similar space velocity). The ALKANOL selectivity appeared to be decreasing over the 6-7 hour test duration while the C_2-C_6 oxygenated fraction of the ALKANOLS was increasing with on-stream time.

UCI L-1124 Catalyst (Run 213-63B)

UCI L-1124 catalyst was screened for initial catalyst performance in the Berty reactor. The catalyst was reduced under the same conditions as those used for reducing UCI L-1122 catalyst with the exception that the maximum reduction temperature was 450°C. This high temperature resulted from a temperature controller malfunction. Only two synthesis tests were made with this catalyst (see Table V-13 for test summary and Appendix for detailed computer run sheets), and the carbon monoxide conversion per pass at the two test conditions were significantly lower than that of the other two UCI catalysts. It is quite probable that the high reduction temperature resulted in a lower catalyst activity than would be expected if a lower maximum reduction temperature was utilized. One interesting point to note is that the concentration of C_2-C_6 oxygenates in the ALKANOL mixtures during the initial activity stages was higher for this catalyst than that of the other two UCI catalysts.

All three of the UCI catalysts appear to result in high selectivity to ALKANOLS and were therefore studied in more detail under conditions of longer-term testing in the process variables studies of Task 2.

3. Screening Studies Using In-House Formulations

The catalysts prepared from in-house formulations have been classified into one of five groups of catalysts as described below:

Group I 5 or 6 component catalyst systems with atomic formula (see Table V-14):

$$Cu_{1.0}Zn_xCo_yM_zA_a$$

TABLE V-13

INITIAL CATALYST PERFORMANCE OF UCI L-1124
CATALYST SCREENED IN THE BERTY REACTOR

Test No. (213-63)	1	2
Test Conditions (1)		
Temperature, °C	359	360
VHSV, l/hr/kg cat	2480	2120
Hours on Stream	1.3	3.6
Run Results		
CO Conversion(2), Vol%	9.0	10.5
ALKANOLS Selectivity, Wt%	96.3	94.8
C_1-C_3 H.C. Selectivity, Wt%	3.7	5.2
ALKANOL Weight Distribution, Wt%		
Methanol	84.4	84.7
C_2-C_6 Oxygenates	10.3	10.5
C_4-C_9 Hydrocarbons	5.3	4.8

(1) Synthesis gas has a 2/1 hydrogen/carbon monoxide ratio with 5 percent carbon dioxide content.
Synthesis pressure fixed at 1500 psig.
Impeller speed fixed at 1500 rpm.

(2) carbon dioxide-free basis.

TABLE V-14

SUMMARY OF STUDIES WITH 5 OR 6 COMPONENT CATALYST SYSTEMS (GROUP I)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
194-62P	197-2	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-71P	197-4	$CuZn_{0.125}CoCrK_{0.11}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-79P	197-9	$CuZn_{0.5}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-83P	197-18	$CuZn_{0.77}CoCr_4K_{0.45}$	Evaporation of $Cu(NO_3)_2$·2-1/2 H_2O, $ZnCO_3$, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-87P	197-10	$CuZn_{0.5}Cr_4K_{0.45}$	Evaporation of $Cu(NO_3)_2$·2-1/2 H_2O, $ZnCO_3$, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-91P	197-11	$CuZn_{0.125}Co_{0.25}CrK_{0.11}$	Evaporation of $Cu(NO_3)_2$·2-1/2 H_2O, $ZnCO_3$, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
194-95P	197-16	$CuZn_{0.5}CoCrK_{0.11}$	Evaporation of $Cu(NO_3)_2$·2-1/2 H_2O, $ZnCO_3$, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-1P	197-17	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of $Cu(NO_3)_2$·2-1/2 H_2O, $ZnCO_3$, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-6P	197-20	$CuZn_{0.49}Co_{0.5}Cr_{0.18}K_{0.09}$	Evaporation of $Cu(NO_3)_2$·2-1.2 H_2O, $ZnCO_3$, cobalt carbonate, and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 2000 VHSV
201-17P	197-29	$CuZn_{0.5}Co_{0.75}Cr_{0.14}K_{0.12}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-34B	197-2	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 2000 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

Continued...

TABLE V-14 (CONTINUED)

SUMMARY OF STUDIES WITH 5 OR 6 COMPONENT CATALYST SYSTEMS (GROUP I)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
201-40P	197-2	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 250°C at 2000 VHSV
201-45B	200-27-2	$CuZn_{0.125}CoFe_{0.5}Th_{0.5}K_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-51B	197-57	$CuZn_{0.125}CoCrK_{0.11}$	Mechanical blending of oxides	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-56B	197-48	$CuZn_{0.125}CoCrK_{0.11}$	Coprecipitation of nitrates with $(NH_4)_2CO_3$	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-58P	197-36	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation using oxalic acid as complexing agent	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-62B	197-16	$CuZn_{0.5}CoCrK_{0.11}$	Evaporation of $Cu(NO_3)_2 \cdot 2\text{-}1/2$ H_2O_3, cobalt carbonate and CrO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-67B	197-2	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates	Catalyst reduced in situ at 900 psig
201-72P	197-59	$CuZn_{0.125}CoMnK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-74B	197-65	30% ($CuZn_{0.125}CoCrK_{0.11}$) 70% (SiO_2)	Impregnation of evaporation	Reduced in situ at ambient pressure
201-77P	197-60	$CuCoVZn_{0.125}K_{0.11}$	Evaporation of nitrates	Reduced in situ at ambient pressure

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

TABLE V-14 (CONTINUED)

SUMMARY OF STUDIES WITH 5 OR 6 COMPONENT CATALYST SYSTEMS (GROUP I)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
201-79B	197-66	55% ($CuZn_{0.125}CoCrK_{0.11}$) 45% (TiO_2)	Impregnation of evaporation onto TiO_2	Reduced in situ at ambient pressure
201-80B	200-57-1	$CuZn_{0.125}CoFe_{0.1}K_{0.11}$	Evaporation of nitrates	Reduced in situ at ambient pressure
201-81P	200-58-1	$CuZn_{0.125}CoMoK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-83B	197-71	$CuZn_{0.125}CoTh_{0.5}Fe_{0.1}K_{0.11}$	Evaporation of nitrates	Reduced in situ at ambient pressure
201-84P	197-67	30% ($CuZn_{0.125}CoCrK_{0.11}$) 70% (TiO_2)	Impregnation of evaporation onto TiO_2	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-85B	197-71	$CuZn_{0.125}CoTh_{0.5}Fe_{0.1}K_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-87B	197-73	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates Pelletized at 10,000 psig	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-89P	197-72	$CuZn_{0.125}CoZrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-90B	197-76	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of metal citrate complexes	Reduced with 2% H_2 in N_2 isothermally at 240°C
201-91B	197-73	$CuZn_{0.125}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-92P	197-78	$CuZn_{0.125}CoCr_{0.125}K_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

TABLE V-14 (CONTINUED)

