2.03	3.43	5.91
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.10	.18	.23	.29	.59

STOICHIOM. H <sub>2</sub> /CO converted	1.91	1.49	1.48	1.61	1.46
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.00	.60	1.18	1.13	1.14
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	3.40	6.80	5.79	7.27	8.54
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	11.50	7.20	5.47	2.01	4.56
CH <sub>4</sub>	48.90	44.60	47.10	48.63	48.34
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	23.50	25.20	25.75	25.19	23.39
C <sub>4</sub> + HYDROCARBONS	12.70	14.30	14.70	15.67	14.12

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	59.9	61.7	62.5	70.8	82.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-9

CATALYST NUMBER : 197-19

DATE : 1/28/80

ATOMIC FORMULA :  $\text{CuCr}_{.18}\text{Zn}_{.49}\text{K}_{.07}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.99 gm/cc  
TEST NUMBER

REACTOR TYPE: Plus Flow

1 2 3 4 5

## TEST CONDITIONS :

	1	2	3	4	5
FEED H <sub>2</sub> /CO RATIO	3.60	3.60	3.60	3.60	3.60
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	279.0	299.0	317.0	335.0	338.0
HOT SPOT, C	280.0	300.0	318.0	337.0	337.0
PRESSURE, psid	910.0	910.0	900.0	900.0	900.0
VHSV, 1/hr/kcm cat.	2062.0	2089.0	2092.0	2063.0	3978.0
HOURS on STREAM	3.1	3.8	4.5	5.1	5.6
RPH	.0	.0	.0	.0	.0

## CONVERSION : \*

CO <sub>2</sub> to Prods., vol%	.81	1.32	1.43	2.89	2.14
CO <sub>2</sub> to CO, vol%	4.49	5.58	6.37	7.41	8.36
CO <sub>2</sub> gm mol/hr/kcm cat.	.60	.80	.90	1.18	2.33
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.09	.15	.16	.30	.44

STOICHIOM. H<sub>2</sub>/CO<sub>2</sub> converted 1.74 1.75 1.25 1.58 1.33

## CARBON SELECTIVITY (Normalized Mol% on CO-free Basis) :

CH <sub>3</sub> OH	97.37	94.79	93.44	89.68	91.67
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.00	.00	.00	.00	.00
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00	.00	.00	.00
CH <sub>4</sub>	1.32	2.08	3.28	6.05	4.41
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	1.32	3.13	3.28	4.27	3.92
C <sub>4</sub> + HYDROCARBONS	.00	.00	.00	.00	.00

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C.

CARBON ACCOUNTABILITY, % (4) 97.3 97.6 115.2 88.1 109.9

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO<sub>2</sub> in feed/100 \* %CO<sub>2</sub> conv./100 \* %Sel to Oxysenates/100.(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* no CO was converted but CO<sub>2</sub> was hydrogenated to CO and H<sub>2</sub>O.

SUMMARY FOR RUN # 201-11

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 CATALYST NUMBER : 197-22 DATE : 1/31/80  
 ATOMIC FORMULA :  $Cu_{0.18}Zn_{0.49}K_{0.07}$   
 CATALYST SUPPORT : NONE

PREP METHOD: Coprecipitation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup> : 1.08 gm/cc REACTOR TYPE: Plug Flow  
 TEST NUMBER 1 2 3 4 5 6

TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	3.60	3.60	3.60	3.60	3.60	3.60
FEED CO2	12.00	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	248.0	249.0	278.0	297.0	318.0	336.0
HOT SPOT, C	249.0	250.0	279.0	299.0	319.0	340.0
PRESSURE, psig	930.0	920.0	910.0	905.0	900.0	900.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3814.0	9000.0	3752.0	3748.0	3805.0	3826.0
HOURS on STREAM	1.2	2.0	3.0	3.7	4.3	5.1
RPM	.0	.0	.0	.0	.0	.0

CONVERSION :\*

CO <sub>2</sub> to Prods., vol%	1.24	.19	1.33	1.46	2.29	3.30
CO <sub>2</sub> to CO, vol%	2.86	2.51	4.57	5.84	6.91	7.50
CO <sub>2</sub> gm mol/hr/k <sub>sm</sub> cat.	.87	1.36	1.23	1.53	1.96	2.31
STY of oxygenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.25	.09	.27	.28	.44	.59

STOICHIOM. H2/CO<sub>2</sub> converted 1.57 .25 1.18 1.22 1.19 1.38

CARBON SELECTIVITY (Normalized Mol% on CO-free Basis) :

CH3OH	95.70	94.37	97.78	91.00	89.16	82.68
C2-C6 ALCOHOLS	.00	.00	.00	.00	.00	.00
C2-C6 ALD. & ESTERS	.00	.00	.00	.00	.00	.00
CH4	4.30	1.41	.89	.50	7.23	12.75
C2-C3 HYDROCARBONS	.00	4.23	1.33	8.50	3.61	4.58
C4+ HYDROCARBONS	.00	.00	.00	.00	.00	.00

APPROACH TO <sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 69.1 101.0 77.8 90.2 85.1 77.2

- (1) Fresh, non-reduced catalyst.  
 (2) Space Time Yield (STY) = VHSV/22.4 \* XCO<sub>2</sub> in feed/100 \* XCO<sub>2</sub> conv./100 \* XSel to Oxygenates/100.  
 (3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.  
 (4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* No CO was converted but CO<sub>2</sub> was hydrogenated to CO and H<sub>2</sub>O

## SUMMARY FOR RUN # 201-13

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CATALYST NUMBER : 197-27 DATE : 2/5/80

ATOMIC FORMULA : CuAl<sub>1.21</sub>Zn<sub>1.36</sub>K<sub>1.07</sub>

CATALYST SUPPORT : NONE

PREP METHOD: Impregnation REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY (1) : 1.04 gm/cc REACTOR TYPE: Plug Flow

TEST NUMBER 1 2 3 4

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## TEST CONDITIONS :

	1	2	3	4
FEED H <sub>2</sub> /CO RATIO	3.60	3.60	3.60	3.60
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00
AVE. TEMP., C	239.0	250.0	261.0	273.0
HOT SPOT, C	240.0	251.0	262.0	274.0
PRESSURE, psia	925.0	920.0	910.0	905.0
WHSV, 1/hr/k <sub>sm</sub> cat.	3898.0	4238.0	4652.0	4249.0
HOURS on STREAM	1.5	2.5	2.9	3.5
RPM	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	13.47	18.65	20.91	24.00
CO to CO <sub>2</sub> , vol%	-3.47	-4.35	-4.01	-5.00
CO, gm mol/hr/k <sub>sm</sub> cat.	2.95	4.59	5.96	6.12
STY of oxidenates (2)				
gm mol/hr/k <sub>sm</sub> cat.	2.95	4.59	5.91	6.10

STOICHIOM. H<sub>2</sub>/CO converted 2.69 2.34 2.39 2.25

CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	99.41	98.94	98.60	98.50
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.00	.00	.00	.00
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.59	1.00	.48	1.11
CH <sub>4</sub>	.00	.08	.89	.40
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	.00	.00	.00	.00
C <sub>4</sub> + HYDROCARBONS	.00	.00	.00	.00

## APPROACH TO (3)

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	81.1	66.6	102.5	50.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxidenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-15

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 CATALYST NUMBER : 197-28  
 ATOMIC FORMULA :  $CuCo_{.32}Al_{.21}Zn_{.36}K_{.09}$   
 CATALYST SUPPORT : NONE

DATE : 2/12/80

PREP METHOD: Impregnation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY <sup>(1)</sup> : 1.78 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	3.60	3.60	3.60	3.60
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00
AVE. TEMP., C	251.0	260.0	271.0	282.0
HOT SPOT, C	252.0	262.0	273.0	283.0
PRESSURE, psig	930.0	920.0	905.0	900.0
VHSV, 1/hr/k <sub>gm</sub> cat.	2261.0	2289.0	2519.0	2555.0
HOURS on STREAM	.8	2.5	3.0	3.5
RPM	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	6.15	6.48	7.60	10.70
CO to CO <sub>2</sub> , vol%	.25	.72	.00	2.30
CO, gm mol/hr/k <sub>gm</sub> cat.	1.09	1.24	1.44	2.50
STY of oxoacetates <sup>(2)</sup>				
gm mol/hr/k <sub>gm</sub> cat.	.21	.20	.67	.49

STOICHIOM. H<sub>2</sub>/CO converted 1.92 1.63 1.98 1.73CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	1.35	.44	10.10	3.16
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	3.64	12.22	11.90	14.34
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	14.57	5.44	24.20	6.44
CH <sub>4</sub>	26.43	35.66	26.70	40.82
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	19.77	26.11	15.60	17.01
C <sub>4</sub> HYDROCARBONS	34.13	20.22	11.50	13.24

APPROACH TO <sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 60.9 60.4 88.6 72.7

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxoacetates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-17

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 CATALYST NUMBER : 197-29  
 ATOMIC FORMULA :  $CuCr_{.14}Co_{.75}Zn_{.5}K_{.12}$   
 CATALYST SUPPORT : NONE

DATE : 2/23/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.29 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

1            2            3            4            5

## TEST CONDITIONS :

FEED H2/CO RATIO	3.60	3.60	3.60	3.60	3.60
FEED CO2	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	242.0	252.0	263.0	274.0	285.0
HOT SPOT, C	244.0	253.0	265.0	276.0	287.0
PRESSURE, psig	910.0	905.0	900.0	900.0	900.0
UHSV, 1/hr/kcm cat.	3214.0	3280.0	3325.0	3355.0	3428.0
HOURS on STREAM	.8	1.4	2.4	3.2	3.7
RPM	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	8.45	8.24	10.29	12.64	19.27
CO to CO2, vol%	.45	.96	2.11	4.06	9.73
CO, gm mol/hr/kcm cat.	2.17	2.29	3.13	4.25	7.54
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	.20	.34	.35	.61	.78

STOICHIOM. H2/CO converted	1.55	1.49	1.56	1.46	1.26
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.00	.22	1.20	1.32	1.20
C2-C6 ALCOHOLS	2.74	12.94	7.93	10.97	8.58
C2-C6 ALD.&ESTERS	6.74	3.35	4.58	6.61	5.72
CH4	37.41	45.42	39.04	42.68	46.94
C2-C3 HYDROCARBONS	33.41	17.19	23.86	24.31	23.32
C4+ HYDROCARBONS	19.60	20.92	23.49	14.01	13.24

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	42.2	50.0	68.1	77.1	83.1
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$  where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-22

CATALYST NUMBER : 197-1  
 ATOMIC FORMULA :  $\text{CuCr}_{.8}\text{CoK}_{.09}$   
 CATALYST SUPPORT : NONE

DATE : 2/29/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup> : 1.46 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1            2            3            4            5            6

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	3.60	3.60	3.60	3.60	2.00	2.00
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00	5.00	5.00
Ave. TEMP., C	251.0	254.0	260.0	261.0	260.0	260.0
HOT SPOT, C	251.0	254.0	260.0	261.0	260.0	260.0
PRESSURE, psig	885.0	885.0	885.0	885.0	885.0	885.0
WHSV, 1/hr/k <sub>sm</sub> cat.	2604.0	688.0	2840.0	779.0	2891.0	746.0
HOURS on STREAM	3.1	5.3	7.6	11.1	13.7	17.0
RPM	1710.0	1720.0	1700.0	1700.0	1700.0	1700.0

## CONVERSION :

CO to Prods., vol%	18.36	36.76	14.53	47.64	4.46	16.24
CO to CO <sub>2</sub> , vol%	5.24	9.54	3.27	15.96	2.14	9.26
CO, gm mol/hr/k <sub>sm</sub> cat.	4.70	2.40	3.80	4.30	2.40	2.40
STY of oxysterates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.33	.27	.46	.38	.34	.31

STOICHIOM. H <sub>2</sub> /CO converted	1.80	1.63	1.54	1.56	.91	1.15
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	2.19	2.14	4.41	3.87	7.69	6.91
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	6.81	11.71	10.17	8.41	13.61	13.66
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00	.00	.00	.00	.00
CH <sub>4</sub>	40.87	35.01	48.15	58.74	44.08	40.50
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	25.06	30.48	23.52	20.16	21.01	27.47
C <sub>4</sub> + HYDROCARBONS	25.06	20.65	12.74	8.81	13.61	11.46

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	84.2	102.3	86.9	104.1	90.5	94.5
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $\text{WHSV}/22.4 * \% \text{CO in feed}/100 * \% \text{CO conv.}/100 * \% \text{Sel to Oxysterates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-22

CHEM SYSTEMS INC.

-----  
 CATALYST NUMBER : 197-1

DATE : 2/29/80

ATOMIC FORMULA :  $CuCr_{.8}CoK_{.09}$

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup> : 1.46 gm/cc

REACTOR TYPE: Bertha

TEST NUMBER

7

8

9

10

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TEST CONDITIONS :

	7	8	9	10
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00	5.00	5.00
AVE. TEMP., C	260.0	259.0	259.0	258.0
HOT SPOT, C	260.0	259.0	259.0	258.0
PRESSURE, psia	885.0	885.0	885.0	885.0
VHSV, 1/hr/gsm cat.	2619.0	2644.0	2643.0	2722.0
HOURS on STREAM	18.3	19.5	20.7	22.1
RPM	2000.0	1700.0	1400.0	1000.0

CONVERSION :

CO to Prods., vol%	4.10	3.93	4.04	4.28
CO to CO <sub>2</sub> , vol%	1.90	1.77	1.66	1.32
CO, gm mol/hr/gsm cat.	2.00	1.90	1.90	1.90
STY of oxysenates <sup>(2)</sup> gm mol/hr/gsm cat.	.30	.29	.35	.42

STOICHIOM. H <sub>2</sub> /CO converted	.89	.99	.86	1.07
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	7.61	8.56	8.76	9.54
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	14.64	13.78	17.37	19.61
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.00	.00	.00	.00
CH <sub>4</sub>	47.87	49.18	47.03	44.05
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	20.20	20.46	19.07	18.56
C <sub>4</sub> + HYDROCARBONS	9.73	8.12	7.77	8.24

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	96.3	90.7	89.4	85.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-32

=====

CATALYST NUMBER : 197-30  
 ATOMIC FORMULA :  $\text{CuCo}_{.65}\text{Al}_{.21}\text{Zn}_{.36}\text{K}_{.1}$   
 CATALYST SUPPORT : NONE

DATE : 3/19/80

PREP METHOD: Impregnation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.69 gm/cc  
 TEST NUMBERREACTOR TYPE: Plug Flow  
 1 2 3

## TEST CONDITIONS :

	1	2	3
FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
AVE. TEMP., C	220.0	241.0	263.0
HOT SPOT, C	220.0	242.0	265.0
PRESSURE, psis	925.0	920.0	920.0
VHSV, 1/hr/kcm cat.	2328.0	2355.0	2391.0
HOURS on STREAM	1.6	2.5	3.4
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	.90	2.62	6.55
CO to CO2, vol%	1.00	1.98	5.65
CO, gm mol/hr/kcm cat.	.54	1.34	3.60
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	.02	.10	.47

STOICHIOM, H2/CO converted 1.19 1.22 .80

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	1.06	1.75	1.86
C2-C6 ALCOHOLS	4.88	3.51	10.61
C2-C6 ALD.&ESTERS	.00	7.72	11.73
CH4	40.71	32.11	28.86
C2-C3 HYDROCARBONS	31.80	28.25	23.28
C4+ HYDROCARBONS	22.05	26.67	23.65

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 60.0 80.1 89.8

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-34

CHEM SYSTEMS INC.

=====  
 CATALYST NUMBER : 197-2 DATE : 3/20/80  
 ATOMIC FORMULA : CuCrCoZn<sub>125</sub>K<sub>11</sub>  
 CATALYST SUPPORT : NONE

PREF METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.69 gm/cc REACTOR TYPE: Bertz  
 TEST NUMBER 1 2 3 4 5 6

TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	250.0	248.0	261.0	260.0	262.0	262.0
HOT SPOT, C	251.0	250.0	263.0	262.0	262.0	263.0
PRESSURE, psig	890.0	890.0	890.0	895.0	895.0	885.0
VHSV, 1/hr/kcm cat.	2475.0	3915.0	2314.0	2354.0	2351.0	4098.0
HOURS on STREAM	1.1	3.7	6.4	7.6	8.6	10.3
RPM	1690.0	1700.0	1740.0	700.0	1420.0	1690.0

CONVERSION :

CO to Prods., vol%	1.59	.99	2.73	2.40	2.15	1.85
CO to CO2, vol%	.51	.11	.97	1.00	.85	.35
CO, gm mol/hr/kcm cat.	.65	.55	1.05	.97	.87	1.13
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.09	.13	.12	.16	.15	.24
STOICHIOM. H2/CO converted	1.89	.65	.83	.02	.14	.23

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.00	.00	.81	.85	1.12	.36
C2-C6 ALCOHOLS	3.97	8.24	3.80	1.84	1.68	1.67
C2-C6 ALD.&ESTERS	14.68	18.82	11.12	19.82	21.95	23.11
CH4	45.50	44.54	41.37	49.41	46.69	55.86
C2-C3 HYDROCARBONS	18.92	16.15	33.64	18.41	17.48	17.63
C4+ HYDROCARBONS	16.93	12.25	9.36	9.77	11.18	7.38

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	102.8	94.0	102.1	86.4	97.4	66.1
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-34

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CATALYST NUMBER : 197-2 DATE : 3/20/80  
 ATOMIC FORMULA : CuCrCoZn .125<sup>K</sup>.11  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.69 gm/cc REACTOR TYPE: Bertw

TEST NUMBER 7 8 9 10

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TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00
AVE. TEMP., C	269.0	271.0	272.0	269.0
HOT SPOT, C	270.0	271.0	273.0	271.0
PRESSURE, psig	900.0	895.0	895.0	895.0
VHSV, 1/hr/kcm cat.	3715.0	2132.0	795.0	766.0
HOURS on STREAM	11.5	12.6	14.5	15.5
RPM	1700.0	1700.0	1710.0	700.0

CONVERSION :

CO to Prods., vol%	2.27	4.03	15.18	12.52
CO to CO2, vol%	.53	1.77	11.02	8.78
CO, gm mol/hr/kcm cat.	1.31	1.54	2.58	2.12
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.29	.26	.36	.32

