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HETEROGENEOUS CATALYTIC PROCESS FOR ALCOHOL FUELS FROM SYNGAS

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1. Executive Summary

The principal objectives of this project are to discover and evaluate novel heterogeneous catalysts for conversion of syngas to oxygenates having use as fuel enhancers, to explore novel reactor and process concepts applicable in this process, and to develop the best total process for converting syngas to liquid fuels.

The project is being pursued as two concurrent tasks. Task 1 involves catalyst research and development and is being largely conducted by catalyst chemists and analytical specialists. Task 2 is largely an engineering activity, and includes process conceptualization and economics and bench-scale process evaluation of systems developed in Task 1.

The current goal of the catalyst development program is to increase selectivities to oxygenates to greater than 90% with methanol making up less than 70% of the oxygenates, and to increase rates to 20 lb/ft³/hr (ca. 350 g/kg-hr). Targets for isobutanol-producing catalysts are to produce a 50/50 split in selectivity between methanol and iso-butanol, a productivity for isobutanol of > 50 g/Kg-hr and an overall process conversion of 40%.

We have completed a catalyst designed set based on promoted zinc-chromium spinel oxides. Various metals were added to the standard spinel in the design: potassium, palladium and cerium, all thought to be beneficial for HAS. The addition of manganese (at the expense of chromium) and excess zinc in the make-up of the spinel itself was also examined. Other preparation variables included drying temperature, drying time, etc.

The designed set consisted of a total of 22 separate runs divided into a center point formulation, whose preparation was repeated three times, repeat tests of two of these center point preparations and sixteen different catalyst formulations. A wide range of activities (0.39-10.9 lb/ft³-hr, 6-174 g/kg-hr), total selectivities to alcohols (26-95%) and specific selectivities to isobutanol (0-34%) are observed. A number of the catalysts tested are highly selective to total alcohols (85-95%) with between 25 - 40% of the alcohols being C₂'s or higher. Isobutanol selectivities between 19-34% are common.

The models derived from this set are of variable quality. The model for C₄ alcohols (isobutanol) selectivity is the best of the group and the models for activity and selectivity to C₃+C₄ alcohols follow the same trend, thus giving a reasonable indication of promoter trends. All three models show the beneficial effect of palladium addition and the deleterious effect of potassium and cerium *at the levels added*. The presence of manganese in the parent spinel promotes the formation of isobutanol. A higher catalyst calcination temperature has a weak, negative effect on isobutanol selectivities and selectivities to C₃+C₄ alcohols.

Addition of the basic components (potassium and cerium) to the parent spinel has a deleterious effect on catalyst performance, contrary to previous literature reports. Examination of the catalyst preparation procedure identified the use of potassium carbonate in the coprecipitation step as a likely source of potassium contamination. The catalysts, nominally "potassium-free", in fact contain up to 2.5% potassium. The system examined in

the design therefore contains a great deal more of the basic component (potassium or potassium/cerium) than intended. The "palladium-only" formulation in actuality contains both palladium and potassium.

To further sort out the effect of the K, Pd, and Ce as promoters, a set of catalysts was prepared from two batches of $\text{Zn}_2\text{Cr}_2\text{Mn}_2\text{O}_4$ prepared using alkali-free coprecipitation methods. These catalysts will be tested shortly.

Modified low temperature methanol catalysts using the alkali-free coprecipitated $\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ were prepared. The catalysts were impregnated with potassium and Pd, Pt or Ag. These catalysts will be tested at temperatures at or below 300°C and may be suitable for slurry-type reactors.

Future plans include examination of (a) "potassium-free" preparation procedures, (b) higher palladium loadings, (c) a process variable (pressure, temperature, syngas ratio, etc.) designed set on the most promising formulations, and (d) extension of testing to some copper-based catalysts.

In Task 2 Process Synthesis work, the Base Case Process for converting coal to fuel alcohols via syngas is now complete and design alternatives have been identified. The Base Case investment for a 1,500 metric tonne/day Fuel Alcohols Unit is \$473 MM. The coal processing and gasification step accounts for 40% of the investment. Due to the processing cost of coal, methane is the preferred route for syngas production. In order to make the coal route economically viable, coal by-products will need to be considered. Optimization of the design variables is the next step, and simulated annealing will be used as the optimization technique.