SUMMARY OF STUDIES WITH 5 OR 6 COMPONENT CATALYST SYSTEMS (GROUP 1)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
201-93B	197-77	$CuZn_{0.125}CoTh_{0.5}K_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-95B	197-79	$CuZn_{0.125}CoThK_{0.11}$	Coprecipitation of KOH	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-97P	197-73	$CuZn_{0.126}CoCrK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 450°C at 500 VHSV
201-98B	197-81	55% $(CuZn_{0.125}CoTh_{0.5}Fe_{0.5}K_{0.11})$ 45% (Mn0)	Coprecipitation of metal nitrates with KOH including manganeous nitrate	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-100P	ICI 51-2	$CuZn_{0.49}Al_{0.21}$	Bottom half of reactor filled with 12.5 g ICI cat. topped with 12.5 g	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
	200-27-2	$CuZn_{0.125}CoTh_{0.5}Fe_{0.5}K_{0.11}$		
213-2B	ICI 51-2	$CuZn_{0.49}Al_{0.21}$	12.5 g ICI cat. charged 12.5 g 200-27-2 charged	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
	200-27-2	$CuZn_{0.125}CoTh_{0.5}Fe_{0.5}K_{0.11}$		
213-4B	197-85	$CuZn_{0.125}CoTh_{0.5}Fe_{0.1}K_{0.11}$	Coprecipitation with KOH	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-29B	200-91	$CuZn_{0.125}CoTh_{0.5}Fe_{0.1}K_{0.11}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

where: M is one or more transition metals;
A is an alkali metal; and
a,x,y,z are the respective atomic ratios
of the metals in the catalyst.

Group II Quarternary catalyst systems with the atomic formula (see Table V-15):

$$CuCo_xM_yA_a \text{ or } CuCr_xM_yA_a$$

where M is Zn, Cr, Ru, or Th and A is K or Cs.

Group III Ternary catalyst systems with the atomic formula (see Table V-16):

$$CuM_xK_a$$

where M = Co, Pd, or Ru.

Group IV Binary catalyst systems comprised of cobalt with either copper or potassium (see Table V-17).

Group V Modified low pressure, methanol synthesis catalysts (see Table V-18).

The detailed summary of computerized test data for each catalyst formulation screened in either the Berty reactor or the diluted-bed, plug-flow reactor is presented in the Appendix.

As discussed in the Overview, the Newtonian approach to catalyst development that was utilized during the formulation and screening studies made it difficult to correlate, on a common basis, all or much of the data obtained. During the course of the program, data correlations were generated for particular sets of data and were reported in the quarterly technical progress reports (43, 44, 45, 46, 47, 48, 49, 50). In general, those in-house catalyst formulations that had good selectivity towards

TABLE V-15

SUMMARY OF STUDIES WITH QUARTERNARY CATALYST SYSTEMS (GROUP II)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
194-39P	197-1	$CuCoCr_{0.8}K_{0.09}$	Evaporation of CrO_3, $Cu(NO_3)_2 \cdot 3H_2O$, and cobalt carbonate with citric acid	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-22B	197-1	$CuCoCr_{0.8}K_{0.09}$	Evaporation of CrO_3, $Cu(NO_3)_2 \cdot 3H_2O$, and cobalt carbonate with citric acid	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-9P	197-19	$CuZn_{0.49}Cr_{0.18}K_{0.07}$	Evaporation of metal nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-11P	197-22	$CuZn_{0.49}Co_{0.18}K_{0.07}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-48B	197-1	$CuCoCr_{0.8}K_{0.09}$	See above	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-60P	200-25-1	$CuZn_{0.125}CoK_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 1000 VSHV
201-65P	200-27-1	$CuZn_{0.125}CoCs_{0.11}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 1000 VSHV
213-9B	197-84	$CuCoRu_{0.1}K_{0.11}$	Coprecipitation with KOH	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-13B	200-76	$CuCoCr_{0.8}K_{0.09}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-14P	200-76	$CuCoCr_{0.8}K_{0.09}$	Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

Continued...

TABLE V-15 (CONTINUED)

SUMMARY OF STUDIES WITH QUARTERNARY CATALYST SYSTEMS (GROUP II)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
213-19B	200-89-1	$CuCo_{0.3}Cr_{0.8}K_{0.09}$	Coprecipitation with Na_2O_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-22P	200-88-1	$Cu_{0.5}Co_{0.2}ZnK_{0.05}$	Coprecipitation with Na_2O_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-25P	200-79	$CuZn_{0.5}CoK_{0.11}$	Evaporation of metal acetates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-28P	200-86	$CuZn_{0.5}CoK_{0.11}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-40P	200-81-1	$CuCoTh_{0.5}K_{0.11}$	Coprecipitation with KOH	In-situ reduction

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

TABLE V-16

SUMMARY OF STUDIES WITH TERNARY CATALYST SYSTEMS (GROUP III)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
213-23B	200-83-1	$CuCoK_{0.11}$	Coprecipitation with KOH	In-situ reduction
213-26B	217-3	$CuCo_{0.3}K_{0.11}$	Coprecipitation with KOH	In-situ reduction
213-31B	217-5	$CuCo_{0.3}K_{0.077}$	Coprecipitation with KOH	In-situ reduction
213-34B	217-7-1	$CuCoK_{0.05}$	Coprecipitation with KOH	In-situ reduction
213-50B	217-23	$CoK_{0.11}Pd_{0.015}$ (50% Al_2O_3)	Impregnation of $Pd(NO_3)_2$ onto 217-15 by evaporation	In-situ reduction
213-52P	217-24	$CuCoK_{0.11}$ (88% α-Al_2O_3)	Impregnation of metal nitrates onto α-Al_2O_3 by evaporation	In-situ reduction
213-54B	217-22	$CuCoK_{0.22}$	Coprecipitation with Na_2CO_3	In-situ reduction
213-56B	217-27	$CoK_{0.11}Ru_{0.016}$ (50% Al_2O_3)	Impregnation of $RuCl_3 \cdot XH_2O$ onto 217-15 by evaporation	In-situ reduction
213-59B	217-29-1	$CuCoK_{0.33}$	Coprecipitation with Na_2CO_3	In-situ reduction
213-61B	217-29-3	$CuCoK_{0.22}$ (88% SiO_2)	Impregnation of metal nitrates onto SiO_2 by evaporaton	In-situ reduction
213-64P	217-22	$CuCoK_{0.22}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 350°C at 500 VHSV
213-65B	217-30	$CuCoK_{0.22}$ (88% Na-Y Zeolite)	Impregnation of metal nitrates onto Linde Zeolite by evaporation	Reduced with 2% H_2 in N_2 up to 240°C at 800 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