STOICHIOM. H2/CO converted 1.07 1.45 1.63 1.54

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	4.07	5.47	5.35	4.93
C2-C6 ALCOHOLS	10.97	9.64	12.42	13.10
C2-C6 ALD.&ESTERS	12.20	9.20	5.87	7.65
CH4	49.93	51.49	51.76	44.22
C2-C3 HYDROCARBONS	16.64	17.55	17.60	21.09
C4+ HYDROCARBONS	6.29	6.76	6.90	9.01

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	89.2	83.6	85.1	99.0
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(1) Fresh, non-reduced catalyst.  
 (2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.  
 (3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.  
 (4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-37

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CATALYST NUMBER : 197-32 DATE : 3/27/80  
 ATOMIC FORMULA : CuCrCoZn<sub>0.125</sub>K<sub>0.11</sub>  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.58 gm/cc REACTOR TYPE: Berty

TEST NUMBER	1	2	3	4	5	6
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TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	249.0	249.0	250.0	266.0	268.0	269.0
HOT SPOT, C	249.0	249.0	250.0	266.0	268.0	269.0
PRESSURE, psig	895.0	895.0	1375.0	895.0	895.0	895.0
WHSV, 1/hr/kgm cat.	2505.0	661.0	680.0	4900.0	2470.0	712.0
HOURS on STREAM	2.1	4.5	6.5	4.5	8.1	10.0
RPM	1700.0	1920.0	1900.0	1680.0	1700.0	1700.0

CONVERSION :

CO to Prods., vol%	1.41	4.80	5.65	1.49	2.76	8.02
CO to CO2, vol%	.19	2.10	2.55	.21	.74	6.08
CO, gm mol/hr/kgm cat.	.50	.80	.69	1.04	1.08	1.57
STY of oxygenates <sup>(2)</sup>						
gm mol/hr/kgm cat.	.11	.12	.12	.24	.23	.21

STOICHIOM. H2/CO converted 1.03 1.50 1.46 .51 1.10 1.05

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.45	.57	.44	.00	.76	1.58
C2-C6 ALCOHOLS	3.40	5.31	4.35	5.49	7.48	6.33
C2-C6 ALD.&ESTERS	22.11	17.09	19.16	20.46	18.51	15.29
CH4	46.03	41.07	40.06	46.76	40.95	42.71
C2-C3 HYDROCARBONS	14.40	16.95	17.27	14.86	14.33	17.22
C4+ HYDROCARBONS	13.61	19.10	18.72	15.43	16.86	16.87

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 63.6 74.8 77.7 55.4 65.8 74.9

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as T = T<sub>eq</sub> - T<sub>hs</sub>

where T<sub>eq</sub> = water gas shift equilibrium temp calculated for reactor eff. composition,

T<sub>hs</sub> = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-37

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CATALYST NUMBER : 197-32 DATE : 3/27/80  
 ATOMIC FORMULA : CuCrCoZn .125<sup>K</sup>.11  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup> : 1.58 gm/cc REACTOR TYPE: Rerts

TEST NUMBER	7	8	9	10	11	12
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TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	271.0	270.0	266.0	287.0	283.0	288.0
HOT SPOT, C	271.0	270.0	266.0	287.0	283.0	288.0
PRESSURE, psia	1275.0	1275.0	425.0	915.0	915.0	910.0
WHSV, 1/hr./ksm cat.	691.0	2498.0	655.0	2713.0	2666.0	716.0
HOURS on STREAM	11.7	12.2	13.1	14.9	16.0	18.1
RPM	1690.0	1700.0	1720.0	1720.0	600.0	1720.0

CONVERSION :

CO to Prods., vol%	10.95	4.09	5.02	4.51	4.11	18.71
CO to CO2, vol%	7.94	2.21	3.98	2.09	1.69	13.39
CO, gm mol/hr./ksm cat.	1.63	1.96	.73	2.23	1.93	2.86
STY of oxides <sup>(2)</sup>						
gm mol/hr./ksm cat.	.18	.32	.12	.31	.29	.44

STOICHIOM. H2/CO converted 1.02    1.01    .87    1.23    1.34    .96

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	1.72	2.31	1.43	[ .00 ]	[ .00 ]	[ .00 ]
C2-C6 ALCOHOLS	4.48	6.93	7.71	[ 20.04 ]	[ 21.47 ]	[ 26.24 ]
C2-C6 ALD. & ESTERS	12.41	15.72	20.43	[ .00 ]	[ .00 ]	[ .00 ]
CH4	46.38	42.53	44.44	50.75	49.86	44.25
C2-C3 HYDROCARBONS	19.83	17.57	9.14	18.58	19.21	18.01
C4+ HYDROCARBONS	15.17	14.95	9.86	10.53	9.46	11.49

APPROACH TO <sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	81.9	74.1	74.1	85.3	88.8	92.5
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxides/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



SUMMARY FOR RUN # 201-37

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 CATALYST NUMBER : 197-32 DATE : 3/27/80  
 ATOMIC FORMULA : CuCrCoZn .125<sup>K</sup> .11  
 CATALYST SUPPORT : NONE  
 PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2  
 BULK DENSITY<sup>(1)</sup> : 1.58 gm/cc REACTOR TYPE: Berty  
 TEST NUMBER 13  
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TEST CONDITIONS :

FEED H2/CO RATIO	2.00
FEED CO2	5.00
AVE. TEMP., C	243.0
HOT SPOT, C	243.0
PRESSURE, psia	910.0
VHSV, 1/hr/kcm cat.	2422.0
HOURS on STREAM	20.0
RPM	1700.0

CONVERSION :

CO to Prods., vol%	.68
CO to CO2, vol%	.02
CO, gm mol/hr/kcm cat.	.21
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/kcm cat.	.06

STOICHIOM. H2/CO converted 2.61

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.00
C2-C6 ALCOHOLS	.00
C2-C6 ALD.&ESTERS	28.79
CH4	45.10
C2-C3 HYDROCARBONS	14.86
C4+ HYDROCARBONS	11.25

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 86.4

-----  
 (1) Fresh, non-reduced catalyst.  
 (2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.  
 (3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.  
 (4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-40

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CATALYST NUMBER : 197-2  
 ATOMIC FORMULA : CuCrCoZn .125<sup>K</sup> .11  
 CATALYST SUPPORT : NONE

DATE : 3/31/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.69 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER	1	2	3	4	5	6
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## TEST CONDITIONS :

FEED H2/CO RATIO	3.50	3.50	3.50	3.50	3.50	3.50
FEED CO2	12.00	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	261.0	267.0	280.0	283.0	280.0	280.0
HOT SPOT, C	262.0	268.0	281.0	286.0	281.0	281.0
PRESSURE, Psig	920.0	940.0	940.0	940.0	920.0	920.0
VHSV, 1/hr/kcm cat.	2275.0	2195.0	2217.0	2284.0	2251.0	2099.0
HOURS on STREAM	.5	25.8	73.5	75.5	80.0	98.5
RPM	.0	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	3.67	7.01	11.14	16.47	13.20	13.61
CO to CO2, vol%	1.53	1.99	4.26	4.83	1.80	2.59
CO, gm mol/hr/kcm cat.	1.40	1.60	2.88	3.80	2.60	2.40
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	.14	.38	.50	.76	.66	.65

STOICHIOM. H2/CO converted	1.56	1.45	1.11	1.51	1.75	1.62
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.14	2.32	2.77	3.10	2.73	3.10
C2-C6 ALCOHOLS	2.27	2.70	3.04	8.02	5.11	4.88
C2-C6 ALD. & ESTERS	10.92	25.67	19.08	14.87	20.91	21.31
CH4	46.81	40.05	43.14	41.39	31.48	38.21
C2-C3 HYDROCARBONS	21.84	17.20	19.77	18.62	25.23	18.33
C4+ HYDROCARBONS	18.01	12.07	12.31	14.10	14.43	14.17

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	84.4	99.5	91.4	92.8	79.3	86.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-45

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CATALYST NUMBER : 200-27-2 DATE : 4/8/80

ATOMIC FORMULA : CuCoFe<sub>.5</sub>Th<sub>.5</sub>Zn<sub>.125</sub>K<sub>.11</sub>

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY (1) : 1.51 gm/cc REACTOR TYPE: Bertu

TEST NUMBER 1 2 3 4 5 6

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TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	2.10	2.10	2.10	2.10	2.10	2.10
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	249.0	248.0	243.0	238.0	248.0	247.0
HOT SPOT, C	250.0	249.0	245.0	239.0	248.0	248.0
PRESURE, psig	895.0	895.0	440.0	885.0	1480.0	885.0
VHSV, 1/hr/kcm cat.	2975.0	2824.0	1526.0	3116.0	4985.0	2857.0
HOURS on STREAM	5.6	10.8	14.9	17.5	19.1	21.4
RPM	1700.0	1700.0	1700.0	1700.0	1700.0	1700.0

CONVERSION :

CO to Prods., vol%	36.56	28.69	19.47	17.59	21.11	21.78
CO to CO2, vol%	30.43	26.63	10.92	14.68	16.54	19.68
CO, gm mol/hr/kcm cat.	24.60	19.30	5.70	12.40	23.50	14.80
STY of oxysenates (2)						
gm mol/hr/kcm cat.	3.51	2.28	.84	1.75	3.65	1.97

STOICHIOM. H2/CO converted .81 .79 1.00 .88 .88 .90

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	2.02	1.89	2.86	1.80	2.51	2.23
C2-C6 ALCOHOLS	18.51	15.04	14.98	14.73	16.25	17.45
C2-C6 ALD. & ESTERS	5.50	5.96	5.03	9.43	8.93	5.67
CH4	20.41	21.58	23.79	17.76	21.26	21.22
C2-C3 HYDROCARBONS	24.11	26.42	27.58	25.68	27.14	27.71
C4+ HYDROCARBONS	29.78	29.12	22.13	30.64	23.93	25.64

APPROACH TO (3)

WGS Equilibrium, C 95.00 120.00 173.00 178.00 178.00 149.00

CARBON ACCOUNTABILITY, % (4) 88.6 82.6 83.0 78.2 79.6 80.1

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-48

CHEM SYSTEMS INC.

CATALYST NUMBER : 197-1

DATE : 4/22/80

ATOMIC FORMULA :  $CuCr_{.8}CoK_{.09}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.46 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1 2 3 4 5 6

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	9.00	13.50	13.50	9.00	9.00	9.00
AVE. TEMP., C	258.0	258.0	259.0	269.0	269.0	269.0
HOT SPOT, C	258.0	258.0	259.0	269.0	269.0	269.0
PRESSURE, psia	920.0	920.0	920.0	920.0	915.0	915.0
VHSV, 1/hr/kcm cat.	3152.0	2679.0	700.0	2719.0	677.0	1345.0
HOURS on STREAM	4.1	6.5	8.6	10.6	12.8	14.5
RPM	1700.0	1700.0	1720.0	1700.0	1700.0	1700.0

## CONVERSION :

CO to Prods., vol%	6.25	4.48	13.79	4.33	18.29	9.44
CO to CO <sub>2</sub> , vol%	2.25	1.25	8.51	2.07	11.21	4.86
CO, gm mol/hr/kcm cat.	3.10	1.72	1.76	2.01	2.31	2.22
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.43	.26	.30	.38	.47	.50

STOICHIOM. H<sub>2</sub>/CO converted

1.15 1.13 1.10 1.04 1.08 .85

CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	9.39	8.95	9.54	14.03	11.77	13.48
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	9.39	10.23	17.63	14.18	20.81	20.61
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00	.00	.00	.00	.00
CH <sub>4</sub>	43.39	35.69	36.71	40.62	39.84	38.94
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	20.41	20.72	20.86	18.02	18.23	18.18
C <sub>4</sub> + HYDROCARBONS	14.83	16.50	15.36	13.15	9.35	8.79

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00 .00 .00 .00 .00

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 84.2 72.8 87.3 91.7 91.8 93.6

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-48

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CATALYST NUMBER : 197-1  
 ATOMIC FORMULA :  $CuCr_2O_7 \cdot 2K_2O$   
 CATALYST SUPPORT : NONE

DATE : 4/22/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.46 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

7

8

9

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	9.00	13.50	13.50
AVE. TEMP., C	255.0	257.0	257.0
HOT SPOT, C	255.0	257.0	257.0
PRESSURE, psia	1200.0	1190.0	1485.0
VHSV, 1/hr/k <sub>cat</sub>	3570.0	3576.0	4322.0
HOURS on STREAM	16.6	19.0	20.8
RPM	1700.0	1700.0	1700.0

## CONVERSION :

CO to Prods., vol%	2.90	3.20	2.40
CO to CO <sub>2</sub> , vol%	.60	.00	.00
CO, gm mol/hr/k <sub>cat</sub>	1.44	1.30	1.17
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/k <sub>cat</sub>	.30	.36	.38

STOICHIOM. H<sub>2</sub>/CO converted 1.92 2.54 2.36CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	16.40	15.10	19.10
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	9.04	13.00	13.40
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00	.00
CH <sub>4</sub>	44.25	48.80	9.40
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	20.14	12.20	14.00
C <sub>4</sub> HYDROCARBONS	10.37	10.90	9.40

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00 .00

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 59.5 51.1 69.6

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-51

=====

CATALYST NUMBER : 197-57  
 ATOMIC FORMULA : CuCrCoZn<sub>.125</sub>K<sub>.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 5/2/80

PREP METHOD: Mech. Blending of Oxides

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.9 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty  
 1 2 3

## TEST CONDITIONS :

	1	2	3
FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
AVE. TEMP., C	252.0	263.0	292.0
HOT SPOT, C	252.0	263.0	293.0
PRESSURE, psig	900.0	900.0	915.0
VHSV, 1/hr/kgm cat.	3192.0	2024.0	2346.0
HOURS on STREAM	2.8	5.5	8.4
RPM	1700.0	1720.0	1730.0

## CONVERSION :

CO to Prods., vol%	2.17	3.93	14.44
CO to CO2, vol%	1.03	1.87	10.46
CO, gm mol/hr/kgm cat.	1.26	1.46	7.22
STY of oxygenates <sup>(2)</sup> gm mol/hr/kgm cat.	.03	.32	1.41

STOICHIOM. H2/CO converted	.97	1.39	1.03
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.00	1.48	2.07
C2-C6 ALCOHOLS	.00	2.36	10.52
C2-C6 ALD. & ESTERS	31.37	28.51	21.03
CH4	31.66	31.91	35.86
C2-C3 HYDROCARBONS	19.59	21.71	18.28
C4+ HYDROCARBONS	17.38	14.03	12.24

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	63.1	85.0	86.9
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* ZCO in feed/100 \* ZCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



## SUMMARY FOR RUN # 201-56

=====  
 CATALYST NUMBER : 197-48  
 ATOMIC FORMULA : CuCrCoZn<sub>1.25</sub>K<sub>1.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 5/12/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup> : 1.52 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1                    2                    3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00	5.00
AVE. TEMP., C	260.0	272.0	287.0
HOT SPOT, C	260.0	272.0	287.0
PRESSURE, Psig	885.0	885.0	885.0
VHSV, 1/hr/k <sub>sm</sub> cat.	2521.0	2492.0	2633.0
HOURS on STREAM	2.9	5.7	7.8
RPM	1690.0	1690.0	1700.0

## CONVERSION :

CO to Prods., vol%	.90	1.10	2.09
CO to CO <sub>2</sub> , vol%	.30	.41	.81
CO, gm mol/hr/k <sub>sm</sub> cat.	.38	.46	.95
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.10	.13	.20

STOICHIOM. H <sub>2</sub> /CO converted	2.78	.74	1.88
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.00	.55	1.39
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	8.95	8.36	3.61
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	26.03	28.90	24.57
CH <sub>4</sub>	30.31	29.73	40.26
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	16.56	16.85	16.94
C <sub>4</sub> + HYDROCARBONS	18.16	15.62	13.33

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	87.1	113.9	71.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* ZCO in feed/100 \* ZCO conv./100 \* ZSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-58

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CATALYST NUMBER ; 197-36 DATE ; 5/11/80  
 ATOMIC FORMULA ; CuCrCoZn<sub>.125</sub><sup>K</sup>.11  
 CATALYST SUPPORT ; NONE

PREP METHOD: Evaporation w/ Oxalic Acid REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> ; 1.45 gm/cc REACTOR TYPE: Plus Flow  
 TEST NUMBER 1 2 3 4

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## TEST CONDITIONS :

	1	2	3	4
FEED H2/CO RATIO	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00
AVE. TEMP., C	265.0	282.0	280.0	293.0
HOT SPOT, C	267.0	285.0	287.0	296.0
PRESSURE, psig	930.0	930.0	1200.0	1200.0
VHSV, l/hr/k <sub>sm</sub> cat.	2654.0	2709.0	3616.0	3655.0
HOURS on STREAM	2.3	3.7	5.7	6.6
RPM	.0	.0	.0	.0

## CONVERSION :

	1	2	3	4
CO to Prods., vol%	7.45	9.74	5.27	8.66
CO to CO2, vol%	.15	4.96	1.73	5.04
CO, gm mol/hr/k <sub>sm</sub> cat.	2.52	4.97	3.16	6.25
STY of oxygenates <sup>(2)</sup>				
gm mol/hr/k <sub>sm</sub> cat.	.30	.60	.63	.99

STOICHIOM. H2/CO converted 1.66 1.29 1.21 1.06

## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

	1	2	3	4
CH3OH	.41	1.21	3.45	3.32
C2-C6 ALCOHOLS	3.16	4.98	22.97	21.68
C2-C6 ALD. & ESTERS	8.77	12.08	[.00]	[.00]
CH4	55.90	51.18	44.08	44.79
C2-C3 HYDROCARBONS	11.12	19.33	18.32	18.20
C4+ HYDROCARBONS	12.04	11.32	13.68	10.60

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 55.7 81.9 75.5 83.9

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-60

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 CATALYST NUMBER : 200-25-1  
 ATOMIC FORMULA : CuCoZn .125<sup>K</sup>.11  
 CATALYST SUPPORT : NONE

DATE : 5/14/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.19 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

1            2            3            4            5  
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## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	259.0	270.0	281.0	295.0	298.0
HOT SPOT, C	160.0	271.0	283.0	298.0	303.0
PRESSURE, psis	910.0	910.0	900.0	900.0	1140.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3267.0	3222.0	3247.0	3376.0	4278.0
HOURS on STREAM	2.3	3.8	5.3	6.6	7.4
RPM	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	2.89	4.10	6.67	12.32	13.24
CO to CO2, vol%	2.91	3.40	6.03	11.78	12.46
CO, gm mol/hr/k <sub>sm</sub> cat.	2.46	3.03	5.17	10.20	13.80
STY of oxoacetates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.32	.53	.89	1.46	2.14