2. Project Objectives

- To discover, study, and evaluate novel heterogeneous catalytic systems for the production of oxygenated fuel enhancers from synthesis gas. In particular, novel heterogeneous catalysts will be studied and optimized for the production of: (a) $\text{C}_1\text{-C}_5$ alcohols using conventional methanol synthesis conditions, and (b) methanol and isobutanol mixtures which may be used for the downstream synthesis of MTBE or related oxygenates.
- To explore, analytically and on the bench scale, novel reactor and process concepts for use in converting syngas to liquid fuel products.
- To develop on the bench scale the best combination of chemistry, catalyst, reactor, and total process configuration to achieve the minimum product cost for the conversion of syngas to liquid products.

3. Project Organization

This project has been divided into two tasks.

Task 1 is concerned with catalyst identification, preparation, performance evaluation, and characterization. This work is being largely conducted by catalyst chemists and analytical specialists. Chemical studies to support the engineering effort in Task 2 are included in this task, but fundamental aspects of the catalytic chemistry are emphasized in this effort.

Task 2 includes process conceptualization and economics, and bench-scale process evaluation of systems developed in Task 1. This is largely an engineering activity.

These tasks are being carried out concurrently throughout the project.

4. Technical Progress

4.1. Task 1 – Catalyst Studies

4.1.1. Catalyst Synthesis

4.1.1.1. Introduction

Synthesis gas can be converted into mixtures of methanol and higher alcohols by use of alkali-modified methanol synthesis catalysts known for many years. Interest in higher alcohol synthesis from syngas has stemmed from the desire to use the alcohol mixtures as high-octane blending stock for gasoline. Currently refining modifications and the use of oxygenated petrochemicals such as methyl tert-butyl ether (MTBE) have been implemented as alternatives. The production of a mixture of methanol and isobutanol is of interest due to its possible use as a feedstock in the production of other oxygenates such as MTBE and related ethers.

The 16-run, 8-variable fractional factorial designed set of experiments to investigate catalyst formulation and preparation variables of the UCC Isobutanol catalyst was finished. We report our current progress with the Isobutanol catalysts and the start of our studies concerning the modified low temperature MeOH catalysts.

4.1.1.2. Catalysts for Isobutanol Synthesis

Preparation of the catalysts for the designed set was completed. Future formulations were to be based upon the results of this designed experiment. The results of the designed set indicate that the presence of potassium was not an important factor in the selectivity of the catalysts. This surprising result led us to wonder if there was alkali metal contamination in these catalysts. Indeed, X-ray fluorescence showed that there was potassium in the Zn-Cr-Mn oxide that had not been impregnated with potassium. Due to the usual matrix effects, quantitative numbers could not be determined with this technique. The rather insoluble nature of the finished catalysts complicated initial ICP analyses. Therefore, three unfired samples of the Zn-Cr-Mn oxides were used in ICP-OES measurements. These ICP-OES analyses showed that the Zn-Cr-Mn oxides contained 0.9 to 2.5% bulk potassium.

This presence of the potassium impurity explains the lack of strong dependence in the selectivity and activity on potassium loadings of the catalysts. The large variation in the levels of the potassium contamination could also explain why the catalytic data were so difficult to model. Even with the error that the uncontrolled levels of potassium contamination introduced in our results, statistical analysis of the data showed that Pd increased the total alcohol production and selectivity to C₃ and C₄ alcohols.

To further clear up the effects of K, Pd, and Ce on the activity and selectivity of these catalysts, Zn₃Mn_{1.5}Cr_{1.5}O_{4.5} and Zn₁Cr₁O_{2.5} were prepared using ammonium hydroxide in the coprecipitation step. Four catalysts — Pd₆Zn₃Mn_{1.5}Cr_{1.5}O_{4.5}, Pd₆Zn₁Cr₁O_{2.5}, K_aPd_bCe_cZn₃Mn_{1.5}Cr_{1.5}O_{4.5}, and K_aPd_bCe_cZn₁Cr₁O_{2.5} — were prepared from this alkali-free material. The first two catalysts are repeats of the best two catalysts in the fractional factorial

design, based on rate and selectivity to total alcohols. These catalysts will be tested soon, and may direct us toward improved isobutanol production.