TABLE V-17

SUMMARY OF STUDIES WITH BINARY CATALYST SYSTEMS (GROUP IV)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
213-36B	200-83-2	CoCo	Coprecipitation with KOH	In-situ reduction
213-38B	217-15	$CoK_{0.11}$ (50% Al_2O_3)	Impregnation by coprecipitation with Na_2CO_3	In-situ reduction
213-41B	217-16	$CoK_{0.34}$ (50% Al_2O_3)	Impregnation by coprecipitation with Na_2CO_3	In-situ reduction
213-42B	217-9	Co (50% Al_2O_3)	Impregnation by coprecipitation with Na_2CO_3	In-situ reduction
213-46B	217-17	$CoK_{0.05}$ (50% Al_2O_3)	Impregnation by coprecipitation with Na_2CO_3	In-situ reduction
213-49B	217-17	$CoK_{0.05}$ (50% Al_2O_3)	Impregnation of coprecipitation with Na_2CO_3	Catalyst was kept under nitrogen from Run 213-46B. No re-reduction was performed

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

TABLE V-18

SUMMARY OF STUDIES WITH MODIFIED LOW PRESSURE, METHANOL SYNTHESIS CATALYSTS (GROUP V)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
201-13P	197-27	$CuZn_{0.36}Al_{0.21}K_{0.07}$	Impregnation of evaporation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-15P	197-28	$CuZn_{0.36}Al_{0.21}Co_{0.32}K_{0.09}$	Impregnation of evaporation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-32P	197-30	$CuZn_{0.36}Al_{0.21}Co_{0.65}K_{0.09}$	Impregnation of evaporation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
201-100P	197-26 200-27-2	$CuZn_{0.49}Al_{0.21}$ $CuZn_{0.125}Co_{1.0}Fe_{0.5}K_{0.11}$	Low Pressure MeOH synthesis catalyst Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-2B	197-26 200-27-2	$CuZn_{0.49}Al_{0.21}$ $CuZn_{0.125}Co_{1.0}Fe_{0.5}K_{0.11}$	Low Pressure MeOH synthesis catalyst Evaporation of nitrates	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-11P	200-78-1	$CuZn_{0.33}Co_{0.5}Al_{0.18}K_{0.05}$	Detergent dispersion	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-16B	200-78-2	$CuZn_{0.33}Co_{0.5}Al_{0.18}$	Detergent dispersion	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-20P	200-93	$CuZn_{0.33}Co_{0.13}Al_{0.18}K_{0.05}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-21B	200-96	$CuZn_{0.33}Co_{0.01}Al_{0.18}K_{0.05}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-24B	200-99	$CuZn_{0.33}Co_{0.17}Al_{0.18}K_{0.05}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

Continued...

TABLE V-18 (CONTINUED)

SUMMARY OF STUDIES WITH MODIFIED LOW PRESSURE, METHANOL SYNTHESIS CATALYSTS (GROUP V)

Run No.	Catalyst Number	Catalyst Formulation	Catalyst Preparation Method	Activation Procedure
213-32B	217-6	$CuZn_{0.33}Co_{0.07}Al_{0.18}K_{0.05}$	Cobalt carbonyl impregnation	Reduced in situ
213-33P	217-1	$CuZn_{0.33}Al_{0.18}K_{0.05}$	Impregnation	Reduced with 2% H_2 in N_2 to 240°C
213-39P	217-8	$CuZn_{0.33}Co_{0.13}Al_{0.18}K_{0.05}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-43	217-2	$CuZn_{0.33}Al_{0.18}$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-44P	217-17	$Cu_{0.5}Zn$	Coprecipitation with Na_2CO_3	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-45B	217-18	$Cu_{0.5}ZnCo_{0.25}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
214-47P	217-19	$Cu_{0.5}ZnCo_{0.25}K_{0.05}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV
213-55P	217-28	$CuZn_{0.33}Co_{0.4}K_{0.05}Al_{0.18}$	Cobalt carbonyl impregnation	Reduced with 2% H_2 in N_2 up to 240°C at 500 VHSV

B denotes test in Berty gradientless reactor
P denotes test in plug-flow reactor

ALKANOLS during the initial catalyst performance studies had relatively low carbon monoxide conversion activity. In the best of cases, the coproduction of light hydrocarbon gases (C_1-C_3) could not be reduced to less than the equivalent of about 26 wt percent selectivity. This compares to the 5-12 wt percent C_1-C_3 selectivities observed during the screening of the three proprietary UCI catalysts.

VI. DISCUSSION OF RESULTS OF PROCESS VARIABLES STUDIES

A. Overview

Three proprietary ALKANOLS synthesis catalysts provided in calcined form by United Catalysts, Inc. were evaluated in bench-scale units containing vapor-phase and slurry-phase reactors, respectively. Several series of process variables studies were performed to elucidate the effects of the key reaction variables on catalyst performance. The following variables were studied:

Reaction Temperature:	245-350°C
Reaction Pressure:	1500-2500 psig
Space Velocity (Fresh Synthesis Gas):	400-5500 SL/Hr/Kg
Hydrogen/Carbon Monoxide Ratios of Synthesis Gas:	0.6/1 - 2.2/1
Carbon Dioxide Content of Synthesis Gas:	0 - 10.8%
On-Stream Time:	up to 590 Hr
Slurry Oil (Slurry Autoclave Unit Only):	n-heptadecane; Witco 40 Mineral Oil
Bed Dilution (Plug-Flow Reactor Only):	66% alumina/34% catalyst

All calcined catalyst samples were reduced in a vapor-phase reactor at similar conditions. The agitator speed for the slurry autoclave reactor was maintained at 720 rpm whereas the agitator speed in the Berty reactor was maintained at 1500 rpm. Catalyst performance was assessed in terms of per pass carbon monoxide conversions, ALKANOLS selectivity, ALKANOLS composition, modified Schulz-Flory probability parameters and reactivity.

All three UCI catalysts were evaluated in the vapor-phase reactors, two in the Berty reactor and one in the diluted-bed, plug-flow reactor. L-1122 catalyst, which was determined to be the most preferred with respect to its activity-catalyst age response, was also evaluated in two campaigns in the slurry autoclave reaction system.

Table VI-1 is a summary of the comparison of the key catalyst performance parameters for the three UCI catalysts. All three catalysts demonstrated good selectivity and activity to ALKANOLS. However, reaction conditions must be closely controlled to prevent catalyst deactivation or catalyst compositional changes that could adversely affect the composition and yield of crude ALKANOLS.

B. Process Variables Studies in Vapor-Phase Reactor Systems

Process variables studies were performed in vapor-phase reactor systems (Berty gradientless reactor and diluted-bed, plug-flow reactor) for evaluation of the performance characteristics of the three proprietary UCI catalysts (L-1122, L-1123, and L-1124) over extended periods of on-stream time. These catalysts had displayed promising initial performances during the catalyst screening tests of Task 1.

UCI Catalyst L-1122 was evaluated in the Berty reactor in two campaigns. The first campaign lasted for 292 hours on-stream time with a freshly reduced catalyst sample. The second campaign consisted of rereducing the catalyst recovered after the first 292 hour campaign followed by an additional 298 hours of synthesis tests. In total, 36 material balance tests were made exploring the effects of space velocity, synthesis gas composition and on-stream time (i.e., catalyst age) on catalyst performance.

UCI catalyst L-1123 was evaluated in the diluted-bed, plug-flow reactor over a 183-hour on-stream period after catalyst activation. A total of seventeen material balance tests were made exploring the effects of reaction temperature, space velocity, syn gas composition and on-stream time on catalyst performance.