STOICHIOM. H2/CO converted	.91	.83	.84	.86	.85
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	2.21	3.84	4.57	4.50	5.44
C2-C6 ALCOHOLS	4.02	4.94	9.14	10.57	12.43
C2-C6 ALD. & ESTERS	19.70	23.24	19.05	12.92	12.23
CH4	31.36	30.19	30.67	34.25	21.94
C2-C3 HYDROCARBONS	22.91	22.87	22.86	24.27	35.92
C4+ HYDROCARBONS	19.90	14.82	13.71	13.50	12.04

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C		-52.00	73.00	69.00	70.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	57.9	72.9	75.0	78.5	78.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxoacetates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-62

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 CATALYST NUMBER : 197-16 DATE : 5/16/80  
 ATOMIC FORMULA : CuCrCoZn .5 .11  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.24 gm/cc

REACTOR TYPE: Bertu

TEST NUMBER 1 2 3 4 5 6

## TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	273.0	275.0	298.0	312.0	297.0	274.0
HOT SPOT, C	273.0	275.0	298.0	312.0	297.0	274.0
PRESSURE, psig	895.0	1350.0	930.0	920.0	915.0	920.0
VHSV, 1/hr/ksm cat.	3375.0	4842.0	3420.0	6766.0	1284.0	3270.0
HOURS on STREAM	4.5	5.9	8.9	10.7	11.9	13.5
RPM	1700.0	1700.0	1720.0	1700.0	1700.0	1710.0

## CONVERSION :

CO to Prods., vol%	10.42	7.81	50.99	57.66	70.43	8.57
CO to CO2, vol%	3.88	4.09	42.31	31.05	27.57	4.03
CO, gm mol/hr/ksm cat.	6.02	7.19	39.80	74.90	15.70	5.10
STY of oxycyanates <sup>(2)</sup> gm mol/hr/ksm cat.	1.05	1.43	.28	.45	.02	.73

STOICHIOM. H2/CO converted	1.43	1.43	1.49	1.45	1.70	1.05
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	4.80	7.47	.18	.15	.00	5.88
C2-C6 ALCOHOLS	19.21	22.87	1.10	.77	.14	15.29
C2-C6 ALD. & ESTERS	.00	.00	.00	.00	.00	.00
CH4	41.58	38.57	46.29	75.69	76.25	32.93
C2-C3 HYDROCARBONS	22.78	21.04	16.28	14.15	15.03	24.40
C4+ HYDROCARBONS	11.53	10.06	11.34	9.23	8.49	21.61

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	165.00	75.00	84.00	104.00	57.00	130.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	94.1	100.2	93.5	92.9	98.8	91.9
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxycyanates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-65

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CATALYST NUMBER : 200-27-1  
 ATOMIC FORMULA : CuCoZn<sub>0.125</sub>Co<sub>0.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 5/21/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.44 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1            2            3

-----

TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
AVE. TEMP., C	272.0	284.0	297.0
HOT SPOT, C	274.0	287.0	300.0
PRESSURE, psis	900.0	900.0	900.0
VHSV, 1/hr/kcm cat.	2557.0	2419.0	2579.0
HOURS on STREAM	2.9	4.6	6.4
RPM	.0	.0	.0

CONVERSION :

CO to Prods., vol%	4.97	7.01	10.64
CO to CO2, vol%	1.53	3.09	5.56
CO, gm mol/hr/kcm cat.	2.07	3.04	5.20
STY of oxygenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	.30	.40	.63

STOICHIOM. H2/CO converted            1.39       1.36       1.23

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	2.23	3.75	3.96
C2-C6 ALCOHOLS	7.46	7.06	7.46
C2-C6 ALD.&ESTERS	9.42	8.36	7.01
CH4	40.71	48.99	51.17
C2-C3 HYDROCARBONS	19.24	20.46	20.71
C4+ HYDROCARBONS	20.94	11.38	9.59

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C            110.00    142.00    119.00

CARBON ACCOUNTABILITY, %<sup>(4)</sup>    65.9       76.3       90.1

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-67

CATALYST NUMBER : 197-2  
 ATOMIC FORMULA : CuCrCoZn<sub>125</sub>K<sub>11</sub>  
 CATALYST SUPPORT : NONE

DATE : 5/22/80

PREP METHOD: Evaporation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.69 gm/cc  
 TEST NUMBER

REACTOR TYPE: Rerty

1            2            3            4            5            6

## TEST CONDITIONS :

	1	2	3	4	5	6
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	270.0	271.0	293.0	294.0	292.0	266.0
HOT SPOT, C	271.0	271.0	294.0	295.0	294.0	267.0
PRESSURE, psis	895.0	1410.0	900.0	895.0	890.0	890.0
VHSV, 1/hr/kcm cat.	648.0	636.0	2541.0	730.0	700.0	622.0
HOURS on STREAM	5.3	6.6	13.6	17.1	35.7	42.8
RPM	1700.0	1700.0	1730.0	1690.0	1700.0	1700.0

## CONVERSION :

CO to Prods., vol%	16.30	20.09	9.77	35.16	27.27	8.02
CO to CO <sub>2</sub> , vol%	12.20	16.31	4.83	23.74	17.73	3.68
CO, gm mol/hr/kcm cat.	2.28	2.87	4.59	5.33	39.00	.90
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	.28	.31	.79	.79	.54	.27

STOICHIOM. H <sub>2</sub> /CO converted	.88	.90	1.13	1.01	.97	.94
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	1.75	1.99	7.03	4.69	6.11	12.40
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.77	4.53	18.54	16.92	16.83	30.48
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	14.16	13.04	.00	3.35	.00	.00
CH <sub>4</sub>	36.19	39.49	47.09	43.89	44.22	34.13
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	25.35	27.90	23.32	27.14	28.22	17.35
C <sub>4</sub> + HYDROCARBONS	16.78	13.04	4.04	4.02	4.62	5.54

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	91.7	87.1	94.1	98.3	99.3	104.4
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-72

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CATALYST NUMBER : 197-59  
 ATOMIC FORMULA : CuCoMnZn<sub>125</sub>K<sub>11</sub>  
 CATALYST SUPPORT : NONE

DATE : 6/5/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.46 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

1            2            3

-----

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
Ave. Temp., C	243.0	274.0	294.0
HOT SPOT, C	245.0	275.0	296.0
PRESSURE, psia	900.0	900.0	895.0
UHSV, 1/hr/kcm cat.	2415.0	2402.0	2382.0
HOURS on STREAM	3.1	4.5	5.6
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	1.37	1.75	8.08
CO to CO2, vol%	.14	.85	4.82
CO, gm mol/hr/kcm cat.	.46	.78	3.80
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.07	.10	.49

STOICHIOM. H2/CO converted

.92	2.52	.70
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CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	2.42	2.67	3.35
C2-C6 ALCOHOLS	13.41	5.94	7.35
C2-C6 ALD. & ESTERS	.00	9.65	9.90
CH4	43.41	44.41	42.17
C2-C3 HYDROCARBONS	21.54	26.29	30.83
C4+ HYDROCARBONS	19.23	11.14	6.39

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

73.00	114.00	82.00
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CARBON ACCOUNTABILITY, %<sup>(4)</sup>

60.3	143.6	90.3
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-74

=====

CATALYST NUMBER : 197-65 DATE : 6/12/80  
 ATOMIC FORMULA : CuCrCoZn<sub>0.125</sub>K<sub>0.11</sub>  
 CATALYST SUPPORT : 70.0% SiO<sub>2</sub>

PREP METHOD: Impregnation REDUCTION: in Situ Reduction

BULK DENSITY <sup>(1)</sup> : .5 gm/cc REACTOR TYPE: Bertu  
 TEST NUMBER 1 2 3

-----

TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
AVE. TEMP., C	267.0	267.0	267.0
HOT SPOT, C	267.0	267.0	267.0
PRESSURE, Psia	905.0	900.0	880.0
VHSV, 1/hr/kcm cat.	7745.0	1744.0	964.0
HOURS on STREAM	.9	2.0	19.1
RPM	1700.0	1700.0	1700.0

CONVERSION :

CO to Prods., vol%	.22	7.12	5.08
CO to CO2, vol%	1.88	.98	1.22
CO, gm mol/hr/kcm cat.	2.01	1.76	.75
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	.00	.52	.12

STOICHIOM. H2/CO converted 3.07 1.72 .18

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	N.A.	7.51	7.69
C2-C6 ALCOHOLS	N.A.	14.90	9.68
C2-C6 ALD. & ESTERS	N.A.	11.38	11.91
CH4	N.A.	32.76	45.15
C2-C3 HYDROCARBONS	N.A.	26.85	22.70
C4+ HYDROCARBONS	N.A.	6.60	2.98

APPROACH TO <sup>(3)</sup>

WGS Equilibrium, C 73.00 139.00

CARBON ACCOUNTABILITY, % <sup>(4)</sup> 89.5 98.8 98.4

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-77

=====  
 CATALYST NUMBER : 197-60  
 ATOMIC FORMULA :  $\text{CuCoVZn}_{.125}^{\text{K}}_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 6/27/80

PREP METHOD: Evaporation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup>: 1.29 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow  
 1 2 3 4 5

## TEST CONDITIONS :

	1	2	3	4	5
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	255.0	277.0	289.0	276.0	288.0
HOT SPOT, C	256.0	279.0	293.0	278.0	292.0
PRESSURE, psia	885.0	885.0	880.0	885.0	885.0
UHSV, 1/hr/k <sub>sm</sub> cat.	2965.0	3084.0	2993.0	3159.0	3135.0
HOURS on STREAM	1.8	3.0	5.4	9.0	10.9
RPM	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	2.54	6.76	8.25	5.24	11.10
CO to CO <sub>2</sub> , vol%	.66	2.44	4.25	2.27	6.80
CO, gm mol/hr/k <sub>sm</sub> cat.	1.18	3.54	4.67	2.91	6.99
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.21	.90	1.01	.67	1.45

STOICHIOM. H<sub>2</sub>/CO converted

1.76	1.41	1.04	1.37	.97
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	4.67	6.94	6.51	7.31	6.77
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	10.34	22.31	18.32	8.02	12.74
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	7.06	5.31	7.87	17.48	14.03
CH <sub>4</sub>	42.37	36.87	35.89	36.25	36.13
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	22.07	19.18	19.08	19.05	19.52
C <sub>4</sub> + HYDROCARBONS	13.49	9.39	12.42	11.89	10.81

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	83.00	107.00	-89.00	62.00	96.00
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CARBON ACCOUNTABILITY, % (4)	90.8	99.4	103.2	104.7	84.7
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{ea} - T_{hs}$ where  $T_{ea}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-79

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CATALYST NUMBER : 197-66	DATE : 6/26/80
ATOMIC FORMULA : $CuCrCoZn_{.125}K_{.11}$	
CATALYST SUPPORT : 45.0% $TiO_2$	
PREP METHOD: Impregnation	REDUCTION: in Situ Reduction
BULK DENSITY <sup>(1)</sup> : 1.14 gm/cc	REACTOR TYPE: Berets
TEST NUMBER	1

-----

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00
FEED CO <sub>2</sub>	5.00
AVE. TEMP., C	272.0
HOT SPOT, C	272.0
PRESSURE, psis	895.0
WHSV, 1/hr/k <sub>sm</sub> cat.	594.0
HOURS on STREAM	9.6
RPM	1700.0

## CONVERSION :

CO to Prods., vol%	1.27
CO to CO <sub>2</sub> , vol%	.00
CO, gm mol/hr/k <sub>sm</sub> cat.	.09
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/k <sub>sm</sub> cat.	.04

STOICHIOM. H <sub>2</sub> /CO converted	2.20
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.50
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	23.80
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	20.50
CH <sub>4</sub>	46.00
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	9.10
C <sub>4</sub> + HYDROCARBONS	.00

APPROACH TO <sup>(3)</sup>	
WGS Equilibrium, C	.00

CARBON ACCOUNTABILITY, % (4)	25.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxygenates}/100.$

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-80

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 CATALYST NUMBER : 200-57-1 DATE : 7/2/80  
 ATOMIC FORMULA : CuCoFe<sub>1</sub>Zn<sub>1.125</sub>K<sub>1.1</sub>  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: in Situ Reduction  
 BULK DENSITY<sup>(1)</sup>: 1.456 gm/cc REACTOR TYPE: Berty  
 TEST NUMBER 1 2  
 -----

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00
AVE. TEMP., C	273.0	288.0
HOT SPOT, C	274.0	289.0
PRESSURE, psig	900.0	900.0
WHSV, 1/hr/ksm cat.	2700.0	638.0
HOURS on STREAM	5.8	12.3
RPM	1720.0	1730.0

## CONVERSION :

CO to Prods., vol%	2.56	7.01
CO to CO <sub>2</sub> , vol%	.95	6.99
CO, gm mol/hr/ksm cat.	1.20	1.10
STY of oxysenates <sup>(2)</sup>		
gm mol/hr/ksm cat.	.43	.25

STOICHIOM. H <sub>2</sub> /CO converted	.79	1.26
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	23.42	30.94
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	19.59	9.58
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	6.85	5.59
CH <sub>4</sub>	21.23	24.15
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	23.97	24.15
C <sub>4</sub> + HYDROCARBONS	4.93	5.59

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	-84.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	50.6	83.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-81

=====

CATALYST NUMBER : 200-58-1  
 ATOMIC FORMULA : CuCoMoZn<sub>0.125</sub>K<sub>0.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 7/10/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.41 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

2

3

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00
AVE. TEMP., C	265.0	275.0	283.0
HOT SPOT, C	267.0	277.0	287.0
PRESSURE, psig	885.0	885.0	885.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3151.0	2972.0	2967.0
HOURS on STREAM	3.3	5.2	6.3
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	5.90	7.19	9.83
CO to CO2, vol%	2.64	3.91	5.57
CO, gm mol/hr/k <sub>sm</sub> cat.	3.38	4.16	5.73
STY of oxygenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.28	.26	.28

STOICHIOM. H2/CO converted 1.24 1.07 1.05

## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	7.23	5.71	4.55
C2-C6 ALCOHOLS	2.89	2.31	1.72
C2-C6 ALD. & ESTERS	.43	.31	.16
CH4	41.08	42.44	44.67
C2-C3 HYDROCARBONS	41.08	37.50	38.09
C4+ HYDROCARBONS	7.09	11.73	10.82

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C 1.00 .00 .00

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 78.8 97.2 102.8

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-83

=====

CATALYST NUMBER : 197-71  
 ATOMIC FORMULA :  $CuCoFe_{.1}Th_{.5}Zn_{.125}K_{.11}$   
 CATALYST SUPPORT : NONE

DATE 1 7/14/80

PREP METHOD: Evaporation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.8 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

	1	2	3
TEST CONDITIONS :			
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.00	5.00	5.00
AVE. TEMP., C	246.0	274.0	275.0
HOT SPOT, C	247.0	275.0	276.0
PRESSURE, psia	900.0	900.0	900.0
WHSV, 1/hr/k <sub>cat</sub>	2063.0	2314.0	533.0
HOURS on STREAM	5.2	9.2	11.4
RPM	1760.0	1700.0	1700.0
CONVERSION :			
CO to Prods., vol%	3.39	5.90	14.38
CO to CO <sub>2</sub> , vol%	.00	.00	4.52
CO, gm mol/hr/k <sub>cat</sub>	.80	1.56	1.16
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/k <sub>cat</sub>	.42	.85	.45
STOICHIOM. H <sub>2</sub> /CO converted	1.72	.30	1.33
CARBON SELECTIVITY (Normalized Mol% on CO <sub>2</sub> -free Basis) :			
CH <sub>3</sub> OH	21.00	19.60	17.87
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	26.50	30.30	27.86
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.80	.60	1.31
CH <sub>4</sub>	27.10	27.70	29.56
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	15.70	15.40	16.42
C <sub>4</sub> + HYDROCARBONS	8.90	6.40	6.57
APPROACH TO <sup>(3)</sup>			
WGS Equilibrium, C			
CARBON ACCOUNTABILITY, % <sup>(4)</sup>	31.7	50.8	76.7

=====

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * X_{CO} \text{ in feed}/100 * X_{CO} \text{ conv.}/100 * X_{Sel} \text{ to Oxysenates}/100$ .