4.1.1.3. Catalysts for Linear Alcohol Synthesis

We also have started preparation of a copper-based low-temperature higher alcohol catalyst. These catalysts may be more suitable for use in slurry-type reactors. It is hypothesized that the introduction of a Fischer-Tropsch metal such as Co induces a classical ASF chain growth mechanism with primary alcohols as the main products. Unfortunately, this also gives rise to the parallel production of hydrocarbons. The active site for alcohol formation is thought to be highly divided Cu-Co clusters that are formed under reaction conditions. We will use this hypothesis to direct our work with this class of catalysts, keeping in mind that higher alcohol (HA) yield increases with the Co/Cu ratio, whereas increasing the Cr/Co ratio leads to decreased activity and an increase in methanol selectivity. We will attempt to increase HA selectivity by alloying the Cu or Cu-Co clusters with another metal or promoter. We will also try to modify the metal-support interactions through the choice of different supports and/or preparation methods. The first additive to be tried will be Pd, since it may be an important component of our isobutanol catalyst.

Initial screening of Fe, Ru, Pd, Pt, and Ag doped $\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ where $x=0, .25$, and 1 will be done first. Preparation of the $\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ where $x=0, .25$, and 1 was repeated using the alkali-free method. A set of catalysts based upon modified low-temperature methanol catalysts using the alkali-free $\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ was prepared. The catalysts have the formulations of $\text{K}_a\text{Pd}_b\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$, $\text{K}_a\text{Pt}_b\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$, and $\text{K}_a\text{Ag}_b\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$. They will be tested at temperatures at and below 300°C .

4.1.2. Catalyst Evaluation

4.1.2.1. Introduction

Higher alcohol synthesis (HAS) catalysts have primarily evolved from modified methanol synthesis catalysts. The original methanol synthesis catalysts were based on a zinc/chromium oxide spinel oxide and operated around 400°C and could tolerate some sulfur impurities in the syngas feed. With the advent of effective desulfurization techniques for the syngas, a second generation methanol synthesis catalyst was developed, based on a more active copper metal based formulation which could operate at substantially lower temperatures ($250\text{--}300^\circ\text{C}$). In both cases, the addition of alkali to the system resulted in the formation of higher alcohols, albeit at a substantially lower overall productivity.

An interesting contrast in the two systems is in the types of alcohols produced: the copper metal based catalysts produce mainly linear alcohols with an Anderson-Schulz-Flory (ASF) distribution similar to that observed in linear condensation polymerization. The original, so-called "high-temperature" catalysts produce branched alcohols with a non-ASF distribution, the major products being methanol and isobutanol.

Our work is focused at the present time on the latter class of materials, with emphasis on discovering a catalyst that has a high selectivity to total alcohols at the expense of hydrocarbons, and a high specific selectivity among the alcohols to isobutanol. A 50/50 mol% mix of methanol and isobutanol would provide an ideal feedstock for the direct production of methyl isobutyl ether (MIBE) via dehydration or the indirect production of methyl tert-butyl ether (MTBE) in two steps by (a) dehydration of the isobutanol to isobutylene, followed by (b) reaction with methanol to produce MTBE. The second route is preferred, as MIBE is not an octane-enhancing agent.

Our initial goals were selectivities to oxygenates > 90% with at least 30% of the oxygenates being C₂'s or higher; total alcohol activities should be > 20 lb/ft³-hr. Working goals specific to isobutanol-producing catalysts are a target of a 50/50 split in selectivity between methanol and isobutanol, a productivity target for isobutanol of 50 g/Kg-hr, and an overall process conversion of 40%.

The catalysts examined in this quarter are high-temperature (400°C) materials, consisting of a spinel oxide support (general formula AB₂O₄, where A = M²⁺ and B = M³⁺), promoted with various other elements. The spinel itself consists of the traditional zinc/chromium oxide formulation, modified by the partial substitution of chromium by manganese in the octahedral sites in the oxygen lattice. This reduces the overall acidity of the spinel (Mn³⁺ is less acidic than Cr³⁺) and should reduce hydrocarbon formation, which is acid-catalyzed.