UCI catalyst L-1124 was evaluated in the Berty reactor over a 141-hour on-stream period. A total of seven material balance tests were made exploring the effects of space velocity, synthesis gas composition and on-stream time on catalyst performance.

TABLE VI-1

COMPARISON OF CATALYST PERFORMANCE
UNDER LONGER-TERM TESTING

Catalyst No. (UCI)	L-1122			L-1123	L-1124
Reactor Type	(1) Berty	(2) Berty	(3) Slurry Autoclave	(4) Plug-Flow	(5) Berty
On-Stream Time, Hr.	292*	298**	558	183	142
Maximum Activity, gmol CO Converted/hr/kg catalyst	10	7	40	7.3	7.9
ALKANOLS Selectivity, Wt%	88	72	60	87	77
C_1-C_3 Hydrocarbon Selectivity, Wt%	12	28	40	13	23
Crude ALKANOL Composition, Wt%					
Methanol	43	34	18	83	42
C_2-C_6 Oxygenates	33	42	57	12.5	36
C_4-C_9 Hydrocarbons	24	24	25	4.5	22
Modified Schulz-Flory Probability Parameter	0.6	0.5	0.48	0.39	0.50
Calculated HHV of ALKANOLS, Btu/Gal	89,700	89,000	93,000	70,370	86,450

(1) Selectivities and compositions at 292 hours on-stream time using 2/1 H_2/CO with 2% CO_2.
(2) Selectivities and compositions at 590 hours cumulative on-stream time using 2/1 H_2/CO with 10.8% CO_2.
(3) Selectivities and compositions at 500 hours on-stream time using 2/1 H_2/CO with 1.3% CO_2 and n-heptadecane as slurry oil.
(4) Selectivities and compositions at 175 hours on-stream time using 2/1 H_2/CO with 10.8% CO_2.
(5) Selectivities and compositions at 141 hours on-stream time using 2/1 H_2/CO with 10.8% CO_2.

* Campaign #1
**Campaign #2

1. UCI L-1122 Catalyst (Run 213-74B)

25.0 gms of UCI L-1122 calcined catalyst pellets were charged to the Berty gradientless reactor. Catalyst activation was accomplished by reduction with a 2% hydrogen/98% nitrogen gas at atmospheric pressure and a volumetric hourly space velocity (VHSV) of 1000 Sl/hr/kg cat. Reduction temperature was gradually increased from an initial temperature of 200°C, to a final temperature of 350°C over a 24-hour period and then maintained at 350°C for an additional 24 hours. At this point, hydrogen uptake was completed based on a gas chromatographic analysis of the reactor effluent. Upon completion of the reduction, the reactor was purged with nitrogen prior to pressurization with synthesis gas.

The catalyst logged 292 hours on-stream time with testing of six different synthesis gas compositions prior to shutdown and removal from the reactor. A sample of the spent catalyst was taken for analysis and the remaining 20.0 gms were later recharged to the Berty reactor. The thus recovered catalyst was re-reduced by the same procedure used for the initial reduction. The re-reduced catalyst was subjected to an additional 298 hours on-stream time. Table VI-2 summarizes the run conditions and results for the first 292-hour campaign while Table VI-3 summarizes the results for the second 298 hour campaign with the rereduced catalyst. Tables VI-4 and -5, respectively, show the crude ALKANOL fuel distributions for the two run campaigns. Throughout run 213-74, difficulties were experienced with the Carle gas chromatograph which was used to determine carbon monoxide conversions. Accordingly, the carbon monoxide conversions were backcalculated from the product carbon concentrations determined in the reactor effluent stream. The corrected carbon monoxide conversions are reported in Table VI-6 (note that the carbon monoxide conversions on the summary sheets of Tables VI-2 and -3 represent the uncorrected values determined by the standard method described in Section IV). It can be readily shown that the corrected carbon monoxide conversion is related to the uncorrected value by the following relationship:

$$X'_{CO} = y_{CO}\left(\frac{\text{\% Carbon Accountability}}{100}\right) - y_{CO/CO2} \qquad (1)$$

CHEM SYSTEMS, INC.

Table VI-2

SUMMARY FOR RUN # 213-74B

TODAY'S DATE :

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.04 gm/cc

TEST NUMBER	1	2	3	4	5	6
TEST CONDITIONS :						
FEED H2/CO Ratio	2.25	2.25	2.16	2.16	2.16	2.13
FEED CO2	10.97	10.97	10.81	5.21	5.21	5.00
AVE. TEMP.,°C	353.0	353.0	353.0	353.0	353.0	353.0
HOT SPOT, °C	353.0	353.0	353.0	353.0	353.0	353.0
PRESSURE, psig	1490.0	1490.0	1495.0	1495.0	1495.0	1495.0
VHSV, l/hr/kgm cat.	3168.4	3169.3	2862.2	2974.4	2970.6	2058.2
HOURS on STREAM	23.2	25.3	117.0	120.5	121.5	140.0
CONVERSION :						
CO to Prods., vol%	13.81	12.90	13.40	15.87	15.29	20.31
CO to CO2, vol%	-1.46	-1.14	1.18	3.81	4.11	7.73
CO, gm mol/hr/kgm cat.	4.08	3.89	4.45	7.02	6.91	7.02
STY of Oxygenates(2) gm mol/hr/kgm cat.	3.53	3.36	3.21	5.47	5.31	4.84
STOICHIOM. H2/CO converted	2.09	1.95	1.76	1.54	1.51	1.26
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :						
CH3OH	75.77	75.69	57.75	62.26	60.78	49.01
C2-C6 ALCOHOLS	8.48	8.04	11.87	12.95	13.09	15.74
C2-C6 ALD.&ESTERS	2.23	2.77	2.40	2.59	2.91	4.17
CH4	6.33	6.32	8.20	6.97	6.91	9.10
C2-C3 HYDROCARBONS	3.64	4.09	8.23	7.06	6.98	10.08
C4+ HYDROCARBONS	3.56	3.10	11.55	8.16	9.33	11.82
APPROACH TO(3) WGS Equilibrium, °C :	16.9	0.1	-30.3	-29.3	-68.7	-13.2
CARBON ACCOUNTABILITY,% (4):	65.4	73.0	97.5	92.8	97.5	85.9
OXYGEN REJECTION RATIO,(5):	0.07	0.06	0.04	0.04	0.02	0.05

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

Continued...