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-84

CATALYST NUMBER : 197-67  
 ATOMIC FORMULA :  $CuCrCoZn_{.125}K_{.11}$   
 CATALYST SUPPORT : 70.0%  $TiO_2$

DATE : 7/18/80

PREP METHOD: Impregnation

REDUCTION: Reduced by 2%  $H_2$  in  $N_2$ 

BULK DENSITY<sup>(1)</sup> : 1.27 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

1 2

## TEST CONDITIONS :

FEED $H_2/CO$ RATIO	2.00	2.00
FEED $CO_2$	5.10	5.10
AVE. TEMP., C	261.0	262.0
HOT SPOT, C	262.0	262.0
PRESSURE, psia	890.0	880.0
WHSV, 1/hr/kgm cat.	3374.0	1000.0
HOURS on STREAM	4.0	6.0
RPM	.0	.0

## CONVERSION :

$CO$ to Prods., vol%	.56	1.65
$CO$ to $CO_2$ , vol%	.44	2.05
$CO$ , gm mol/hr/kgm cat.	.42	.45
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/kgm cat.	.03	.05

STOICHIOM. $H_2/CO$ converted	.56	.75
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CARBON SELECTIVITY (Normalized Mol% on  $CO_2$ -free Basis) :

$CH_3OH$	.36	.22
$C_2-C_4$ ALCOHOLS	.89	.67
$C_2-C_6$ ALB. ESTERS	9.07	22.70
$CH_4$	76.16	57.98
$C_2-C_3$ HYDROCARBONS	10.14	13.26
$C_4+$ HYDROCARBONS	3.38	5.17

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	69.3	89.2
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO$  in feed/100 \*  $\%CO$  conv./100 \*  $\%Sel$  to Oxygenates/100.(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp. calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-85

=====						
CATALYST NUMBER : 197-71	DATE : 7/22/80					
ATOMIC FORMULA : $CuCoFe_{.1}Th_{.5}Zn_{.125}K_{.11}$						
CATALYST SUPPORT : NONE						
PREP METHOD: Evaporation	REDUCTION: Reduced by 2% H <sub>2</sub> in N <sub>2</sub>					
BULK DENSITY <sup>(1)</sup> : 1.73 gm/cc	REACTOR TYPE: Berts					
TEST NUMBER	1	2	3	4	5	6
-----						
TEST CONDITIONS :						
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.10	5.10	5.10	5.10	5.10	5.10
AVE. TEMP., C	257.0	258.0	270.0	271.0	279.0	280.0
HOT SPOT, C	258.0	259.0	271.0	272.0	280.0	281.0
PRESSURE, psig	905.0	900.0	905.0	905.0	905.0	905.0
VHSV, l/hr/k <sub>sm</sub> cat.	3597.0	882.0	3351.0	976.0	3258.0	1005.0
HOURS on STREAM	4.2	5.9	10.3	12.8	16.1	19.1
RPM	1740.0	1740.0	1740.0	1740.0	1730.0	1720.0
CONVERSION :						
CO to Prods., vol%	3.90	10.43	5.50	13.04	4.92	14.61
CO to CO <sub>2</sub> , vol%	.00	2.67	.80	4.46	1.48	5.79
CO, gm mol/hr/k <sub>sm</sub> cat.	1.70	1.39	2.60	2.13	2.61	2.57
STY of oxoates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.85	.54	1.12	.70	.94	.75
STOICHIOM. H <sub>2</sub> /CO converted	1.33	1.44	.82	.70	.85	.78
CARBON SELECTIVITY (Normalized Mol% on CO <sub>2</sub> -free Basis) :						
CH <sub>3</sub> OH	14.80	13.44	17.41	13.69	17.82	13.69
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	32.00	33.17	29.55	28.19	27.05	24.44
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	3.30	2.26	2.41	2.15	2.21	2.93
CH <sub>4</sub>	24.40	26.88	28.75	33.15	32.51	35.89
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	16.10	17.34	16.27	18.26	16.38	18.02
C <sub>4</sub> + HYDROCARBONS	9.40	6.91	5.61	4.56	4.03	5.03
APPROACH TO <sup>(3)</sup>						
WGS Equilibrium, C	147.00	176.00	134.00	169.00	67.00	148.00
CARBON ACCOUNTABILITY, % (4)						
	73.3	91.1	80.3	91.5	97.5	98.0
-----						

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxoates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-87

=====  
 CATALYST NUMBER : 197-73  
 ATOMIC FORMULA : CuCrCoZn<sub>0.125</sub>K<sub>0.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 7/31/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.28 gm/cc

REACTOR TYPE: Berty

TEST NUMBER                    1                    2                    3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.10	5.10	5.10
AVE. TEMP., C	260.0	260.0	272.0
HOT SPOT, C	260.0	261.0	273.0
PRESSURE, psia	935.0	930.0	935.0
WHSV, 1/hr/kgm cat.	3406.0	892.0	877.0
HOURS on STREAM	4.0	6.0	9.3
RPM	1720.0	1720.0	1720.0

## CONVERSION :

CO to Prods., vol%	3.81	9.14	18.68
CO to CO <sub>2</sub> , vol%	1.79	6.76	10.42
CO, gm mol/hr/kgm cat.	2.41	1.79	3.22
STY of oxides <sup>(2)</sup>			
gm mol/hr/kgm cat.	.48	.28	.56

STOICHIOM. H <sub>2</sub> /CO converted	.34	.62	.52
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	3.82	3.65	6.23
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	11.62	11.83	18.85
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	13.97	11.30	1.87
CH <sub>4</sub>	42.94	43.13	46.26
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	19.12	20.52	19.47
C <sub>4</sub> + HYDROCARBONS	8.53	9.57	7.32

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	68.2	99.8	93.4
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxides/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-B9

\*\*\*\*\*  
 CATALYST NUMBER : 197-72  
 ATOMIC FORMULA :  $\text{CuCoZrZn}_{.125\text{K}.11}$   
 CATALYST SUPPORT : NONE

DATE : 8/6/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY <sup>(1)</sup> : 1.3 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

1            2            3            4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	5.10	5.10	5.10	5.10
AVE. TEMP., C	264.0	264.0	273.0	273.0
HOT SPOT, C	265.0	265.0	273.0	273.0
PRESSURE, psia	880.0	875.0	910.0	910.0
VHSV, l/hr/kcm cat.	3548.0	857.0	2791.0	932.0
HOURS on STREAM	4.1	6.9	10.0	14.9
RPH	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	.72	2.70	1.31	6.63
CO to CO <sub>2</sub> , vol%	.28	1.20	.09	.57
CO, gm mol/hr/kcm cat.	.45	.42	.49	.83
STY of oxoacetates <sup>(2)</sup> gm mol/hr/kcm cat.	.11	.12	.20	.34

STOICHIOM. H <sub>2</sub> /CO converted	1.60	.89	.78	.96
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	22.42	22.54	25.80	23.78
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	9.33	13.01	12.10	18.35
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	2.51	5.20	5.67	4.34
CH <sub>4</sub>	48.47	41.47	38.01	33.33
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	12.81	11.85	14.99	14.66
C <sub>4</sub> + HYDROCARBONS	4.46	5.92	3.43	5.54

APPROACH TO <sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	96.6	106.1	95.8	55.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxacetates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



## SUMMARY FOR RUN # 201-90

CATALYST NUMBER : 197-76  
 ATOMIC FORMULA :  $\text{CuCrCoZn}_{125}^{\text{K}}.11$   
 CATALYST SUPPORT : NONE

DATE : 8/4/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.35 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	4.90	4.90	4.90	4.90
AVE. TEMP., C	271.0	273.0	238.0	246.0
HOT SPOT, C	272.0	273.0	238.0	246.0
PRESSURE, psia	935.0	930.0	1600.0	1600.0
UHSV, 1/hr/kcm cat.	3509.0	854.0	322.0	309.0
HOURS on STREAM	3.0	6.0	8.5	12.1
RPM	1730.0	1750.0	1720.0	1720.0

## CONVERSION :

CO to Prods., vol%	3.07	14.39	6.39	10.94
CO to CO <sub>2</sub> , vol%	1.73	10.21	2.21	6.16
CO, gm mol/hr/kcm cat.	2.07	2.61	.34	.65
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.36	.36	.07	.10

STOICHIOM. H <sub>2</sub> /CO converted	.61	.51	1.00	.67
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	5.32	4.62	7.94	5.78
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	7.98	7.86	8.34	7.97
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	14.24	10.77	11.44	11.41
CH <sub>4</sub>	45.70	46.32	43.20	43.59
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	18.62	20.85	19.38	19.84
C <sub>4</sub> + HYDROCARBONS	8.14	9.57	9.69	11.41

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	112.9	100.0	98.3	101.7
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-91

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=====
CATALYST NUMBER : 197-73
ATOMIC FORMULA : CuCrCoZn .125K.11
CATALYST SUPPORT : NONE
PREP METHOD: Evaporation
REDUCTION: Reduced by 2% H2 in N2
BULK DENSITY(1) : 1.47 gm/cc
REACTOR TYPE: Bertu
TEST NUMBER 1
=====

```

## TEST CONDITIONS :

```

FEED H2/CO RATIO      2.10
FEED CO2              5.20
AVE. TEMP., C        271.0
HOT SPOT, C          272.0
PRESSURE, psia       915.0
VHSV, l/hr/ksm cat.  918.0
HOURS on STREAM      9.2
RPM                  1720.0

```

## CONVERSION :

```

CO to Prods., vol%   13.82
CO to CO2, vol%      7.38
CO, gm mol/hr/ksm cat.  2.40
STY of oxygenates(2)
  gm mol/hr/ksm cat.  .46

```

```

STOICHIOM. H2/CO converted .49

```

## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

```

CH3OH                8.59
C2-C6 ALCOHOLS       19.79
C2-C6 ALD. & ESTERS   .92
CH4                   44.48
C2-C3 HYDROCARBONS   18.10
C4+ HYDROCARBONS     8.13

```

APPROACH TO<sup>(3)</sup>

```

WGS Equilibrium, C    91.00

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CARBON ACCOUNTABILITY, %(4)  103.5
=====

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-92

=====

CATALYST NUMBER : 197-78	DATE : 8/15/80
ATOMIC FORMULA : $\text{CuCr}_{.125}\text{CoZn}_{.125}\text{K}_{.11}$	
CATALYST SUPPORT : NONE	

PREP METHOD: Evaporation                      REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.41 gm/cc                      REACTOR TYPE: Plus Flow

TEST NUMBER	1	2	3
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TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.10	5.10	5.10
AVE. TEMP., C	262.0	276.0	279.0
HOT SPOT, C	263.0	279.0	284.0
PRESSURE, psig	905.0	920.0	910.0
VHSV, 1/hr/kcm cat.	3677.0	3361.0	969.0
HOURS on STREAM	3.6	6.1	9.0
RPM	.0	.0	.0

CONVERSION :

CO to Prods., vol%	3.42	5.89	30.03
CO to CO2, vol%	.58	2.01	20.87
CO, gm mol/hr/kcm cat.	1.82	3.20	5.94
STY of oxygenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	.48	.83	.93

STOICHIOM. H2/CO converted                      .65                      .59                      .56

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis)

CH3OH	4.21	4.69	4.07
C2-C6 ALCOHOLS	7.13	8.71	15.76
C2-C6 ALD. & ESTERS	19.63	21.45	6.61
CH4	35.16	32.98	39.49
C2-C3 HYDROCARBONS	21.85	22.25	23.90
C4+ HYDROCARBONS	12.03	9.92	10.17

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	142.00	72.00	19.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	83.9	112.8	104.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

    where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-93

CATALYST NUMBER : 197-77  
 ATOMIC FORMULA :  $CuCoTh_{.5}Zn_{.125}K_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 8/19/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 0 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1            2            3            4            5            6

## TEST CONDITIONS :

FEED H2/CO RATIO	2.10	2.10	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.10	5.10	5.10	5.10
AVE. TEMP., C	262.0	268.0	270.0	270.0	282.0	284.0
HOT SPOT, C	262.0	268.0	270.0	270.0	283.0	284.0
PRESSURE, psig	920.0	915.0	920.0	920.0	920.0	915.0
VHSV, 1/hr/kcm cat.	3607.0	900.0	3239.0	931.0	3431.0	984.0
HOURS on STREAM	4.0	7.0	10.2	13.1	18.1	20.2
RPM	1760.0	1760.0	1720.0	1720.0	1770.0	1730.0

## CONVERSION :

CO to Prods., vol%	3.61	19.06	5.53	20.50	11.11	42.62
CO to CO2, vol%	.69	11.44	1.97	9.30	2.49	21.18
CO, gm mol/hr/kcm cat.	1.90	3.37	2.98	3.41	5.73	7.71
STY of oxogenates <sup>(2)</sup> gm mol/hr/kcm cat.	.59	.87	.75	.72	1.67	1.33

STOICHIOM. H2/CO converted

1.02	.57	.92	.61	.76	.57
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CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	9.64	8.80	10.45	7.70	8.94	6.29
C2-C6 ALCOHOLS	19.40	28.64	20.35	20.20	21.66	17.37
C2-C6 ALD.&ESTERS	7.98	3.68	3.12	2.62	5.02	2.10
CH4	39.88	31.68	37.72	39.83	34.96	45.81
C2-C3 HYDROCARBONS	17.50	19.36	24.83	25.29	23.75	24.40
C4+ HYDROCARBONS	5.60	7.84	3.53	4.36	3.67	4.04

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

88.00	70.00	72.00	142.00	170.00	122.00
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CARBON ACCOUNTABILITY, %<sup>(4)</sup>

106.2	100.8	109.0	105.3	100.2	103.1
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxogenates/100.

(3) Defined as  $T = T_{ea} - T_{hs}$ where  $T_{ea}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-93

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CATALYST NUMBER : 197-77	DATE : 8/19/80
ATOMIC FORMULA : $CuCoTh_{.5}Zn_{.125}K_{.11}$	
CATALYST SUPPORT : NONE	
PREP METHOD: Evaporation	REDUCTION: Reduced by 2% H2 in N2
BULK DENSITY <sup>(1)</sup> : 0 gm/cc	REACTOR TYPE: Berty
TEST NUMBER 7	

-----

TEST CONDITIONS :

FEED H2/CO RATIO	2.10
FEED CO2	5.00
AVE. TEMP., C	257.0
HOT SPOT, C	257.0
PRESSURE, psis	925.0
VHSV, 1/hr/kcm cat.	3248.0
HOURS on STREAM	22.7
RPM	1730.0

CONVERSION :

CO to Prods., vol%	2.65
CO to CO2, vol%	.05
CO, gm mol/hr/kcm cat.	1.08
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/kcm cat.	.35

STOICHIOM. H2/CO converted .63

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	13.37
C2-C6 ALCOHOLS	17.14
C2-C6 ALD.&ESTERS	3.06
CH4	40.00
C2-C3 HYDROCARBONS	23.67
C4+ HYDROCARBONS	2.76

APPROACH TO <sup>(3)</sup>  
WGS Equilibrium, C 93.00

CARBON ACCOUNTABILITY, % (4) 101.7

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 201-95

CATALYST NUMBER : 197-79  
 ATOMIC FORMULA : CuCoThZn<sub>.125</sub><sup>K</sup>.<sub>.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 8/28/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.52 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1 2 3

TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	5.20	5.20	5.20
AVE. TEMP., C	260.0	261.0	273.0
HOT SPOT, C	260.0	261.0	273.0
PRESSURE, psis	920.0	1530.0	910.0
VHSV, 1/hr/ksm cat.	3202.0	3237.0	3364.0
HOURS on STREAM	4.6	7.3	12.2
RPM	1710.0	1700.0	1720.0

CONVERSION :

CO to Prods., vol%	3.48	4.69	4.27
CO to CO2, vol%	.02	2.61	.43
CO, gm mol/hr/ksm cat.	1.39	2.93	1.96
STY of oxysenates <sup>(2)</sup> gm mol/hr/ksm cat.	.52	.77	.70

STOICHIOM. H2/CO converted 1.29 .93 2.06

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	12.68	14.00	15.75
C2-C6 ALCOHOLS	23.74	25.04	22.36
C2-C6 ALD. & ESTERS	1.31	1.71	.99
CH4	32.09	30.79	37.56
C2-C3 HYDROCARBONS	24.35	22.24	20.26
C4+ HYDROCARBONS	5.84	6.22	3.08

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00 .00

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 90.3 89.0 104.9

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 201-97

CATALYST NUMBER : 197-73

DATE : 9/5/80

ATOMIC FORMULA : CuCrCoZn<sub>1.25</sub><sup>K</sup>.11

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.38 gm/cc

REACTOR TYPE: Plug Flow

TEST NUMBER 1

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10
FEED CO <sub>2</sub>	5.10
AVE. TEMP., C	273.0
HOT SPOT, C	273.0
PRESSURE, psig	910.0
WHSV, 1/hr/kgm cat.	1030.0
HOURS on STREAM	35.6
RPM	.0

## CONVERSION :

CO to Prods., vol%	5.40
CO to CO <sub>2</sub> , vol%	1.80
CO, gm mol/hr/kgm cat.	.92
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/kgm cat.	.19

STOICHIOM. H<sub>2</sub>/CO converted .51CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	6.40
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	8.26
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	13.33
CH <sub>4</sub>	38.79
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	25.19
C <sub>4</sub> + HYDROCARBONS	8.13

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00

CARBON ACCOUNTABILITY, % (4) 99.1

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxygenates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 201-98

CATALYST NUMBER : 197-81

DATE : 9/8/80

ATOMIC FORMULA :  $CuFe_{.5}Th_{.5}Mn_{3.24}Zn_{.125}K_{.11}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.02 gm/cc

REACTOR TYPE: Bertw

TEST NUMBER

1 2 3 4

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00	2.00
FEED CO2	5.00	5.00	5.00	5.00
AVE. TEMP., C	267.0	262.0	262.0	239.0
HOT SPOT, C	268.0	262.0	263.0	242.0
PRESSURE, psia	920.0	920.0	1500.0	900.0
VHSV, 1/hr/kcm cat.	1619.0	4487.0	5162.0	1797.0
HOURS on STREAM	3.8	8.2	11.1	15.1
RPM	1730.0	1730.0	1740.0	1700.0

## CONVERSION :

CO to Prods., vol%	37.84	10.21	10.41	7.91
CO to CO2, vol%	11.76	1.69	1.89	1.19
CO, gm mol/hr/kcm cat.	10.10	6.71	7.78	2.06
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	1.27	1.14	1.70	.44

STOICHIOM. H2/CO converted	.70	.87	1.06	.56
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	1.70	4.78	5.44	5.75
C2-C6 ALCOHOLS	14.15	14.10	17.38	16.46
C2-C6 ALD., ESTERS	.66	.93	3.07	2.65
CH4	26.61	28.21	26.60	28.65
C2-C3 HYDROCARBONS	36.30	37.41	33.33	34.06
C4+ HYDROCARBONS	20.58	14.57	14.18	12.43

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	101.2	95.3	114.4	90.1
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $VHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxysenates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$   
where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC

## SUMMARY FOR RUN # 201-100

-----  
 CATALYST NUMBER : Methanol synthesis cat. / 200-27-2 \*      DATE : 9/12/80  
 ATOMIC FORMULA : CuAl<sub>1.21</sub>Zn<sub>1.49</sub> / CuCoTh<sub>5</sub>Fe<sub>5</sub>Zn<sub>1.25</sub>K<sub>1.11</sub>  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation (200-27-1)      REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup>: 1.23 gm/cc      REACTOR TYPE: Plus Flow  
 TEST NUMBER                              1                              2                              3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10
FEED CO <sub>2</sub>	4.90	4.90	4.90
AVE. TEMP., C	182.0	193.0	209.0
HOT SPOT, C	183.0	193.0	219.0
PRESSURE, psis	920.0	920.0	920.0
VHSV, 1/hr/kcm cat.	3402.0	3388.0	3669.0
HOURS on STREAM	4.0	5.8	10.4
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	1.40	1.80	27.45
CO to CO <sub>2</sub> , vol%	.00	.00	.45
CO, gm mol/hr/kcm cat.	.58	.75	12.50
STY of oxygenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	.40	.58	11.60

STOICHIOM. H <sub>2</sub> /CO converted	.86	7.60	1.06
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	68.90	71.90	92.38
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	2.10	1.70	1.42
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	6.70	3.50	.30
CH <sub>4</sub>	10.60	9.90	1.63
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	7.90	9.90	2.54
C <sub>4</sub> + HYDROCARBONS	3.80	3.10	1.73

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	87.2	121.3	88.5
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as T = T<sub>eq</sub> - T<sub>hs</sub>

where T<sub>eq</sub> = water gas shift equilibrium temp calculated for reactor eff. composition.