HAS requires at least two complementary, yet competing reactions: carbon-carbon bond formation and hydrogenation. In the copper metal-based, low-temperature system, carbon-carbon bond formation is thought to occur via a classical CO insertion mechanism, followed by hydrogenation. In contrast, the high-temperature catalysts utilize an aldol condensation mechanism to form the carbon-carbon bonds. The aldol reaction can proceed via acid or base catalysis. Clearly, in HAS, the base-catalyzed route will be preferred, as acid sites will promote hydrocarbon formation. Basic components included in the design are alkali (specifically potassium) and ceria (the rare earth oxides are basic materials).

The hydrogenation components necessary to produce higher alcohols included in this design are palladium and excess zinc. Copper metal cannot be used, as it sinters rapidly above 300°C. A fractional factorial design was utilized to determine the importance of each catalyst component.

4.1.2.4. Catalyst Tests

We have completed testing the catalyst designed set based on promoted zinc-chromium spinel oxides. (This set is designated design #2, to distinguish it from the catalyst preparation designed set used as a basis for this work; see the Third Quarterly Report, 1992.) Various metals were added to the standard spinel in the design: potassium, palladium and cerium, all thought to be beneficial for HAS. The addition of manganese (at the expense of chromium)

and excess zinc in the make-up of the spinel itself were also examined. Other preparation variables included drying temperature, drying time, etc.

Basis for Design #2

The designed set consisted of a total of 22 separate runs divided into a center-point formulation, whose preparation was repeated three times (catalysts 10-DAN-50, 10-DAN-57 and 10-DAN-66), repeat tests of two of these center-point preparations (10-DAN-50R and 10-DAN-57R) and sixteen different catalyst formulations. The results are displayed in Table 1.

Center-Point Catalysts

The center-point formulations have all the promoters present in intermediate amounts and show reasonable agreement for two out of the three: 10-DAN-57 and 10-DAN-66. In contrast, 10-DAN-50 is less active and produces a significant amount of C₃ products. This C₃ split contains significant quantities of both the normal and branched products (n-propanol and isopropanol), suggesting some difference in the preparation. A likely scenario is incomplete incorporation of all of the promoters; 10-DAN-50 was made early in the campaign and may have suffered as a consequence of the learning process.

Alcohol activities for the two "good" catalysts are 6-7 lb/ft³-hr (96-112 g/kg-hr), with selectivities, on a carbon dioxide-free basis, of 57-67%. The amount of isobutanol produced on a wt% basis is 18-20% of the total alcohols (11% on a mol% basis), giving isobutanol productivities of 17-22 g/kg-hr.

Scope of the Design

The results are summarized in Table 1. A wide range of activities (0.39-10.9 lb/ft³-hr, 6-174 g/kg-hr), total selectivities to alcohols (26-95%) and specific selectivities to isobutanol (0-34%) are observed. A number of the catalysts tested are highly selective to total alcohols (85-95%) with between 25 and 40% of the alcohols being C₂'s or higher. Isobutanol selectivities of 19-34% are common. This indicates that the design limits chosen were wide enough to give meaningful models.

Design Models

The models derived from this set (see Table 2) are of variable quality. The model for C₄ alcohols (isobutanol) selectivity is the best of the group and the models for activity and selectivity to C₃+C₄ alcohols follow the same trend, thus giving a reasonable indication of promoter trends. All three models show the beneficial effect of palladium addition and the deleterious effect of potassium and cerium *at the levels added*. The presence of manganese in the parent spinel promotes the formation of isobutanol. A higher catalyst calcination

temperature has a weak, negative effect on isobutanol selectivities and selectivities to C_3+C_4 alcohols.

Alcohol Product Distribution

12 of the 22 catalysts make significant quantities of isobutanol (14 wt% or greater). Four catalysts (highlighted in Table 1) have been selected for illustrative purposes. The alcohol distributions for these catalysts appear in Figures 1-4.