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Table VI-2 (Continued)

SUMMARY FOR RUN # 213-748

TODAY'S DATE : 07/17/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.04 gm/cc

TEST NUMBER	7	8	9	10	11	12
TEST CONDITIONS :						
FEED H2/CO Ratio	2.13	2.13	2.03	2.03	2.20	2.20
FEED CO2	5.00	5.00	2.77	2.77	10.95	10.95
AVE. TEMP., °C	353.0	0.0	352.0	353.0	354.0	354.0
HOT SPOT, °C	353.0	353.0	352.0	353.0	354.0	354.0
PRESSURE, psig	1490.0	1495.0	1500.0	1500.0	1500.0	1500.0
VHSV, l/hr/kgm cat.	3039.0	3039.0	2038.1	2880.4	1961.5	2843.8
HOURS on STREAM	142.0	145.0	165.5	168.3	189.0	191.7
CONVERSION :						
CO to Prods., vol%	17.14	17.63	19.41	17.79	20.81	15.54
CO to CO2, vol%	5.17	5.53	12.79	5.13	5.58	3.04
CO, gm mol/hr/kgm cat.	8.25	8.56	8.34	8.39	5.47	5.72
STY of Oxygenates(2) gm mol/hr/kgm cat.	6.09	6.24	5.36	5.79	3.38	3.80
STOICHIOM. H2/CO converted	1.39	1.38	1.13	1.54	1.44	0.43
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :						
CH3OH	56.90	56.86	39.85	48.47	35.70	41.29
C2-C6 ALCOHOLS	14.32	13.06	19.53	15.47	21.90	19.71
C2-C6 ALD.&ESTERS	2.67	2.96	4.88	4.07	4.58	5.36
CH4	7.51	8.05	8.61	8.37	9.24	7.17
C2-C3 HYDROCARBONS	8.17	8.87	9.47	9.11	11.46	9.11
C4+ HYDROCARBONS	10.42	10.21	17.66	13.51	17.51	17.36
APPROACH TO(3) WGS Equilibrium, °C :	-13.7	-8.5		2.1	-26.8	-56.2
CARBON ACCOUNTABILITY,% (4):	88.0	85.9	107.3	103.7	105.3	119.9
OXYGEN REJECTION RATIO,(5):	0.05	0.06		0.06	0.05	0.03

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

Table VI-2 (Continued)

CHEM SYSTEMS, INC.

SUMMARY FOR RUN # 213-74B

TODAY'S DATE : 07/14/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.04 gm/cc

TEST NUMBER	13	14	15	16	17	18
TEST CONDITIONS :						
FEED H2/CO Ratio	2.20	2.14	2.17	0.59	0.59	2.21
FEED CO2	10.95	10.84	10.88	5.80	5.80	10.96
AVE. TEMP.,°C	353.0	354.0	353.0	353.0	353.0	353.0
HOT SPOT, °C	353.0	354.0	353.0	353.0	353.0	353.0
PRESSURE, psig	1500.0	1505.0	1505.0	1505.0	1505.0	1505.0
VHSV, l/hr/kgm cat.	3891.8	2868.9	2844.4	2723.3	1972.1	2899.9
HOURS on STREAM	193.2	197.2	217.0	222.0	223.3	240.8
CONVERSION :						
CO to Prods. , vol%	13.59	14.12	13.45	4.30	-0.48	16.82
CO to CO2, vol%	1.33	2.79	2.76	3.57	5.31	3.12
CO, gm mol/hr/kgm cat.	6.14	5.18	4.89	5.39	2.40	6.07
STY of Oxygenates(2) gm mol/hr/kgm cat.	4.39	3.16	2.95	3.52	1.47	3.52
STOICHIOM. H2/CO converted	1.72	1.65	1.57	1.11	0.93	1.54
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :						
CH3OH	45.94	39.77	38.12	26.44	24.80	31.04
C2-C6 ALCOHOLS	20.67	15.89	19.24	25.67	24.02	26.35
C2-C6 ALD.&ESTERS	4.98	5.40	2.93	13.17	12.55	0.60
CH4	6.48	10.24	8.83	4.87	6.52	8.08
C2-C3 HYDROCARBONS	7.86	12.87	11.30	6.19	7.57	11.15
C4+ HYDROCARBONS	14.08	15.84	19.58	23.67	24.53	22.78
APPROACH TO(3) WGS Equilibrium, °C :	-42.5	-34.0	-43.4	2.1	-26.8	-4.7
CARBON ACCOUNTABILITY,% (4):	118.7	107.7	115.4	155.5	301.6	111.3
OXYGEN REJECTION RATIO,(5):	0.03	0.04	0.03			0.06

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

CHEM SYSTEMS, INC.

Table VI-2 (Continued)

SUMMARY FOR RUN # 213-74B

TODAY'S DATE : 07/17/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.04 gm/cc

TEST NUMBER	19	20	21	22	23	24
TEST CONDITIONS :						
FEED H2/CO Ratio	1.48	1.48	2.11	2.06	2.06	2.06
FEED CO2	6.07	6.07	5.15	5.00	0.00	0.00
AVE. TEMP.,°C	354.0	353.0	353.0	353.0	353.0	353.0
HOT SPOT, °C	354.0	353.0	353.0	353.0	353.0	353.0
PRESSURE, psig	1505.0	1505.0	1500.0	1500.0	1500.0	1500.0
VHSV, l/hr/kgm cat.	2762.2	4679.3	2755.9	3141.2	2810.4	4508.2
HOURS on STREAM	243.7	244.7	246.0	264.7	267.4	268.7
CONVERSION :						
CO to Prods., vol%	13.58	9.15	14.88	13.35	5.28	3.77
CO to CO2, vol%	5.92	3.09	7.82	7.02	9.68	6.67
CO, gm mol/hr/kgm cat.	7.79	8.28	7.61	7.93	6.08	6.90
STY of Oxygenates(2) gm mol/hr/kgm cat.	4.99	5.07	3.64	4.31	3.42	4.24
STOICHIOM. H2/CO converted	1.27	1.42	1.30	1.25	1.16	1.20
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :						
CH3OH	31.03	31.84	22.52	23.66	28.81	34.56
C2-C6 ALCOHOLS	29.94	23.46	23.02	27.65	25.07	25.27
C2-C6 ALD.&ESTERS	3.19	5.94	2.23	3.06	2.40	2.55
CH4	6.29	5.21	11.73	7.49	7.27	6.59
C2-C3 HYDROCARBONS	8.96	6.97	12.70	10.18	9.31	8.54
C4+ HYDROCARBONS	20.67	26.59	27.80	27.97	27.13	22.49
APPROACH TO(3) WGS Equilibrium, °C :	-45.5	-42.2	-93.7	0.0	0.0	0.0
CARBON ACCOUNTABILITY,% (4):	113.0	129.5	121.9	133.4	182.3	198.9
OXYGEN REJECTION RATIO,(5):	0.02	0.02	0.02			

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

CHEM SYSTEMS, INC.