T<sub>hs</sub> = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* 12.5g of MeOH catalyst in first stage, 12.5g 200-27-2 in second stage.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-2

=====

CATALYST NUMBER : Methanol synthesis cat. / 200-27-2\*      DATE : 9/17/80  
 ATOMIC FORMULA : CuAl<sub>1.21</sub>Zn<sub>1.49</sub> / CuCoTh<sub>1.5</sub>Fe<sub>1.5</sub>Zn<sub>1.125</sub>K<sub>1.11</sub>  
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation (200-27-1)      REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY <sup>(1)</sup>: 1.23 gm/cc      REACTOR TYPE: Berts

TEST NUMBER	1	2	3	4	5
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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10	2.10	2.10
FEED CO <sub>2</sub>	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	225.0	225.0	208.0	208.0	250.0
HOT SPOT, C	225.0	225.0	208.0	208.0	250.0
PRESSURE, psig	910.0	905.0	905.0	905.0	910.0
UHSV, 1/hr/kcm cat.	3632.0	1251.0	673.0	3521.0	3972.0
HOURS on STREAM	3.8	7.7	11.3	14.1	19.4
RPM	1740.0	1735.0	1740.0	1745.0	1715.0

## CONVERSION :

CO to Prods., vol%	28.37	50.71	38.57	16.56	26.72
CO to CO <sub>2</sub> , vol%	5.93	14.89	13.93	.74	9.48
CO, gm mol/hr/kcm cat.	14.80	9.81	4.30	7.40	17.40
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	10.10	5.71	2.45	6.50	8.31

STOICHIOM. H<sub>2</sub>/CO converted

1.50	1.51	1.53	2.18	1.50
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	77.25	64.42	73.22	87.88	53.12
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.20	10.48	4.36	3.76	10.57
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.00	.39	.00	.00	.68
CH <sub>4</sub>	4.96	8.02	6.40	2.82	14.63
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	6.53	9.44	9.12	3.24	13.82
C <sub>4</sub> + HYDROCARBONS	6.17	7.24	6.81	2.30	7.18

APPROACH TO <sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	100.6	90.6	95.1	95.5	103.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* Random mixture of 12.5g Methanol synthesis catalyst and 12.5g 200-27-2

## SUMMARY FOR RUN # 213-4

=====  
 CATALYST NUMBER : 197-85  
 ATOMIC FORMULA :  $CuCoFe_{.1}Th_{.5}Zn_{.125}K_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 9/24/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.04 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

3

4\*

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10	2.10
FEED CO <sub>2</sub>	4.80	4.80	4.80	4.80
AVE. TEMP., C	263.0	263.0	245.0	267.0
HOT SPOT, C	263.0	263.0	245.0	267.0
PRESSURE, psia	910.0	905.0	910.0	920.0
VHSV, 1/hr/kcm cat.	3574.0	1092.0	3262.0	3763.0
HOURS on STREAM	3.7	6.3	11.6	18.1
RPM	1740.0	1735.0	1715.0	1700.0

## CONVERSION :

CO to Prods., vol%	13.68	35.72	4.07	9.11 (11.1 MeOH Conv.)
CO to CO <sub>2</sub> , vol%	4.32	20.18	1.13	4.39 (1.36 MeOH Conv.)
CO, gm mol/hr/kcm cat.	7.60	7.21	2.09	5.06
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	1.91	1.28	.59	.87

STOICHIOM. H<sub>2</sub>/CO converted .91 1.09 1.74 1.45CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	5.13	4.69	8.18	.00
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	22.37	20.34	22.12	18.37
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	5.53	2.82	5.37	1.63
CH <sub>4</sub>	22.89	34.59	28.64	44.89
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	29.21	25.98	27.11	26.37
C <sub>4</sub> + HYDROCARBONS	14.87	11.58	8.57	8.74

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00 .00 .00

CARBON ACCOUNTABILITY, % (4) 103.0 102.9 105.9 97.9

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

\* 7 mole % MeOH added to feed gas

## SUMMARY FOR RUN # 213-9

=====  
 CATALYST NUMBER : 197-84  
 ATOMIC FORMULA : CuCoRu<sub>1K.11</sub>  
 CATALYST SUPPORT : NONE

DATE : 10/6/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.67 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1                    2                    3

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	11.90	11.90	11.90
AVE. TEMP., C	263.0	264.0	280.0
HOT SPOT, C	264.0	265.0	280.0
PRESSURE, psia	930.0	925.0	925.0
VHSV, 1/hr/k <sub>sm</sub> cat.	2954.0	917.0	3357.0
HOURS on STREAM	4.9	6.7	11.6
RPM	1690.0	1680.0	1700.0

## CONVERSION :

CO to Prods., vol%	3.66	10.91	5.48
CO to CO2, vol%	1.84	8.99	3.92
CO, gm mol/hr/k <sub>sm</sub> cat.	1.77	1.99	3.36
STY of oxoates <sup>(2)</sup>			
gm mol/hr/k <sub>sm</sub> cat.	.40	.30	.59

STOICHIOM. H2/CO converted	1.41	1.18	1.57
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CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	3.45	3.10	3.09
C2-C6 ALCOHOLS	1.95	4.38	4.63
C2-C6 ALD.&ESTERS	28.53	20.06	22.28
CH4	32.88	33.37	35.31
C2-C3 HYDROCARBONS	23.27	25.71	24.68
C4+ HYDROCARBONS	9.91	13.49	10.11

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	96.0	90.8	85.4
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxoates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-11

CATALYST NUMBER : 200-78-1

DATE : 10/9/80

ATOMIC FORMULA :  $\text{CuCo}_{.5}\text{Al}_{.18}\text{Zn}_{.33}\text{K}_{.05}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Detergent Dispersion

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.3 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

2

3

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	11.50	11.50	11.50
AVE. TEMP., C	250.0	271.0	283.0
HOT SPOT, C	251.0	271.0	284.0
PRESSURE, psig	880.0	900.0	900.0
VHSV, 1/hr/kcm cat.	3550.0	3322.0	3404.0
HOURS on STREAM	6.1	9.2	14.9
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	2.30	5.56	9.38
CO to CO2, vol%	.30	.14	.72
CO, gm mol/hr/kcm cat.	.99	2.06	3.82
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.24	.68	1.30

STOICHIOM. H2/CO converted	4.73	1.62	.87
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	7.35	8.61	7.64
C2-C6 ALCOHOLS	13.01	20.90	24.11
C2-C6 ALD.&ESTERS	7.35	4.51	4.84
CH4	36.32	35.96	33.48
C2-C3 HYDROCARBONS	24.10	23.57	23.04
C4+ HYDROCARBONS	11.65	6.45	6.89

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	76.4	100.4	94.2
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 213-13

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CATALYST NUMBER : 200-76 DATE : 10/14/80  
 ATOMIC FORMULA :  $CuCr_{.8}CoK_{.09}$   
 CATALYST SUPPORT : NONE

PREP METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup>: 1.16 gm/cc REACTOR TYPE: Bertw

TEST NUMBER 1      2      3      4      5      6

-----

TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	1.98	1.98	1.98	1.98	1.98	1.98
FEED CO2	11.52	11.52	11.52	11.52	11.52	11.52
AVE. TEMP., C	266.0	267.0	280.0	280.0	257.0	257.0
HOT SPOT, C	266.0	267.0	280.0	280.0	257.0	258.0
PRESSURE, Psia	930.0	940.0	930.0	930.0	930.0	930.0
UHSV, 1/hr/ksm cat.	3567.0	1050.0	4147.0	8413.0	3523.0	1036.0
HOURS on STREAM	4.2	7.4	17.3	13.7	19.3	20.9
RPM	1640.0	1640.0	1640.0	1645.0	1630.0	1635.0

CONVERSION :

CO to Prods., vol%	13.12	29.58	8.37	5.13	3.80	12.77
CO to CO2, vol%	2.28	11.72	3.13	1.67	.00	3.23
CO, gm mol/hr/ksm cat.	5.86	4.63	5.02	6.26	1.45	1.80
STY of oxysenates <sup>(2)</sup>						
gm mol/hr/ksm cat.	1.28	.59	.86	1.03	.36	.35

STOICHIOM. H2/CO converted 1.44    1.19    2.25    71.78    1.23    1.52

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	4.93	3.91	8.93	9.67	11.30	10.03
C2-C6 ALCOHOLS	19.37	13.54	14.29	11.39	12.70	13.91
C2-C6 ALD.&ESTERS	1.41	.42	.41	.79	1.00	.50
CH4	31.92	37.97	49.31	46.75	46.10	46.49
C2-C3 HYDROCARBONS	25.12	26.39	21.02	22.91	21.90	21.88
C4+ HYDROCARBONS	17.25	17.87	6.04	8.48	7.00	7.39

APPROACH TO <sup>(3)</sup>

WGS Equilibrium, C .00    .00    .00    .00    .00    .00

CARBON ACCOUNTABILITY, % <sup>(4)</sup> 91.1    108.1    135.5    95.7    100.0    95.2

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

    where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-14

CHEM SYSTEMS INC.

CATALYST NUMBER : 200-76

DATE : 10/23/80

ATOMIC FORMULA :  $\text{CuCr}_{.8}\text{CoK}_{.09}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.14 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER 1 2 3 4 5 6

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.06	2.06	2.06	2.06	2.06	2.06
FEED CO <sub>2</sub>	11.70	11.70	11.70	11.70	11.70	11.70
AVE. TEMP., C	257.0	259.0	273.0	274.0	292.0	295.0
HOT SPOT, C	257.0	259.0	273.0	278.0	292.0	295.0
PRESSURE, Psig	925.0	900.0	935.0	930.0	930.0	930.0
WHSV, 1/hr/k <sub>cat</sub>	4021.0	968.0	3516.0	1007.0	3290.0	3589.0
HOURS on STREAM	12.9	14.6	17.8	20.8	76.9	100.0
RPM	.0	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	3.54	8.75	3.93	10.51	6.46	8.23
CO to CO <sub>2</sub> , vol%	.66	3.05	.97	3.79	.54	1.47
CO, gm mol/hr/k <sub>cat</sub>	1.86	1.26	1.92	1.61	2.48	3.75
STY of oxygenates <sup>(2)</sup> gm mol/hr/k <sub>cat</sub>	.65	.19	.43	.29	.80	.99

STOICHIOM. H <sub>2</sub> /CO converted	13.86	1.35	1.60	1.36	2.07	1.86
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	8.06	7.82	10.85	8.71	17.33	14.84
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	28.79	11.06	15.33	14.69	16.47	15.43
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	4.27	2.02	1.99	1.22	.98	.71
CH <sub>4</sub>	34.12	45.86	46.37	48.98	44.96	47.83
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	16.59	24.01	19.32	20.41	17.66	18.61
C <sub>4</sub> + HYDROCARBONS	8.18	8.63	6.23	5.99	2.60	2.47

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	66.6	88.4	98.2	104.3	101.5	98.3
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $\text{WHSV}/22.4 * \% \text{CO in feed}/100 * \% \text{CO conv.}/100 * \% \text{Sel to Oxygenates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-14

=====

CATALYST NUMBER : 200-76  
 ATOMIC FORMULA :  $CuCr_{.8}CoK_{.09}$   
 CATALYST SUPPORT : NONE

DATE : 10/23/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup> : 1.14 gm/cc  
 TEST NUMBER 7

REACTOR TYPE: Plus Flow

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.06
FEED CO <sub>2</sub>	11.70
AVE. TEMP., C	297.0
HOT SPOT, C	297.0
PRESSURE, psig	930.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3496.0
HOURS on STREAM	122.8
RPM	.0

## CONVERSION :

CO to Prods., vol%	7.52
CO to CO <sub>2</sub> , vol%	2.78
CO, gm mol/hr/k <sub>sm</sub> cat.	3.90
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/k <sub>sm</sub> cat.	.90

STOICHIOM. H<sub>2</sub>/CO converted 2.05CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	13.56
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	16.30
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	1.64
CH <sub>4</sub>	44.79
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	17.95
C <sub>4</sub> + HYDROCARBONS	5.75

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C .00

CARBON ACCOUNTABILITY, % (4) 118.2

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



SUMMARY FOR RUN # 213-16

=====  
 CATALYST NUMBER : 200-78-2 DATE : 10/27/80  
 ATOMIC FORMULA :  $\text{CuCo}_{.5}\text{Al}_{.18}\text{Zn}_{.33}$   
 CATALYST SUPPORT : NONE

PREP METHOD: Detergent Dispersion REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup>: 1.08 gm/cc REACTOR TYPE: Bertu  
 TEST NUMBER 1

-----  
 TEST CONDITIONS :

FEED H2/CO RATIO 2.00  
 FEED CO2 10.00  
 AVE. TEMP., C 270.0  
 HOT SPOT, C 272.0  
 PRESSURE, psig 870.0  
 VHSV, 1/hr/ksm cat. 4628.0  
 HOURS on STREAM 7.4  
 RPM 1510.0

CONVERSION :

CO to Prods., vol% 9.54  
 CO to CO2, vol% 2.86  
 CO, gm mol/hr/ksm cat. 6.16  
 STY of oxygenates <sup>(2)</sup>  
 gm mol/hr/ksm cat. .52

STOICHIOM. H2/CO converted 1.93

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH 2.34  
 C2-C6 ALCOHOLS 8.32  
 C2-C6 ALD. ESTERS .26  
 CH4 45.77  
 C2-C3 HYDROCARBONS 30.56  
 C4+ HYDROCARBONS 12.74

APPROACH TO <sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup> 113.4  
 -----

- (1) Fresh, non-reduced catalyst.  
 (2) Space Time Yield (STY) =  $\text{VHSV}/22.4 * \text{ZCO in feed}/100 * \text{ZCO conv.}/100 * \text{ZSel to Oxygenates}/100$ .  
 (3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.  
 (4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-19

-----  
 CATALYST NUMBER : 200-89-1  
 ATOMIC FORMULA :  $\text{CuCr}_{.8}\text{Co}_{.3}\text{K}_{.09}$   
 CATALYST SUPPORT : NONE

DATE : 10/30/80

PREP METHOD: Evaporation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup>: 1.47 gm/cc  
 TEST NUMBER 1

REACTOR TYPE: Bertz

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00
FEED CO <sub>2</sub>	12.00
AVE. TEMP., C	282.0
HOT SPOT, C	283.0
PRESSURE, psig	915.0
VHSV, 1/hr/k <sub>sm</sub> cat.	876.0
HOURS on STREAM	6.9
RPM	1590.0

## CONVERSION :

CO to Prods., vol%	2.88
CO to CO <sub>2</sub> , vol%	.02
CO, gm mol/hr/k <sub>sm</sub> cat.	.27
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.18

STOICHIOM. H<sub>2</sub>/CO converted 2.41CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	60.83
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.44
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00
CH <sub>4</sub>	22.96
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	8.06
C <sub>4</sub> + HYDROCARBONS	2.62

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 48.4

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-20

=====

CATALYST NUMBER : 200-93 DATE : 11/5/80

ATOMIC FORMULA :  $CuCo_{.13}Al_{.18}Zn_{.33}K_{.05}$

CATALYST SUPPORT : NONE

PREP METHOD: Cobalt Carbonyl Impregnation REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY <sup>(1)</sup> : 1.04 gm/cc REACTOR TYPE: Plug Flow

TEST NUMBER 1 2 3 4

-----

## TEST CONDITIONS :

	1	2	3	4
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.90	11.90	11.90	11.90
AVE. TEMP., C	307.0	304.0	297.0	303.0
HOT SPOT, C	310.0	305.0	298.0	304.0
PRESSURE, psia	950.0	950.0	9500.0	950.0
VHSV, 1/hr/kcm cat.	3531.0	3379.0	1010.0	6995.0
HOURS on STREAM	5.2	13.0	18.0	20.5
RPM	.0	.0	.0	.0

## CONVERSION :

	1	2	3	4
CO to Prods., vol%	14.26	9.63	17.54	6.25
CO to CO <sub>2</sub> , vol%	4.34	1.97	8.66	.55
CO, gm mol/hr/kcm cat.	7.34	4.33	2.84	5.08
STY of oxygenates <sup>(2)</sup>				
gm mol/hr/kcm cat.	.97	1.42	.55	1.60

STOICHIOM. H<sub>2</sub>/CO converted 1.41 1.65 1.38 1.63

CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

	1	2	3	4
CH <sub>3</sub> OH	3.65	17.83	15.84	17.85
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	1.17	10.97	6.42	10.77
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	12.39	10.85	6.87	5.55
CH <sub>4</sub>	41.08	32.78	41.53	36.24
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	26.74	18.44	22.11	20.89
C <sub>4</sub> + HYDROCARBONS	14.87	9.04	7.32	8.71

APPROACH TO <sup>(3)</sup>

WGS Equilibrium, C .00 .00 .00 .00

CARBON ACCOUNTABILITY, % (4) 95.1 106.3 102.8 82.5

-----

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{ea} - T_{hs}$   
 where  $T_{ea}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-21

CATALYST NUMBER : 200-96

DATE : 11/8/80

ATOMIC FORMULA :  $\text{CuCo}_{.01}\text{Al}_{.18}\text{Zn}_{.33}\text{K}_{.05}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Cobalt Carbonyl Impregnation      REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.08 gm/cc

REACTOR TYPE: Bertw

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10
FEED CO <sub>2</sub>	12.40	12.40
AVE. TEMP., C	298.0	298.0
HOT SPOT, C	299.0	298.0
PRESSURE, psia	920.0	920.0
VHSV, 1/hr/kcm cat.	3361.0	877.0
HOURS on STREAM	6.7	13.1
RPM	1590.0	1540.0

## CONVERSION :

CO to Prods., vol%	2.20	5.40
CO to CO <sub>2</sub> , vol%	.00	.00
CO, gm mol/hr/kcm cat.	.82	.28
STY of oxysenates <sup>(2)</sup>		
gm mol/hr/kcm cat.	.70	.25

STOICHIOM. H<sub>2</sub>/CO converted      3.76      2.02CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	83.80	85.30
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	2.00	2.30
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00
CH <sub>4</sub>	11.40	9.10
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	1.80	2.10
C <sub>4</sub> + HYDROCARBONS	.80	1.20

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)      97.8      91.9

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-22

-----  
 CATALYST NUMBER : 200-88-1  
 ATOMIC FORMULA :  $Cu_{.5}Co_{.2}ZnK_{.05}$   
 CATALYST SUPPORT : NONE

DATE : 11/10/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : 1.7 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.05
FEED CO <sub>2</sub>	11.70
Ave. TEMP., C	272.0
HOT SPOT, C	273.0
PRESSURE, psia	950.0
VHSV, 1/hr/kcm cat.	3122.0
HOURS on STREAM	3.5
RPM	.0

## CONVERSION :

CO to Prods., vol%	5.26
CO to CO <sub>2</sub> , vol%	1.24
CO, gm mol/hr/kcm cat.	2.17
STY of oxygenates <sup>(2)</sup>	
gm mol/hr/kcm cat.	.52

STOICHIOM. H<sub>2</sub>/CO converted 1.64CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	3.96
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.94
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	20.16
CH <sub>4</sub>	27.70
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	19.54
C <sub>4</sub> + HYDROCARBONS	11.01

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00

CARBON ACCOUNTABILITY, % (4) 88.3

-----  
 (1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-23

-----  
 CATALYST NUMBER : 200-83-1  
 ATOMIC FORMULA : CuCoK<sub>11</sub>  
 CATALYST SUPPORT : NONE

DATE : 11/11/80

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.22 gm/cc  
 TEST NUMBER

REACTOR TYPE: Bertz

1 2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	12.10	12.10
AVE. TEMP., C	290.0	288.0
HOT SPOT, C	290.0	289.0
PRESSURE, psia	920.0	920.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3778.0	6964.0
HOURS on STREAM	6.4	8.4
RPM	1505.0	1505.0

## CONVERSION :

CO to Prods., vol%	33.65	14.48
CO to CO <sub>2</sub> , vol%	20.25	7.12
CO, gm mol/hr/k <sub>sm</sub> cat.	21.90	16.20
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	3.47	3.52

STOICHIOM. H <sub>2</sub> /CO converted	1.27	1.27
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	3.68	4.33
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	15.70	10.89
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	5.93	17.16
CH <sub>4</sub>	40.68	33.86
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	23.86	22.23
C <sub>4</sub> + HYDROCARBONS	10.25	11.64

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	103.3	103.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* ZCO in feed/100 \* ZCO conv./100 \* ZSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-24

CATALYST NUMBER : 200-99

DATE : 11/12/80

ATOMIC FORMULA :  $\text{CuCo}_{.25}\text{Al}_{.18}\text{Zn}_{.33}\text{K}_{.05}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Cobalt Carbonyl Impregnation      REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : .93 gm/cc

REACTOR TYPE: Bertu

TEST NUMBER

1

2

3

4

5

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10	2.10	2.10
FEED CO <sub>2</sub>	12.10	12.10	12.10	12.10	12.10
AVE. TEMP., C	273.0	273.0	302.0	302.0	302.0
HOT SPOT, C	273.0	273.0	302.0	302.0	302.0
PRESSURE, psia	920.0	920.0	915.0	915.0	915.0
VHSV, 1/hr/k <sub>sm</sub> cat.	3220.0	3220.0	3760.0	3760.0	2050.0
HOURS on STREAM	4.5	6.0	10.5	10.5	12.5
RPM	1480.0	1490.0	1500.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	7.49	5.74	5.80	5.74	11.00
CO to CO <sub>2</sub> , vol%	2.61	2.56	1.30	1.36	3.80
CO, gm mol/hr/k <sub>sm</sub> cat.	3.50	2.90	3.00	2.70	3.40
STY of oxigenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	1.05	.78	1.09	.96	1.07

STOICHIOM. H <sub>2</sub> /CO converted	1.39	1.31	2.09	2.23	1.61
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	6.88	9.54	22.28	23.12	21.40
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	29.41	27.60	19.95	19.78	19.25
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	3.78	1.59	1.35	.74	.67
CH <sub>4</sub>	21.58	24.71	33.41	34.25	35.53
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	19.56	19.65	16.03	15.45	16.82
C <sub>4</sub> + HYDROCARBONS	18.89	16.91	6.98	6.06	6.33

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, % (4)	103.1	101.8	135.6	127.9	107.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxigenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 213-25

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CATALYST NUMBER : 200-79 DATE : 11/20/80  
 ATOMIC FORMULA : CuCoZn<sub>5</sub>K<sub>11</sub>  
 CATALYST SUPPORT : NONE

PREF METHOD: Evaporation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup> : 0 gm/cc REACTOR TYPE: Plus Flow

TEST NUMBER 1      2      3      4

-----

TEST CONDITIONS :

	1	2	3	4
FEED H2/CO RATIO	2.10	2.10	2.10	2.10
FEED CO2	12.10	12.10	12.10	12.10
AVE. TEMP., C	262.0	298.0	287.0	287.0
HOT SPOT, C	264.0	300.0	288.0	288.0
PRESSURE, psia	945.0	950.0	950.0	950.0
UHSV, 1/hr/kcm cat.	2820.0	2820.0	3100.0	3100.0
HOURS on STREAM	3.3	5.2	7.7	9.2
RPM	.0	.0	.0	.0

CONVERSION :

	1	2	3	4
CO to Prods., vol%	4.47	19.11	10.79	11.13
CO to CO2, vol%	2.03	14.39	6.61	6.07
CO, gm mol/hr/kcm cat.	2.00	10.40	5.90	5.80
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.39	1.09	.97	1.39

STOICHIOM. H2/CO converted 2.30    1.19    1.33    1.23

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

	1	2	3	4
CH3OH	3.49	2.28	4.52	8.50
C2-C6 ALCOHOLS	5.23	7.36	8.39	14.37
C2-C6 ALD. & ESTERS	20.77	8.76	13.55	13.91
CH4	32.54	43.64	30.48	29.52
C2-C3 HYDROCARBONS	22.08	25.94	27.74	21.02
C4+ HYDROCARBONS	15.69	11.92	15.32	12.67

APPROACH TO <sup>(3)</sup>  
WGS Equilibrium, C

	1	2	3	4
WGS Equilibrium, C	.00	.00	.00	.00

CARBON ACCOUNTABILITY, % <sup>(4)</sup> 105.7    92.0    105.6    114.2

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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-26

=====  
 CATALYST NUMBER : 217-3  
 ATOMIC FORMULA :  $\text{CuCo}_{.3}\text{K}_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 11/26/80

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 0 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10	2.10
FEED CO <sub>2</sub>	12.00	12.00	12.00	12.00
AVE. TEMP., C	267.0	286.0	293.0	293.0
HOT SPOT, C	268.0	287.0	294.0	294.0
PRESSURE, psia	925.0	925.0	950.0	950.0
VHSV, 1/hr/kcm cat.	3950.0	3950.0	3975.0	3975.0
HOURS on STREAM	2.0	3.6	8.0	9.2
RPM	1500.0	1490.0	1490.0	1500.0

## CONVERSION :

CO to Prods., vol%	1.62	6.33	8.25	8.51
CO to CO <sub>2</sub> , vol%	1.88	4.68	4.55	3.79
CO, gm mol/hr/kcm cat.	1.50	4.80	5.50	5.30
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	.28	.99	1.26	1.33

STOICHIOM. H <sub>2</sub> /CO converted	3.11	1.70	1.67	1.49
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	4.31	4.87	6.36	6.65
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	4.53	6.96	10.71	11.56
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	30.17	24.00	17.54	17.34
CH <sub>4</sub>	29.96	32.52	33.53	32.80
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	17.03	19.30	20.02	19.51
C <sub>4</sub> + HYDROCARBONS	14.01	12.35	11.64	12.14

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	217.0	127.9	113.7	105.1
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-28 CHEM SYSTEMS INC.

CATALYST NUMBER : 200-86  
 ATOMIC FORMULA :  $\text{CuCoZn}_{.5}^{\text{K}}.11$   
 CATALYST SUPPORT : NONE

DATE : 12/12/80

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 0 gm/cc

REACTOR TYPE: Plug Flow

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10
FEED CO <sub>2</sub>	12.00	12.00
AVE. TEMP., C	281.0	302.0
HOT SPOT, C	282.0	302.0
PRESSURE, psig	960.0	960.0
UHSV, 1/hr/k <sub>sm</sub> cat.	4740.0	4740.0
HOURS on STREAM	3.7	4.5
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	1.49	3.16
CO to CO <sub>2</sub> , vol%	.41	.74
CO, gm mol/hr/k <sub>sm</sub> cat.	.97	2.00
STY of oxogenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	.17	.32

STOICHIOM. H <sub>2</sub> /CO converted	3.12	4.45
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	5.60	4.94
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.85	5.92
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	11.19	8.76
CH <sub>4</sub>	39.05	39.61
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	24.55	25.91
C <sub>4</sub> + HYDROCARBONS	13.86	15.05

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	133.0	144.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxogenates/100.

(3) Defined as  $T = T_{ea} - T_{hs}$   
 where  $T_{ea}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-29

CHEM SYSTEMS INC.

CATALYST NUMBER : 200-91

DATE : 12/10/80

ATOMIC FORMULA :  $CuCoFe_{.1}Th_{.5}Zn_{.125}K_{.11}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup>: 1.2 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

3

4

5

## TEST CONDITIONS :

FEED H2/CO RATIO	2.10	2.10	2.10	2.10	2.10
FEED CO2	12.00	12.00	12.00	12.00	12.00
Ave. TEMP., C	263.0	252.0	222.0	232.0	245.0
HOT SPOT, C	264.0	253.0	223.0	233.0	246.0
PRESSURE, psig	920.0	920.0	945.0	945.0	945.0
VHSV, 1/hr/k <sub>cat</sub>	3800.0	3250.0	3780.0	3950.0	7670.0
HOURS on STREAM	2.0	3.3	8.0	9.5	10.5
RPM	1480.0	1480.0	1510.0	1500.0	1490.0

## CONVERSION :

CO to Prods., vol%	75.37	71.22	7.36	10.87	12.00
CO to CO2, vol%	17.33	14.78	1.84	3.93	4.00
CO, $\mu$ m mol/hr/k <sub>cat</sub>	37.40	30.00	3.77	6.34	13.30

STY of oxygenates<sup>(2)</sup>

$\mu$ m mol/hr/k <sub>cat</sub>	.64	1.53	.87	1.30	2.68
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STOICHIOM. H2/CO converted

	1.78	1.68	2.99	2.55	2.37
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	.00	.24	5.12	5.04	5.20
C2-C6 ALCOHOLS	.98	4.47	20.24	19.88	18.94
C2-C6 ALD.&ESTERS	1.11	1.45	3.37	3.00	2.67
CH4	28.91	25.48	25.74	26.41	29.08
C2-C3 HYDROCARBONS	33.83	33.21	28.62	27.91	27.08
C4+ HYDROCARBONS	35.18	35.26	17.00	17.97	16.94

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

	.00	.00	.00	.00	.00
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CARBON ACCOUNTABILITY, %<sup>(4)</sup>

	120.1	138.4	94.7	100.9	108.3
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-31

=====  
 CATALYST NUMBER : 217-5  
 ATOMIC FORMULA :  $CuCo_{3K}.077$   
 CATALYST SUPPORT : NONE

DATE : 12/12/80

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.2 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berts

1            2            3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10	2.10
FEED CO <sub>2</sub>	12.00	12.00	12.00
AVE. TEMP., C	279.0	289.0	298.0
HOT SPOT, C	280.0	290.0	299.0
PRESSURE, psig	920.0	920.0	920.0
VHSV, 1/hr/kcm cat.	3540.0	3660.0	3660.0
HOURS on STREAM	4.3	5.5	6.5
RPM	1500.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	8.62	11.91	16.46
CO to CO <sub>2</sub> , vol%	3.48	5.79	9.74
CO, gm mol/hr/kcm cat.	4.69	7.09	10.50
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	1.25	1.74	2.13

STOICHIOM. H <sub>2</sub> /CO converted	1.22	1.42	1.20
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	4.21	4.61	4.94
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	6.04	10.55	13.69
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	27.24	21.25	13.69
CH <sub>4</sub>	29.76	31.95	34.55
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	19.23	19.32	21.17
C <sub>4</sub> + HYDROCARBONS	13.62	12.63	12.26

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	93.9	100.5	107.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-32

CATALYST NUMBER : 217-6

DATE : 12/16/80

ATOMIC FORMULA :  $\text{CuCo}_{.07}\text{Al}_{.18}\text{Zn}_{.33}\text{K}_{.05}$ 

CATALYST SUPPORT : NONE

PREP METHOD: Cobalt Carbonyl Impregnation      REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : .96 gm/cc

REACTOR TYPE: Berts

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.68	11.68	11.68	11.68
AVE. TEMP., C	271.0	273.0	300.0	300.0
HOT SPOT, C	272.0	273.0	301.0	301.0
PRESSURE, psig	950.0	950.0	950.0	950.0
WHSV, 1/hr/k <sub>sm</sub> cat.	3787.0	910.0	3605.0	3605.0
HOURS on STREAM	4.3	6.7	10.7	10.7
RPM	1500.0	1500.0	1490.0	1500.0

## CONVERSION :

CO to Prods., vol%	1.90	5.19	3.10	8.34
CO to CO <sub>2</sub> , vol%	.00	1.01	.00	1.26
CO, gm mol/hr/k <sub>sm</sub> cat.	.78	.61	1.38	1.05
STY of oxygenates <sup>(2)</sup>				
gm mol/hr/k <sub>sm</sub> cat.	.38	.29	.86	.51

STOICHIOM. H <sub>2</sub> /CO converted	7.65	2.61	3.80	2.04
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	40.50	40.02	51.90	44.54
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	8.70	16.01	10.50	11.03
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.00	.00	.00	.00
CH <sub>4</sub>	32.30	16.13	24.90	26.13
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	16.40	16.13	10.00	13.12
C <sub>4</sub> + HYDROCARBONS	2.00	2.51	2.70	5.06

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	84.1	100.1	89.2	108.3
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $\text{WHSV}/22.4 * \% \text{CO in feed}/100 * \% \text{CO conv.}/100 * \% \text{Sel to Oxygenates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-33

CATALYST NUMBER : 217-1  
 ATOMIC FORMULA :  $\text{CuAl}_{.18}\text{Zn}_{.33}\text{K}_{.05}$   
 CATALYST SUPPORT : NONE

DATE : 1/6/81

PREP METHOD: Impregnation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.36 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	11.94	11.94
AVE. TEMP., C	270.0	297.0
HOT SPOT, C	273.0	299.0
PRESSURE, psid	960.0	965.0
VHSV, 1/hr/k <sub>sm</sub> cat.	2869.0	2670.0
HOURS on STREAM	2.0	3.3
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	29.52	20.25
CO to CO <sub>2</sub> , vol%	.18	.65
CO, gm mol/hr/k <sub>sm</sub> cat.	9.30	6.10
STY of oxigenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	9.10	3.70

STOICHIOM. H <sub>2</sub> /CO converted	2.12	2.12
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	97.28	92.67
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.80	2.68
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.72
CH <sub>4</sub>	1.11	1.65
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	.70	.52
C <sub>4</sub> + HYDROCARBONS	.60	1.75

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C	.00	.00
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CARBON ACCOUNTABILITY, % <sup>(4)</sup>	98.3	104.2
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxigenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-34

CHEM SYSTEMS INC

=====  
 CATALYST NUMBER : 217-7-1  
 ATOMIC FORMULA : CuCoK<sub>0.05</sub>  
 CATALYST SUPPORT : NONE

DATE : 12/22/80

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 0 gm/cc  
 TEST NUMBER

REACTOR TYPE: Bertu

1                    2                    3                    4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.80	11.80	11.80	11.80
AVE. TEMP., C	272.0	273.0	281.0	291.0
HOT SPOT, C	273.0	274.0	281.0	292.0
PRESSURE, psig	955.0	955.0	955.0	905.0
VHSV, 1/hr/ksm cat.	3630.0	1139.0	8538.0	6760.0
HOURS on STREAM	4.9	6.8	12.3	14.6
RPM	1700.0	1770.0	1730.0	1750.0

## CONVERSION :

CO to Prods., vol%	11.87	37.58	4.49	7.63
CO to CO <sub>2</sub> , vol%	5.13	23.82	1.41	3.67
CO, gm mol/hr/ksm cat.	6.74	7.64	5.57	8.35
STY of oxysenates <sup>(2)</sup> gm mol/hr/ksm cat.	1.72	1.34	1.59	1.90

STOICHIOM. H <sub>2</sub> /CO converted	1.29	1.07	1.92	1.24
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	5.01	4.08	4.20	5.04
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	9.31	17.97	5.65	9.78
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	22.21	6.54	27.60	18.52
CH <sub>4</sub>	30.80	31.37	32.72	36.74
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	21.35	27.12	18.79	21.18
C <sub>4</sub> + HYDROCARBONS	11.32	12.91	11.04	8.44

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	98.0	98.6	102.6	110.9
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=====  
 (1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{wg} - T_{hs}$   
 where  $T_{wg}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-36

CATALYST NUMBER : 200-83-2

DATE : 1/7/81

ATOMIC FORMULA : CuCo

CATALYST SUPPORT : NONE

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 0 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1 2 3 4 5 6

## TEST CONDITIONS :

	1	2	3	4	5	6
FEED H2/CO RATIO	2.00	2.00	2.00	2.00	2.00	2.00
FEED CO2	12.00	12.00	12.00	12.00	12.00	12.00
AVE. TEMP., C	271.0	271.0	291.0	291.0	290.0	251.0
HOT SPOT, C	271.0	271.0	291.0	291.0	290.0	251.0
PRESSURE, Psia	908.0	907.0	908.0	910.0	910.0	910.0
UHSV, 1/hr/kgm cat.	1930.0	3780.0	3565.0	5000.0	5060.0	2040.0
HOURS on STREAM	2.5	4.0	5.7	8.8	10.3	11.8
RPM	1510.0	1510.0	1520.0	1490.0	1480.0	1520.0