Table VI-2 (Concluded)

SUMMARY FOR RUN # 213-74B

TODAY'S DATE : 07/17/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.04 gm/cc

TEST NUMBER	25	26
TEST CONDITIONS :		
FEED H2/CO Ratio	2.15	2.11
FEED CO2	10.94	1.95
AVE. TEMP.,°C	352.0	354.0
HOT SPOT, °C	352.0	354.0
PRESSURE, psig	1500.0	1500.0
VHSV, l/hr/kgm cat.	4784.9	2993.2
HOURS on STREAM	289.0	291.5
CONVERSION :		
CO to Prods. , vol%	8.35	18.27
CO to CO2, vol%	1.57	8.51
CO, gm mol/hr/kgm cat.	5.06	10.00
STY of Oxygenates(2) gm mol/hr/kgm cat.	2.74	5.31
STOICHIOM. H2/CO converted	1.65	1.29
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :		
CH3OH	21.88	23.08
C2-C6 ALCOHOLS	28.62	26.96
C2-C6 ALD.&ESTERS	3.72	3.04
CH4	7.96	7.33
C2-C3 HYDROCARBONS	10.74	10.12
C4+ HYDROCARBONS	27.07	29.46
APPROACH TO(3) WGS Equilibrium, °C :	-65.6	-11.7
CARBON ACCOUNTABILITY,% (4):	162.0	122.5
OXYGEN REJECTION RATIO,(5):	0.02	0.06

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

Table VI-3

SUMMARY FOR RUN # 213-748-R

TODAY'S DATE : 08/11/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.15 gm/cc

TEST NUMBER	1	2	3	4	5	6
TEST CONDITIONS :						
FEED H2/CO Ratio	2.04	2.04	2.24	2.24	2.21	2.16
FEED CO2	10.70	10.70	11.01	11.01	10.79	10.93
AVE. TEMP., °C	354.0	354.0	354.0	353.0	355.0	354.0
HOT SPOT, °C	354.0	354.0	354.0	353.0	355.0	355.0
PRESSURE, psig	1525.0	1525.0	1530.0	1520.0	1525.0	1520.0
VHSV, l/hr/kgm cat.	2905.4	2604.3	2897.9	2918.2	2224.7	3322.1
HOURS on STREAM	5.5	6.5	27.0	29.0	52.7	176.6
CONVERSION :						
CO to Prods., vol%	7.14	11.38	7.78	14.06	23.21	9.52
CO to CO2, vol%	4.65	1.51	3.68	2.71	6.58	4.84
CO, gm mol/hr/kgm cat.	3.81	3.73	3.44	5.07	6.95	5.10
STY of Oxygenates(2) gm mol/hr/kgm cat.	1.85	1.79	1.61	2.31	2.94	2.67
STOICHIOM. H2/CO converted	1.29	1.69	1.43	1.49	1.39	1.46
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :						
CH3OH	25.63	28.70	20.27	19.78	14.82	12.71
C2-C6 ALCOHOLS	21.33	17.21	21.05	22.01	23.48	29.66
C2-C6 ALD.&ESTERS	1.64	2.09	5.43	3.81	3.92	9.94
CH4	15.29	17.00	13.25	13.40	14.48	9.84
C2-C3 HYDROCARBONS	18.35	20.80	20.03	20.14	20.48	14.60
C4+ HYDROCARBONS	17.76	14.39	19.98	20.86	22.82	23.25
APPROACH TO(3) WGS Equilibrium, °C :	0.0	14.8		13.0	32.4	0.0
CARBON ACCOUNTABILITY,% (4):	134.9	93.4	153.6	92.9	86.7	150.7
OXYGEN REJECTION RATIO,(5):		0.07	0.00	0.07	0.10	

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

Continued...

CHEM SYSTEMS, INC.

Table VI-3 (Concluded)

SUMMARY FOR RUN # 213-74B-R

TODAY'S DATE : 08/24/81

CATALYST NUMBER : UCI L-1122
ATOMIC FORMULA :
PREP. METHOD : UCI PREP
SURFACE AREA(1) : 0 m^2/gm
BULK DENSITY(1) : 1.15 gm/cc

TEST NUMBER	7	8	9	10
TEST CONDITIONS :				
FEED H2/CO Ratio	2.13	2.25	2.09	2.19
FEED CO2	9.92	11.00	10.93	10.99
AVE. TEMP.,°C	354.0	353.0	354.0	354.0
HOT SPOT, °C	354.0	354.0	355.0	355.0
PRESSURE, psig	1530.0	1525.0	1510.0	1530.0
VHSV, l/hr/kgm cat.	2954.9	2902.5	3087.2	2921.2
HOURS on STREAM	200.9	249.5	274.0	298.0
CONVERSION :				
CO to Prods. , vol%	11.85	14.22	11.98	17.70
CO to CO2, vol%	5.65	3.68	3.56	3.11
CO, gm mol/hr/kgm cat.	5.62	5.41	5.24	6.41
STY of Oxygenates(2) gm mol/hr/kgm cat.	2.85	2.34	2.30	2.77
STOICHIOM. H2/CO converted	1.37	1.55	1.54	1.60
CARBON SELECTIVITY (Normalized Mol % on CO2-free Basis) :				
CH3OH	12.38	13.72	14.62	14.60
C2-C6 ALCOHOLS	28.30	23.10	21.85	23.46
C2-C6 ALD.&ESTERS	9.93	6.47	7.47	5.18
CH4	9.91	14.29	13.81	14.02
C2-C3 HYDROCARBONS	14.73	20.59	19.91	20.59
C4+ HYDROCARBONS	24.76	21.83	22.34	22.16
APPROACH TO(3) WGS Equilibrium, °C :		-10.4	-23.1	36.1
CARBON ACCOUNTABILITY,% (4):	144.3	112.7	120.9	90.8
OXYGEN REJECTION RATIO,(5):	0.01	0.06	0.04	0.10

(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.
(5) Defined as ratio of oxygen removed as water, to that removed as CO2.

CHEM SYSTEMS INC.

Table VI-4

CRUDE ALKANOL FUEL WT DISTRIBUTION

RUN 213-74 B

Catalyst Number : UCI L-1122 Date : 7/13/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

	TEST #					
COMPONENT	1	2	3	4	5	6
METHANOL	90.182	90.343	80.392	82.343	81.172	73.599
ETHANOL	2.091	2.094	3.294	3.498	3.199	3.848
N-PROP OL	2.727	2.811	4.597	4.957	4.951	7.132
N-BUT OL	1.088	.991	2.045	1.945	2.744	3.388
N-PENT OL	.235	.118	.442	.330	.000	.465
N-HEX OL	.273	.137	.128	.192	.189	.090
ACET ALD	.000	.000	.166	.000	.000	.310
PROP ALD	.698	.776	.364	.327	.376	.511
BUT ALD	.000	.096	.362	.473	.534	.824
PENT ALD	.805	.576	.864	.807	.957	1.060
HEX ALD	.000	.402	.126	.282	.278	.792
C4 H.C.	.620	.699	2.113	1.416	1.721	2.554
C5 H.C.	.193	.193	1.266	1.081	1.335	1.775
C6 H.C.	.230	.230	1.512	.727	.718	1.212
C7 H.C.	.401	.535	1.382	1.408	1.391	2.113
C8 H.C.	.457	.000	.143	.214	.317	.100
C9 H.C.	.000	.000	.804	.000	.119	.225
TOTAL	100.000	100.000	100.000	100.000	100.000	100.000
METHANOL	90.182	90.343	80.392	82.343	81.172	73.599
C2 - C6 ALCOHOLS	6.414	6.150	10.506	10.922	11.083	14.923
OTHER C2 - C6 OXYGENATES	1.503	1.850	1.882	1.889	2.145	3.498
C4 - C9 HYDROCARBONS	1.901	1.657	7.220	4.846	5.600	7.980
CALCULATED HIGHER HEATING VALUE Btu/gal	67399.	67244.	71768.	70607.	71220.	74217.