## CONVERSION :

CO to Prods., vol%	23.00	12.58	43.49	18.19	17.14	2.95
CO to CO2, vol%	19.20	10.62	29.51	10.11	9.56	3.55
CO, gm mol/hr/kgm cat.	9.10	9.80	29.20	15.90	15.20	1.49
STY of oxysenates <sup>(2)</sup> gm mol/hr/kgm cat.	1.23	1.90	3.33	2.96	2.81	.37

STOICHIOM. H2/CO converted

.95 1.02 1.07 1.10 1.61 1.61

## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	3.85	3.69	2.18	4.51	4.36	5.42
C2-C6 ALCOHOLS	9.36	16.41	13.76	11.05	10.59	4.23
C2-C6 ALD. & ESTERS	12.29	15.49	3.19	13.38	13.86	28.70
CH4	42.94	30.43	46.99	36.56	35.83	28.17
C2-C3 HYDROCARBONS	21.10	21.21	24.00	23.81	23.68	20.22
C4+ HYDROCARBONS	10.46	13.28	10.07	10.89	11.68	13.24

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	89.8	119.4	101.1	108.7	110.2	166.5
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



## SUMMARY FOR RUN # 213-38

=====

CATALYST NUMBER : 217-15	DATE : 1/16/81
ATOMIC FORMULA : CoK <sub>11</sub>	
CATALYST SUPPORT : 50.0% Al <sub>2</sub> O <sub>3</sub>	

PREP METHOD: Coprecipitation Impregnation     REDUCTION: in Situ Reduction

BULK DENSITY <sup>(1)</sup> : 1.16 gm/cc	REACTOR TYPE: Bertu
TEST NUMBER	1            2            3

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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	1.96	1.96	1.96
FEED CO <sub>2</sub>	11.92	11.92	11.92
AVE. TEMP., C	249.0	268.0	287.0
HOT SPOT, C	250.0	267.0	270.0
PRESSURE, psig	915.0	915.0	915.0
VHSV, 1/hr/k <sub>sm</sub> cat.	2080.0	4070.0	7080.0
HOURS on STREAM	1.5	3.0	5.0
RPM	1500.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	14.79	17.55	28.21
CO to CO <sub>2</sub> , vol%	9.91	9.15	14.89
CO, gm mol/hr/k <sub>sm</sub> cat.	5.57	11.80	33.10
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/k <sub>sm</sub> cat.	1.02	2.61	5.96

STOICHIOM. H <sub>2</sub> /CO converted	1.08	.88	.99
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.33	.30	.31
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	1.84	3.35	4.43
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	28.40	29.97	22.77
CH <sub>4</sub>	23.56	25.41	16.81
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	22.22	20.84	34.38
C <sub>4</sub> + HYDROCARBONS	23.56	19.93	16.81

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	87.7	100.6	115.8
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-39

=====

CATALYST NUMBER : 217-8 DATE : 1/19/81  
 ATOMIC FORMULA :  $\text{CuCo}_{.13}\text{Al}_{.18}\text{Zn}_{.33}\text{K}_{.05}$   
 CATALYST SUPPORT : NONE

PREP. METHOD: Cobalt Carbonyl Impregnation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.25 gm/cc REACTOR TYPE: Plus Flow

TEST NUMBER 1 2 3

-----

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00	2.00
FEED CO2	11.71	11.71	11.71
AVE. TEMP., C	270.0	302.0	302.0
HOT SPOT, C	271.0	303.0	303.0
PRESSURE, psig	955.0	955.0	965.0
UHSV, 1/hr/kcm cat.	2660.0	2660.0	5170.0
HOURS on STREAM	1.1	2.7	4.1
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	3.27	9.08	2.77
CO to CO2, vol%	5.73	1.82	.13
CO, gm mol/hr/kcm cat.	2.58	3.13	.82
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	.70	.78	.62

STOICHIOM. H2/CO converted 1.74 1.77 4.23

## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	3.30	9.73	15.20
C2-C6 ALCOHOLS	21.19	20.89	20.86
C2-C6 ALD. & ESTERS	2.75	2.04	3.98
CH4	27.80	32.66	33.23
C2-C3 HYDROCARBONS	23.67	20.29	17.61
C4+ HYDROCARBONS	21.19	14.29	9.12

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, Z<sup>(4)</sup> 187.0 80.4 140.5

-----

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* ZCO in feed/100 \* ZCO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-40

=====  
 CATALYST NUMBER : 200-81-1  
 ATOMIC FORMULA :  $\text{CuCoTh}_{.5}\text{K}_{.11}$   
 CATALYST SUPPORT : NONE

DATE : 1/22/81

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.14 gm/cc

REACTOR TYPE: Plug Flow

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.07	2.07
FEED CO <sub>2</sub>	11.41	11.41
AVE. TEMP., C	255.0	272.0
HOT SPOT, C	256.0	273.0
PRESSURE, psig	965.0	960.0
VHSV, 1/hr/kcm cat.	4340.0	4450.0
HOURS on STREAM	1.1	2.5
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	4.91	10.19
CO to CO <sub>2</sub> , vol%	.69	.71
CO, gm mol/hr/kcm cat.	2.60	5.14
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.50	1.09

STOICHIOM. H<sub>2</sub>/CO converted 2.81 2.39CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	4.68	5.35
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	12.89	14.33
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	4.45	3.10
CH <sub>4</sub>	36.95	39.57
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	25.55	23.74
C <sub>4</sub> + HYDROCARBONS	15.28	13.80

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4) 80.3 78.3

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-41

-----  
 CATALYST NUMBER : 217-16 DATE : 1/23/81  
 ATOMIC FORMULA : CoK<sub>0.34</sub>  
 CATALYST SUPPORT : 50.0% Al<sub>2</sub>O<sub>3</sub>

FREP METHOD: Coprecipitation Impregnation REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.19 gm/cc REACTOR TYPE: Berty  
 TEST NUMBER 1 2 3  
 -----

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.02	2.02	2.02
FEED CO <sub>2</sub>	11.24	11.24	11.24
Ave. TEMP., C	269.0	279.0	289.0
HOT SPOT, C	269.0	279.0	289.0
PRESSURE, psig	915.0	918.0	918.0
UHSV, 1/hr/k <sub>sm</sub> cat.	3700.0	3720.0	6980.0
HOURS on STREAM	1.1	3.1	4.0
RPM	1480.0	1490.0	1510.0

## CONVERSION :

CO to Prods., vol%	9.73	15.20	13.41
CO to CO <sub>2</sub> , vol%	6.97	8.10	6.99
CO, gm mol/hr/k <sub>sm</sub> cat.	6.50	9.10	15.00
STY of oxoacetates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	1.16	1.64	2.54

STOICHIOM. H <sub>2</sub> /CO converted	1.22	1.22	1.30
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.34	.46	.46
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	2.06	4.29	4.56
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	28.15	22.84	19.93
CH <sub>4</sub>	29.52	34.79	35.90
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	21.63	24.06	24.80
C <sub>4</sub> HYDROCARBONS	18.19	14.25	14.45

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	90.3	100.7	104.1
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 (1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxoacetates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-42

CATALYST NUMBER : 217-9

DATE : 1/28/81

ATOMIC FORMULA : Co

CATALYST SUPPORT : 50.0% Al<sub>2</sub>O<sub>3</sub>

PREP METHOD: Coprecipitation Impregnation      REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.19 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00
AVE. TEMP., C	259.0	259.0
HOT SPOT, C	259.0	259.0
PRESSURE, psia	925.0	925.0
VHSV, 1/hr/kcm cat.	2520.0	3780.0
HOURS on STREAM	1.4	2.5
RPM	1530.0	1550.0

## CONVERSION :

CO to Prods., vol%	52.72	20.86
CO to CO <sub>2</sub> , vol%	8.08	1.14
CO, gm mol/hr/kcm cat.	16.20	8.80
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/kcm cat.	.29	.23

STOICHIOM. H<sub>2</sub>/CO converted      2.06      2.34CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.12	.42
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	1.27	1.48
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.69	.84
CH <sub>4</sub>	40.36	35.86
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	18.91	16.24
C <sub>4</sub> + HYDROCARBONS	38.75	45.25

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, %<sup>(4)</sup>      71.5      53.8

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition, $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-43

=====  
 CATALYST NUMBER : 217-2  
 ATOMIC FORMULA : CuAl<sub>1.18</sub>Zn<sub>0.33</sub>  
 CATALYST SUPPORT : NONE

DATE : 1/29/81

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.27 gm/cc

REACTOR TYPE: Plus Flow

TEST NUMBER

1 2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00
AVE. TEMP., C	269.0	297.0
HOT SPOT, C	271.0	299.0
PRESSURE, psig	965.0	965.0
WHSV, 1/hr/ksm cat.	3300.0	4650.0
HOURS on STREAM	1.5	3.7
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	30.70	17.97
CO to CO <sub>2</sub> , vol%	.00	1.03
CO, gm mol/hr/ksm cat.	10.60	9.20
STY of oxysenates <sup>(2)</sup>		
gm mol/hr/ksm cat.	10.40	8.24

STOICHIOM. H<sub>2</sub>/CO converted 2.39 2.88CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	97.20	92.28
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.90	2.01
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.00	.00
CH <sub>4</sub>	.90	2.75
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	.00	1.06
C <sub>4</sub> + HYDROCARBONS	.90	1.90

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00

CARBON ACCOUNTABILITY, % (4) 84.8 72.6

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* ZCO in feed/100 \* ZCO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-44

CATALYST NUMBER : 217-10

DATE : 2/2/81

ATOMIC FORMULA : Cu<sub>5</sub>Zn

CATALYST SUPPORT : NONE

PREP METHOD: Coprecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup>: 1.46 gm/cc

REACTOR TYPE: Plug Flow

TEST NUMBER

1

2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00
AVE. TEMP., C	271.0	298.0
HOT SPOT, C	271.0	298.0
PRESSURE, psia	900.0	900.0
UHSV, 1/hr/k <sub>sm</sub> cat.	3690.0	3850.0
HOURS on STREAM	2.2	3.5
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	24.62	19.95
CO to CO <sub>2</sub> , vol%	-1.22	-.75
CO, gm mol/hr/k <sub>sm</sub> cat.	9.40	8.07
STY of oxysenates <sup>(2)</sup>		
gm mol/hr/k <sub>sm</sub> cat.	9.40	8.20

STOICHIOM. H<sub>2</sub>/CO converted 2.22 2.15CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	97.91	95.38
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.57	2.41
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	.00	.00
CH <sub>4</sub>	.76	1.06
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	.00	.29
C <sub>4</sub> + HYDROCARBONS	.86	.77

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C .00 .00

CARBON ACCOUNTABILITY, % (4) 110.8 106.2

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = UHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp. calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC.

SUMMARY FOR RUN # 213-45

CATALYST NUMBER : 217-18  
 ATOMIC FORMULA :  $Cu_{.5}Co_{.25}Zn$   
 CATALYST SUPPORT : NONE

DATE : 2/3/81

PREP METHOD: Cobalt Carbonyl Impregnation      REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY <sup>(1)</sup>: 1.2 gm/cc  
 TEST NUMBER    1    2

REACTOR TYPE: Bertu

TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00
FEED CO2	11.00	11.00
AVE. TEMP., C	270.0	270.0
HOT SPOT, C	270.0	270.0
PRESSURE, psig	910.0	910.0
WHSV, 1/hr/kcm cat.	4400.0	7580.0
HOURS on STREAM	1.3	2.5
RPM	1510.0	1520.0

CONVERSION :

CO to Prods., vol%	32.07	18.00
CO to CO2, vol%	6.33	3.20
CO, gm mol/hr/kcm cat.	18.80	17.90
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/kcm cat.	1.64	2.45

STOICHIOM. H2/CO converted                          1.84                          1.97

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	1.08	1.41
C2-C6 ALCOHOLS	8.50	13.90
C2-C6 ALD. & ESTERS	.84	.82
CH4	23.83	23.32
C2-C3 HYDROCARBONS	23.83	22.61
C4+ HYDROCARBONS	38.43	38.04

APPROACH TO <sup>(3)</sup>

WGS Equilibrium, C    .00    .00

CARBON ACCOUNTABILITY, % <sup>(4)</sup>                          94.0                          106.2

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxygenates}/100$ .

(3) Defined as  $T = T_{eq} - T_{hs}$

    where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



## SUMMARY FOR RUN # 213-46

CATALYST NUMBER : 217-17

DATE : 2/3/81

ATOMIC FORMULA : CoK<sub>0.05</sub>CATALYST SUPPORT : 150.0% Al<sub>2</sub>O<sub>3</sub>

PREP METHOD: Coprecipitation Impregnation      REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.11 gm/cc

REACTOR TYPE: Berty

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00	11.00	11.00
AVE. TEMP., C	263.0	272.0	291.0	290.0
HOT SPOT, C	263.0	272.0	291.0	290.0
PRESSURE, psia	910.0	905.0	900.0	900.0
WHSV, 1/hr/k <sub>sm</sub> cat.	3870.0	2251.0	6360.0	7520.0
HOURS on STREAM	1.7	2.8	4.7	5.5
RPM	1500.0	1500.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	8.13	18.89	20.13	15.86
CO to CO <sub>2</sub> , vol%	3.27	8.91	9.97	6.04
CO, gm mol/hr/k <sub>sm</sub> cat.	4.63	6.57	20.10	17.30
STY of oxysulfates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	1.24	1.62	4.41	4.23

STOICHIOM. H <sub>2</sub> /CO converted	1.95	1.38	1.42	1.53
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.28	.29	.45	.28
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	2.81	4.12	4.79	4.69
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	34.50	31.94	27.52	28.72
CH <sub>4</sub>	22.16	27.09	27.07	24.02
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	17.25	18.70	19.29	17.39
C <sub>4</sub> + HYDROCARBONS	23.00	17.96	18.69	18.50

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	106.7	115.4	130.8	141.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * XCO \text{ in feed}/100 * XCO \text{ conv.}/100 * XSel \text{ to Oxysulfates}/100$ .(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.



CHEM SYSTEMS INC.

## SUMMARY FOR RUN # 213-49

=====  
 CATALYST NUMBER : 217-17 DATE : 2/24/80  
 ATOMIC FORMULA :  $C_{20}K_{10}O_{50}$   
 CATALYST SUPPORT : 50.0%  $Al_2O_3$

PREP METHOD: Impregnation Coprecipitation REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.11 gm/cc REACTOR TYPE: Berly  
 TEST NUMBER 1 2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	.00	.00
AVE. TEMP., C	272.0	290.0
HOT SPOT, C	272.0	290.0
PRESSURE, psia	935.0	935.0
WHSV, 1/hr/gsm cat.	2420.0	5130.0
HOURS on STREAM	1.0	2.1
RPM	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	5.60	9.20
CO to CO <sub>2</sub> , vol%	2.50	4.90
CO, gm mol/hr/gsm cat.	2.94	10.49
STY of oxygenates <sup>(2)</sup> gm mol/hr/gsm cat.	.78	2.54

STOICHIOM. H <sub>2</sub> /CO converted	.91	.67
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.58	.46
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.50	5.56
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	33.57	31.10
CH <sub>4</sub>	27.06	29.87
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	21.13	21.45
C <sub>4</sub> + HYDROCARBONS	12.16	11.49

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	211.0	209.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) =  $WHSV/22.4 * \%CO \text{ in feed}/100 * \%CO \text{ conv.}/100 * \%Sel \text{ to Oxygenates}/100$ .

(3) Defined as  $T = T_{ea} - T_{hs}$

where  $T_{ea}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 213-50

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CATALYST NUMBER : 217-23 DATE : 2/27/81  
 ATOMIC FORMULA : CoPd<sub>0.05</sub>K<sub>0.11</sub>  
 CATALYST SUPPORT : 50.0% Al<sub>2</sub>O<sub>3</sub>  
 PREP METHOD: Pd(NO<sub>3</sub>)<sub>2</sub> Impres. onto 217-15 REDUCTION: in Situ Reduction  
 BULK DENSITY<sup>(1)</sup> : 0 gm/cc REACTOR TYPE: Bertu  
 TEST NUMBER 1 2 3

-----

TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.13	2.13	2.13
FEED CO <sub>2</sub>	10.89	10.89	10.89
AVE. TEMP., C	271.0	273.0	292.0
HOT SPOT, C	272.0	274.0	293.0
PRESSURE, psia	910.0	910.0	905.0
VHSV, 1/hr/kcm cat.	4340.0	4370.0	7460.0
HOURS on STREAM	1.3	2.3	3.5
RPM	1510.0	1510.0	1470.0

CONVERSION :

CO to Prods., vol%	15.96	19.82	24.54
CO to CO <sub>2</sub> , vol%	7.84	7.48	11.06
CO, gm mol/hr/kcm cat.	11.27	13.02	28.98
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/kcm cat.	3.47	3.53	5.80

STOICHIOM. H<sub>2</sub>/CO converted 1.10 .92 .96

CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.45	.41	.44
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	7.75	5.92	4.35
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	3.43	30.99	24.23
CH <sub>4</sub>	29.53	27.96	35.11
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	23.56	21.90	24.08
C <sub>4</sub> + HYDROCARBONS	12.38	12.81	11.90

APPROACH TO<sup>(3)</sup>

WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	129.4	114.5	118.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water-gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-52

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=====
CATALYST NUMBER : 217-24          DATE : 3/9/81
ATOMIC FORMULA : CuCoK11
CATALYST SUPPORT : 88.0% Al2O3

PREP METHOD: Impregnation by Evaporation    REDUCTION: in Situ Reduction

BULK DENSITY(1) : .91 gm/cc          REACTOR TYPE: Plus Flow
TEST NUMBER          1          2          3
=====

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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00	11.00
Ave. TEMP., C	272.0	290.0	299.0
HOT SPOT, C	273.0	292.0	301.0
PRESSURE, psia	935.0	935.0	935.0
WHSV, 1/hr/kgm cat.	2530.0	2550.0	4610.0
HOURS on STREAM	1.1	3.3	4.2
RPM	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	9.82	15.34	10.85
CO to CO <sub>2</sub> , vol%	.38	.46	.15
CO, gm mol/hr/kgm cat.	2.80	4.40	5.60
STY of oxysenates <sup>(2)</sup>			
gm mol/hr/kgm cat.	.10	.20	.25

STOICHIOM. H <sub>2</sub> /CO converted	1.46	1.64	1.39
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	1.04	.82	1.12
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	2.18	3.60	3.25
C <sub>2</sub> -C <sub>6</sub> ALD. ESTERS	.31	.21	.20
CH <sub>4</sub>	35.41	33.89	37.83
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	24.09	23.69	24.65
C <sub>4</sub> + HYDROCARBONS	36.97	37.49	32.86

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	95.0	250.0	259.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

$T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-54

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CATALYST NUMBER : 217-22  
 ATOMIC FORMULA : CuCoK<sub>.22</sub>  
 CATALYST SUPPORT : NONE

DATE : 3/11/81

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup>: 1.56 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1            2            3            4            5

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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00	11.00	11.00	11.00
Ave. TEMP., C	272.0	272.0	292.0	293.0	291.0
HOT SPOT, C	272.0	272.0	292.0	293.0	291.0
PRESSURE, psia	915.0	915.0	915.0	915.0	915.0
VHSV, 1/hr/k <sub>sm</sub> cat.	4650.0	6850.0	7050.0	9800.0	13400.0
HOURS on STREAM	.9	2.0	4.0	4.8	5.6
RPM	1510.0	1510.0	1510.0	1520.0	1510.0

## CONVERSION :

CO to Prods., vol%	34.50	14.89	40.92	23.73	14.47
CO to CO <sub>2</sub> , vol%	10.60	5.11	12.48	11.07	7.43
CO, gm mol/hr/k <sub>sm</sub> cat.	22.58	14.75	40.54	36.72	31.60
STY of oxysenates <sup>(2)</sup>					
gm mol/hr/k <sub>sm</sub> cat.	4.90	3.80	5.70	5.10	5.70

STOICHIOM. H <sub>2</sub> /CO converted	.90	.83	1.11	.96	.76
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	1.57	1.88	1.31	1.61	1.97
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	9.54	9.81	10.44	10.41	11.05
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	16.99	22.71	6.53	8.50	14.08
CH <sub>4</sub>	35.82	30.63	46.59	47.95	40.87
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	22.35	20.02	25.45	21.55	21.49
C <sub>4</sub> + HYDROCARBONS	13.73	15.05	9.79	9.97	10.75

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	170.9	176.0	167.0	214.0	215.9
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ 

where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.

 $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-56

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CATALYST NUMBER : 217-27                       DATE : 3/17/81
ATOMIC FORMULA : CoRu .016K .11
CATALYST SUPPORT : 50.0% Al2O3
PREP METHOD: RuCl3 impres. onto 217-15      REDUCTION: in Situ Reduction
BULK DENSITY(1) : 1.22 gm/cc                REACTOR TYPE: Bertv
TEST NUMBER                     1         2         3
=====

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## TEST CONDITIONS :

	1	2	3
FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00	11.00
AVE. TEMP., C	272.0	295.0	295.0
HOT SPOT, C	272.0	295.0	295.0
PRESSURE, psig	910.0	910.0	910.0
VHSV <sup>(2)</sup> /hr/kcm cat.	4050.0	5280.0	12960.0
HOURS on STREAM	1.1	3.3	4.3
RPM	1500.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	34.30	61.12	22.13
CO to CO <sub>2</sub> , vol%	18.20	26.78	9.67
CO, gm mol/hr/kcm cat.	22.90	49.97	44.38
STY of oxygenates <sup>(2)</sup> gm mol/hr/kcm cat.	5.70	8.24	10.80

STOICHIOM. H <sub>2</sub> /CO converted	N/A.	N/A.	N/A.
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.46	.29	.72
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	5.05	6.04	5.46
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	28.01	16.97	28.16
CH <sub>4</sub>	30.31	42.43	32.33
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	21.43	25.46	22.41
C <sub>4</sub> + HYDROCARBONS	14.85	8.92	10.92

 APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	105.6	107.4	106.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

SUMMARY FOR RUN # 213-55

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 CATALYST NUMBER : 217-28 DATE : 3/19/81  
 ATOMIC FORMULA :  $CuCo_{.4}Al_{.18}Zn_{.33}K_{.05}$   
 CATALYST SUPPORT : NONE

PREP METHOD: Cobalt Carbonyl Impregnation REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.27 gm/cc REACTOR TYPE: Plus Flow  
 TEST NUMBER 1 2 3 4

TEST CONDITIONS :

	1	2	3	4
FEED H2/CO RATIO	2.00	2.00	2.00	2.00
FEED CO2	11.00	11.00	11.00	11.00
AVE. TEMP., C	271.0	301.0	298.0	312.0
HOT SPOT, C	271.0	302.0	299.0	315.0
PRESSURE, psig	940.0	945.0	940.0	940.0
VHSV, 1/hr/kcm cat.	3490.0	6460.0	3570.0	3550.0
HOURS on STREAM	1.7	3.3	4.5	5.6
RPM	.0	.0	.0	.0

CONVERSION :

	1	2	3	4
CO to Prods., vol%	6.14	8.44	9.52	14.30
CO to CO2, vol%	1.26	2.16	6.18	7.30
CO, gm mol/hr/kcm cat.	2.78	7.37	6.04	8.26
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	.75	2.01	1.30	1.55

STOICHIOM. H2/CO converted N.A. N.A. N.A. N.A.

CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

	1	2	3	4
CH3OH	5.90	7.54	7.75	5.29
C2-C6 ALCOHOLS	19.64	19.97	19.30	16.47
C2-C6 ALD.&ESTERS	7.11	7.16	7.92	6.19
CH4	31.08	33.79	33.00	35.35
C2-C3 HYDROCARBONS	20.24	19.97	20.46	21.90
C4+ HYDROCARBONS	16.02	11.56	12.37	14.20

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

	1	2	3	4
CARBON ACCOUNTABILITY, % <sup>(4)</sup>	93.9	111.0	100.8	99.4

- 
- (1) Fresh, non-reduced catalyst.  
 (2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.  
 (3) Defined as  $T = T_{eq} - T_{hs}$   
 where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition.  
 $T_{hs}$  = hot spot temperature.  
 (4) Defined as Carbon observed in Products to Feed Carbon Converted.



## SUMMARY FOR RUN # 213-57

CATALYST NUMBER : UCI L-1122  
 ATOMIC FORMULA : Proprietary Catalyst

DATE : 3/25/81

PREP METHOD: UCI Prep.

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.04 gm/cc

REACTOR TYPE: Berby

TEST NUMBER

1

2

3

4

## TEST CONDITIONS :

FEED H2/CO RATIO	2.10	2.10	2.10	2.10
FEED CO2	5.00	5.00	5.00	5.00
AVE. TEMP., C	299.0	348.0	301.0	350.0
HOT SPOT, C	299.0	348.0	301.0	350.0
PRESSURE, psis	1485.0	1480.0	1480.0	1480.0
VHSV, 1/hr/kcm cat.	2480.0	2425.0	5680.0	6240.0
HOURS on STREAM	.5	2.3	4.6	5.3
RPM	1500.0	1490.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	25.85	18.62	9.57	17.16
CO to CO2, vol%	.75	2.78	-.17	-.26
CO, gm mol/hr/kcm cat.	8.12	6.38	6.57	12.97
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	7.68	5.04	6.42	11.84

STOICHIOM. H2/CO converted	1.99	1.49	2.01	1.66
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	95.69	78.16	94.87	81.26
C2-C4 ALCOHOLS	1.54	10.80	1.08	7.49
C2-C4 ALD., ESTERS	.10	1.72	.00	.89
CH4	1.23	4.37	1.47	3.94
C2-C3 HYDROCARBONS	.31	1.84	.29	2.17
C4+ HYDROCARBONS	.82	3.10	1.08	2.86

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % (4)	82.6	109.3	122.0	69.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-59

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 CATALYST NUMBER : 217-29-1  
 ATOMIC FORMULA : CuCoK<sub>33</sub>  
 CATALYST SUPPORT : NONE

DATE : 3/26/81

PREP METHOD: Coprecipitation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : 1.6 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berete

1 2 3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00	11.00
AVE. TEMP., C	272.0	290.0	292.0
HOT SPOT, C	272.0	290.0	292.0
PRESSURE, psia	940.0	940.0	1470.0
VHSV, l/hr/k <sub>sm</sub> cat.	4490.0	7524.0	8930.0
HOURS on STREAM	1.8	3.6	4.8
RPM	1480.0	1490.0	1490.0

## CONVERSION :

CO to Prods., vol%	12.56	18.81	18.52
CO to CO <sub>2</sub> , vol%	7.54	9.69	8.38
CO, gm mol/hr/k <sub>sm</sub> cat.	9.59	22.78	25.52
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>sm</sub> cat.	1.90	4.40	4.90

STOICHIOM. H <sub>2</sub> /CO converted	.86	.92	1.07
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	2.72	1.82	3.78
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	4.80	8.48	9.30
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	23.68	18.79	14.67
CH <sub>4</sub>	29.92	35.91	40.39
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	21.12	21.36	19.03
C <sub>4</sub> HYDROCARBONS	17.76	13.64	12.93

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	114.6	120.2	125.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-60

CATALYST NUMBER : UCI L-1123  
 ATOMIC FORMULA : Proprietary Catalyst

DATE : 3/27/81

PREP METHOD: UCI Prep.

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.14 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plug Flow

1            2            3            4            5            6

## TEST CONDITIONS :

FEED H2/CO RATIO	2.04	2.04	2.04	2.04	2.04	2.04
FEED CO2	5.00	5.00	5.00	5.00	5.00	5.00
AVE. TEMP., C	306.0	349.0	352.0	349.0	351.0	350.0
HOT SPOT, C	307.0	352.0	353.0	349.0	351.0	351.0
PRESSURE, psig	1480.0	1480.0	1480.0	1470.0	1470.0	1470.0
VHSV, 1/hr/kcm cat.	3100.0	4120.0	2960.0	2820.0	2770.0	1930.0
HOURS on STREAM	.4	2.1	3.3	4.8	6.1	6.8
RPM	.0	.0	.0	.0	.0	.0

## CONVERSION :

CO to Prods., vol%	22.42	20.91	21.55	12.70	12.14	14.39
CO to CO2, vol%	-.02	2.59	3.95	1.60	1.96	3.41
CO, gm mol/hr/kcm cat.	8.44	11.77	9.17	4.90	4.75	4.17
STY of oxysenates <sup>(2)</sup> gm mol/hr/kcm cat.	8.20	9.14	6.14	3.10	2.80	2.20

STOICHIOM. H2/CO converted	1.90	1.40	1.25	1.60	1.65	1.53
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	95.80	75.75	64.85	72.07	69.21	63.60
C2-C6 ALCOHOLS	1.30	9.67	12.07	7.55	7.66	8.91
C2-C6 ALD. & ESTERS	.00	1.91	2.25	1.01	.93	1.24
CH4	1.80	4.83	7.93	9.91	11.03	13.61
C2-C3 HYDROCARBONS	.30	2.70	5.80	5.52	6.15	7.55
C4+ HYDROCARBONS	.80	4.95	7.10	3.94	5.11	5.20

APPROACH TO<sup>(3)</sup>  
WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	103.1	111.0	102.6	127.0	114.2	112.0
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-61

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CATALYST NUMBER : 217-29-3  
 ATOMIC FORMULA : CuCoK<sub>22</sub>  
 CATALYST SUPPORT : 88.0% SiO<sub>2</sub>

DATE : 3/30/81

PREP METHOD: Evaporation Impregnation

REDUCTION: in Situ Reduction

BULK DENSITY<sup>(1)</sup> : .38 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1 2

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.10	2.10
FEED CO <sub>2</sub>	11.00	11.00
AVE. TEMP., C	293.0	294.0
HOT SPOT, C	293.0	294.0
PRESSURE, psia	940.0	940.0
WHSV, 1/hr/gsm cat.	4915.0	4910.0
HOURS on STREAM	4.8	5.5
RPM	1500.0	1480.0

## CONVERSION :

CO to Prods., vol%	10.86	4.16
CO to CO <sub>2</sub> , vol%	.14	2.54
CO, gm mol/hr/gsm cat.	5.82	3.54
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/gsm cat.	1.18	.38

STOICHIOM. H<sub>2</sub>/CO converted 2.33 3.16CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	1.52	1.77
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	10.03	8.53
C <sub>2</sub> -C <sub>6</sub> ALD. & ESTERS	9.02	6.76
CH <sub>4</sub>	23.10	26.06
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	26.85	29.44
C <sub>4</sub> + HYDROCARBONS	29.58	29.44

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, %<sup>(4)</sup> 104.8 231.6

(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-63

CHEM SYSTEMS INC.

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 CATALYST NUMBER : UCI L-1124  
 ATOMIC FORMULA : Proprietary Catalyst

DATE : 4/6/81

PREP METHOD: UCI preparation

REDUCTION: Reduced by 2% H2 in N2

BULK DENSITY<sup>(1)</sup> : 1.14 gm/cc  
 TEST NUMBER

REACTOR TYPE: Berty

1 2

## TEST CONDITIONS :

FEED H2/CO RATIO	2.00	2.00
FEED CO2	5.00	5.00
AVE. TEMP., C	359.0	360.0
HOT SPOT, C	359.0	360.0
PRESSURE, psia	1505.0	1500.0
VHSV, 1/hr/ksa cat.	2480.0	2120.0
HOURS on STREAM	1.3	3.6
RPM	1500.0	1490.0

## CONVERSION :

CO to Prods., vol%	9.00	10.52
CO to CO2, vol%	.50	.88
CO, gm mol/hr/ksa cat.	2.95	3.00
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/ksa cat.	2.30	2.20

STOICHIOM. H2/CO converted	2.15	1.85
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## CARBON SELECTIVITY (Normalized Mol% on CO2-free Basis) :

CH3OH	70.33	68.26
C2-C6 ALCOHOLS	10.03	9.97
C2-C6 ALD. & ESTERS	4.01	4.12
CH4	4.44	5.74
C2-C3 HYDROCARBONS	2.22	3.25
C4+ HYDROCARBONS	8.98	8.67

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	122.0	106.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* XCO in feed/100 \* XCO conv./100 \* XSel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

## SUMMARY FOR RUN # 213-64

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 CATALYST NUMBER : 217-22 (used)  
 ATOMIC FORMULA : CuCoK<sub>22</sub>  
 CATALYST SUPPORT : NONE

DATE : 4/8/81

PREP METHOD: Corecipitation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>

BULK DENSITY<sup>(1)</sup> : 1.52 gm/cc  
 TEST NUMBER

REACTOR TYPE: Plus Flow

TEST NUMBER	1	2
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## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.00	2.00
FEED CO <sub>2</sub>	11.00	11.00
AVE. TEMP., C	269.0	292.0
HOT SPOT, C	269.0	292.0
PRESSURE, psig	940.0	935.0
WHSV, 1/hr/ksm cat.	4100.0	6840.0
HOURS on STREAM	1.5	3.0
RPM	.0	.0

## CONVERSION :

CO to Prods., vol%	7.51	10.45
CO to CO <sub>2</sub> , vol%	6.19	5.35
CO, gm mol/hr/ksm cat.	6.00	11.54
STY of oxygenates <sup>(2)</sup>		
gm mol/hr/ksm cat.	.95	2.50

STOICHIOM. H <sub>2</sub> /CO converted	.96	1.14
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	3.28	3.78
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	8.21	9.37
C <sub>2</sub> -C <sub>6</sub> ALD. ESTERS	17.52	19.65
CH <sub>4</sub>	32.66	32.65
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	20.80	20.55
C <sub>4</sub> + HYDROCARBONS	17.52	13.90

APPROACH TO<sup>(3)</sup>

WGS Equilibrium: C

CARBON ACCOUNTABILITY, % (4)	85.1	96.6
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = WHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxygenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.

CHEM SYSTEMS INC

## SUMMARY FOR RUN # 213-65

CATALYST NUMBER : 217-30  
 ATOMIC FORMULA :  $\text{CuCoK}_{.22}$   
 CATALYST SUPPORT : 88.0% Na-Y Zeolite

DATE : 4/9/81

PREP METHOD: Evaporation Impregnation

REDUCTION: Reduced by 2% H<sub>2</sub> in N<sub>2</sub>BULK DENSITY<sup>(1)</sup> : .64 gm/cc

REACTOR TYPE: Bertx

TEST NUMBER

1

2

3

## TEST CONDITIONS :

FEED H <sub>2</sub> /CO RATIO	2.40	2.40	2.40
FEED CO <sub>2</sub>	11.00	11.00	11.00
AVE. TEMP., C	272.0	275.0	291.0
HOT SPOT, C	272.0	275.0	291.0
PRESSURE, psia	920.0	915.0	915.0
VHSV, 1/hr/k <sub>gm</sub> cat.	3980.0	2310.0	2200.0
HOURS on STREAM	1.4	3.8	3.8
RPM	1490.0	1500.0	1500.0

## CONVERSION :

CO to Prods., vol%	6.52	11.74	18.66
CO to CO <sub>2</sub> , vol%	.48	1.06	1.74
CO, gm mol/hr/k <sub>gm</sub> cat.	3.01	3.20	4.85
STY of oxysenates <sup>(2)</sup> gm mol/hr/k <sub>gm</sub> cat.	.01	.01	.08

STOICHIOM. H <sub>2</sub> /CO converted	2.22	2.59	2.32
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CARBON SELECTIVITY (Normalized Mol% on CO<sub>2</sub>-free Basis) :

CH <sub>3</sub> OH	.43	.22	.33
C <sub>2</sub> -C <sub>6</sub> ALCOHOLS	.11	.22	1.31
C <sub>2</sub> -C <sub>6</sub> ALD.&ESTERS	.00	.11	.11
CH <sub>4</sub>	40.17	36.75	36.18
C <sub>2</sub> -C <sub>3</sub> HYDROCARBONS	22.77	22.25	21.64
C <sub>4</sub> + HYDROCARBONS	36.42	40.35	41.32

APPROACH TO<sup>(3)</sup>  
 WGS Equilibrium, C

CARBON ACCOUNTABILITY, % <sup>(4)</sup>	85.2	97.3	105.2
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(1) Fresh, non-reduced catalyst.

(2) Space Time Yield (STY) = VHSV/22.4 \* %CO in feed/100 \* %CO conv./100 \* %Sel to Oxysenates/100.

(3) Defined as  $T = T_{eq} - T_{hs}$ where  $T_{eq}$  = water gas shift equilibrium temp calculated for reactor eff. composition. $T_{hs}$  = hot spot temperature.

(4) Defined as Carbon observed in Products to Feed Carbon Converted.