Continued...

CHEM SYSTEMS INC.

Table VI-4 (Continued)

CRUDE ALKANOL FUEL WT DISTRIBUTION

RUN 213-74B

Catalyst Number : UCI L-1122 Date : 5/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

COMPONENT	TEST # 7	8	9	10	11	12
METHANOL	78.893	79.511	63.586	71.902	59.649	63.333
ETHANOL	3.623	3.857	4.115	4.195	5.409	4.583
N-PROP OL	5.523	5.783	9.000	7.010	11.425	8.824
N-BUT OL	2.458	1.997	4.580	3.012	4.549	4.353
N-PENT OL	.752	.000	.651	.000	.902	.751
N-HEX OL	.194	.098	1.029	1.153	.348	.581
ACET ALD	.000	.170	.118	.265	.113	.125
PROP ALD	.440	.447	.585	.568	.693	.550
BUT ALD	.615	.694	1.114	1.465	1.598	2.254
PENT ALD	.816	.829	1.331	1.102	.881	.898
HEX ALD	.190	.193	1.144	.377	1.110	1.803
C4 H.C.	2.036	2.236	2.965	2.623	3.566	2.751
C5 H.C.	1.435	1.388	1.937	1.899	2.705	2.186
C6 H.C.	1.061	.912	1.851	1.426	2.056	1.795
C7 H.C.	1.518	1.542	2.825	2.186	3.501	3.700
C8 H.C.	.325	.220	.844	.430	.292	.541
C9 H.C.	.121	.123	2.325	.386	1.202	.972
TOTAL	100.000	100.000	100.000	100.000	100.000	100.000
METHANOL	78.893	79.511	63.586	71.902	59.649	63.333
C2 - C6 ALCOHOLS	12.549	11.735	19.375	15.370	22.633	19.091
OTHER C2 - C6 OXYGENATES	2.061	2.332	4.292	3.778	4.396	5.630
C4 - C9 HYDROCARBONS	6.497	6.421	12.747	8.950	13.322	11.945
CALCULATED HIGHER HEATING VALUE Btu/gal	72145.	71697.	79124.	75041.	80060.	78913.

CHEM SYSTEMS INC.

Table VI-4 (Continued)

CRUDE ALKANOL FUEL WT DISTRIBUTION

RUN 213-74B

Catalyst Number : UCI L-1122 Date : 5/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

	TEST #					
COMPONENT	13	14	15	16	17	18
METHANOL	67.135	66.319	63.041	44.484	43.368	53.962
ETHANOL	4.042	5.002	4.962	2.098	2.086	5.049
N-PROP OL	8.936	7.369	7.588	9.281	8.512	8.329
N-BUT OL	2.854	3.881	4.863	8.071	7.709	6.610
N-PENT OL	3.677	.563	1.091	3.054	.000	6.345
N-HEX OL	.109	.000	1.265	3.135	6.477	1.317
ACET ALD	.189	.507	.000	.175	.087	.142
PROP ALD	.435	.445	.431	.863	1.036	.499
BUT ALD	1.543	1.197	1.250	3.213	3.214	.000
PENT ALD	.461	1.320	.000	4.349	4.351	.000
HEX ALD	1.393	1.535	.992	3.470	3.274	.000
C4 H.C.	2.175	3.413	3.236	2.300	2.877	3.308
C5 H.C.	1.620	2.395	2.499	1.785	2.286	2.634
C6 H.C.	1.382	1.980	1.919	2.473	3.242	2.591
C7 H.C.	2.143	3.198	4.339	3.371	6.548	4.520
C8 H.C.	.122	.875	1.413	5.087	4.298	4.417
C9 H.C.	1.783	.000	1.111	2.792	.635	.275
TOTAL	100.000	100.000	100.000	100.000	100.000	100.000
METHANOL	67.135	66.319	63.041	44.484	43.368	53.962
C2 - C6 ALCOHOLS	19.619	16.815	19.767	25.639	24.783	27.651
OTHER C2 - C6 OXYGENATES	4.020	5.005	2.673	12.069	11.963	.641
C4 - C9 HYDROCARBONS	9.226	11.862	14.518	17.808	19.886	17.746
CALCULATED HIGHER HEATING VALUE Btu/gal	77215.	77452.	79575.	88690.	89413.	83907.

CHEM SYSTEMS INC.

Table VI-4 (Continued)

CRUDE ALKANOL FUEL WT DISTRIBUTION

RUN 213-74B

Catalyst Number : UCI L-1122 Date : 5/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

COMPONENT	TEST # 19	20	21	22	23	24
METHANOL	51.698	52.011	44.839	43.120	47.871	56.214
ETHANOL	3.981	3.778	6.044	6.156	5.264	6.271
N-PROP OL	11.904	7.459	7.822	8.965	7.469	7.186
N-BUT OL	5.309	6.668	5.317	5.901	5.673	4.179
N-PENT OL	5.144	3.112	6.215	5.485	6.932	3.599
N-HEX OL	3.614	2.094	2.408	4.207	4.304	3.774
ACET ALD	.117	.201	.136	.121	.155	.129
PROP ALD	.616	.529	.655	.585	.530	.508
BUT ALD	.957	2.956	1.774	2.508	1.620	1.753
PENT ALD	1.219	1.766	.000	.000	.000	.000
HEX ALD	.000	.000	.000	.000	.000	.000
C4 H.C.	3.545	2.382	4.704	4.041	3.427	3.163
C5 H.C.	2.551	2.053	3.030	2.904	2.481	2.314
C6 H.C.	2.209	2.354	3.002	3.153	2.540	2.345
C7 H.C.	3.277	4.790	5.851	7.242	5.205	3.408
C8 H.C.	2.726	6.241	5.968	3.030	3.287	2.664
C9 H.C.	1.134	1.606	2.234	2.581	3.241	2.493
TOTAL	100.000	100.000	100.000	100.000	100.000	100.000
METHANOL	51.698	52.011	44.839	43.120	47.871	56.214
C2 - C6 ALCOHOLS	29.952	23.111	27.807	30.715	29.642	25.010
OTHER C2 - C6 OXYGENATES	2.909	5.452	2.564	3.214	2.305	2.390
C4 - C9 HYDROCARBONS	15.442	19.427	24.789	22.951	20.181	16.387
CALCULATED HIGHER HEATING VALUE Btu/gal	84419.	85410.	88472.	88885.	87118.	82725.

CHEM SYSTEMS INC.

Table VI-4 (Concluded)

CRUDE ALKANOL FUEL WI DISTRIBUTION

RUN 213-74B

Catalyst Number : UCI L-1122 Date : 5/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

COMPONENT	TEST # 25	26
METHANOL	41.123	42.611
ETHANOL	6.682	5.743
N-PROP OL	7.567	8.020
N-BUT OL	5.434	5.924
N-PENT OL	5.057	6.722
N-HEX OL	7.327	3.446
ACET ALD	.281	.000
PROP ALD	.648	.554
BUT ALD	3.103	2.644
PENT ALD	.000	.000
HEX ALD	.000	.000
C4 H.C.	3.704	3.493
C5 H.C.	2.873	2.644
C6 H.C.	3.295	3.032
C7 H.C.	5.268	6.463
C8 H.C.	4.368	6.447
C9 H.C.	3.269	2.256
TOTAL	100.000	100.000
METHANOL	41.123	42.611
C2 - C6 ALCOHOLS	32.068	29.856
OTHER C2 - C6 OXYGENATES	4.032	3.198
C4 - C9 HYDROCARBONS	22.777	24.336
CALCULATED HIGHER HEATING VALUE Btu/gal	89936.	89701.

CHEM SYSTEMS INC.

Table VI-5

CRUDE ALKANOL FUEL WT DISTRIBUTION

RUN 213-74B-R

Catalyst Number : UCI L-1122 Date : 7/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

COMPONENT	TEST # 1	2	3	4	5	6
METHANOL	53.679	60.659	44.376	43.649	35.048	16.789
ETHANOL	8.299	9.441	10.904	11.513	13.233	6.412
N-PROP OL	8.892	7.472	9.364	9.761	12.461	6.766
N-BUT OL	5.245	2.048	3.362	3.241	3.479	42.300
N-PENT OL	4.725	1.826	3.477	2.937	3.766	2.205
N-HEX OL	.657	2.352	2.015	3.191	2.290	4.313
ACET ALD	.284	.304	1.565	1.652	1.544	1.464
PROP ALD	.747	.803	1.146	1.210	1.343	.681
BUT ALD	.773	.498	.853	.901	1.111	.620
PENT ALD	.000	.000	1.699	.000	.000	3.098
HEX ALD	.000	.922	1.580	1.251	1.473	1.566
C4 H.C.	4.858	5.484	6.989	7.258	8.627	3.543
C5 H.C.	2.474	2.857	3.556	4.055	4.799	2.481
C6 H.C.	2.217	1.785	2.718	2.870	3.500	2.896
C7 H.C.	6.658	1.845	3.556	2.711	3.789	2.036
C8 H.C.	.490	1.314	1.576	1.664	1.920	1.428
C9 H.C.	.000	.590	1.264	2.136	1.617	1.403
TOTAL	100.000	100.000	100.000	100.000	100.000	100.000
METHANOL	53.679	60.659	44.376	43.649	35.048	16.789
C2 - C6 ALCOHOLS	27.819	23.139	29.122	30.643	35.229	61.996
OTHER C2 - C6 OXYGENATES	1.804	2.527	6.843	5.014	5.471	7.430
C4 - C9 HYDROCARBONS	16.697	13.675	19.659	20.694	24.251	13.786
CALCULATED HIGHER HEATING VALUE Btu/gal	82604.	79154.	85657.	85908.	89015.	97732.

Continued...

CHEM SYSTEMS INC.

Table VI-5 (Concluded)

CRUDE ALKANOL FUEL WI DISTRIBUTION

RUN 213-74 B-R

Catalyst Number : UCI L-1122 Date : 7/29/81

Catalyst Formulation: Proprietary Wt% (H_2O FREE)

COMPONENT	TEST # 7	8	9	10
METHANOL	26.769	32.670	33.937	34.339
ETHANOL	9.847	15.437	15.332	14.825
N-PROP OL	10.407	9.801	10.374	10.200
N-BUT OL	6.661	3.679	3.693	3.800
N-PENT OL	5.990	3.125	3.137	2.493
N-HEX OL	4.479	3.079	.364	3.793
ACET ALD	1.304	1.953	1.961	1.792
PROP ALD	.828	1.339	1.344	1.335
BUT ALD	1.107	1.278	1.155	1.020
PENT ALD	4.532	2.138	2.912	2.437
HEX ALD	4.062	2.131	2.495	.531
C4 H.C.	5.858	8.239	7.650	8.114
C5 H.C.	4.110	4.730	5.005	4.972
C6 H.C.	3.965	3.970	3.832	4.112
C7 H.C.	4.830	2.841	2.495	3.010
C8 H.C.	3.004	2.227	2.032	1.413
C9 H.C.	2.248	1.364	2.281	1.813
TOTAL	100.000	100.000	100.000	100.000
METHANOL	26.769	32.670	33.937	34.339
C2 - C6 ALCOHOLS	37.384	35.121	32.900	35.111
OTHER C2 - C6 OXYGENATES	11.832	8.839	9.867	7.115
C4 - C9 HYDROCARBONS	24.015	23.370	23.296	23.435
CALCULATED HIGHER HEATING VALUE Btu/gal	94304.	89602.	88980.	89022.

TABLE VI-6

CARBON MONOXIDE CONVERSION FOR UCI L-1122
CATALYST DURING TEST CAMPAIGNS IN THE BERTY REACTOR

Run 213-74-	Ratio of Syn Gas H_2/CO	% CO_2 Content of Syn Gas	Hours On-Stream	VHSV, Sl/Hr/Kg Cat.	Volume % CO(1) Conversion
1	2	10.8	23	3170	9.5
2	2	10.8	25	3170	9.7
3	2	10.8	117	2860	13.0
4	2	5	120	2970	14.4
5	2	5	121	2970	14.8
6	2	5	140	2060	16.4
7	2	5	142	3040	14.5
8	2	5	145	3040	14.4
9	2	1.5	166	2040	21.8
10	2	1.5	168	2880	18.6
11	2	10.8	189	1960	22.2
12	2	10.8	191	2840	19.2
13	2	10.8	193	3890	16.4
14	2	10.8	197	2870	15.4
15	2	10.8	217	2840	15.9
16	0.56	5.3	222	2720	8.7
17	0.56	5.3	223	1970	9.3
18	2	10.8	240	2900	19.1
19	1.35	6.0	243	2860	16.1
20	1.35	6.0	244	4680	12.8
21	2	5.0	246	2760	19.9
22	2	5.0	264	3140	20.2
23	2	0	267	3280	17.6
24	2	0	268	5050	14.1
25	2	10.8	289	4780	14.5
26	2	1.5	291	2990	24.3
Run 213-74R-					
1	2	10.8	297	2900	11.3
2	2	10.8	298	2600	10.5
3	2	10.8	319	2900	13.9
4	2	10.8	321	2920	12.9
5	2	10.8	344	2220	19.2
6	2	10.8	468	3320	16.8
7	2	10.8	492	2950	19.6
8	2	10.8	541	2900	16.5
9	2	10.8	566	3090	15.2
10	2	10.8	590	2920	15.8

(1) CO_2-free basis; calculated from carbon concentration of synthesis products

Nominal Reaction Temperature: 355°C; Nominal Reaction Pressure: 1500 psig; Agitator Speed: 1200 rpm.