- 3-DAN-90: (see Figure 1). This catalyst is the most active of the set and the least selective for total alcohols, producing hydrocarbons instead. The formulation consists of the basic zinc/chromium spinel support with added potassium and gives a unique alcohol distribution, with the major components being the propanols (isopropanol and n-propanol). The ratio of branched to normal product is also unusual, with nearly a 1:1 split between iso- and n-propanol. The usual split is roughly 10:1.

- 10-DAN-47 and 10-DAN-52: (see Figures 2 and 3). These two formulations consist of a zinc/chromium/manganese spinel with excess zinc as the basis. Additionally, 10-DAN-47 has potassium and 10-DAN-52 has cerium. Both exhibit lower activities than the mean, are very selective to alcohols (93-94%), and produce relatively large quantities of methanol as the major alcohol product. Notice once more that potassium addition appears to favor products in the C_2-C_4 range (contrast this with 10-DAN-52).

- 10-DAN-54: (see Figure 4). This formulation is identical to 10-DAN-47 and 10-DAN-52, except palladium is the additional promoter instead of potassium or cerium. The catalyst is more active than its two counterparts, slightly less selective to total alcohols (but still a very respectable 86%) and the most selective of the whole design for isobutanol (34 wt%).

These results are promising, but somewhat surprising. The addition of the basic components (potassium and cerium) to the parent spinel has a deleterious effect on catalyst performance, contrary to previous literature reports. Examination of the catalyst preparation procedure (as described in Section 4.1.1.2), identified the use of potassium carbonate in the coprecipitation step as a likely source of potassium contamination. The catalysts, nominally "potassium-free", in fact contain up to 2.5% potassium. The system examined in the design therefore contains a great deal more of the basic component (potassium or potassium/cerium) than intended. The "palladium-only" formulation, 10-DAN-54, in actuality contains both palladium and potassium. Some catalysts prepared using a "potassium-free" precipitation step need to be tested to sort out the real effect of potassium (and base) in this system.

4.1.3. Task 1 Conclusions

We have discovered that the catalysts tested contained moderate levels of potassium as an impurity. ICP-OES showed that the levels of potassium in the bulk varied from 0.8 to 2.5%. The potassium contamination was probably due to the use of potassium carbonate in the coprecipitation step. The statistical analysis of the catalytic data resulted in poorly fitting models, but still showed that Pd had a beneficial effect in alcohol productivity and higher alcohol selectivity. To further sort out the effect of the K, Pd, and Ce as promoters, a set of catalysts was prepared from two batches of $\text{Zn}_a\text{Cr}_b\text{Mn}_c\text{O}_d$ prepared using alkali-free coprecipitation methods. These catalysts will be tested soon.

A set of catalysts based upon modified low-temperature methanol catalysts using the alkali-free $\text{Cu}_{1-x}\text{Co}_x\text{Cr}_2\text{O}_4$ was prepared. The catalysts were impregnated with potassium and Pd, Pt or Ag. These catalysts will be tested at temperatures of 300°C or below and may be suitable for slurry-type reactors.

Results from the iso-alcohol designed set show that a number of the catalysts tested are highly selective to total alcohols (85-95%) with between 25 and 40% of the alcohols being C_2 's or higher. Isobutanol selectivities of 19-34% are common.

The activities range from < 1 $\text{lb/ft}^3\text{-hr}$ to as high as 10.9 $\text{lb/ft}^3\text{-hr}$ (6-174 g/kg-hr) with values of 5-7 $\text{lb/ft}^3\text{-hr}$ (80-112 g/kg-hr) being common.

The alcohols produced are almost exclusively methanol and iso-butanol. The isobutanol is believed to be formed because the HAS proceeds predominately via an aldol condensation mechanism over the promoted spinel oxide catalysts.

The statistical models themselves are of variable quality. All three models show the beneficial effect of palladium addition and the deleterious effect of potassium and cerium *at the levels added*. The presence of manganese in the parent spinel promotes the formation of isobutanol. A higher catalyst calcination temperature has a weak, negative effect on isobutanol selectivities and selectivities to C_3+C_4 alcohols.

Addition of the basic components (potassium and cerium) to the parent spinel has a deleterious effect on catalyst performance, contrary to previous literature reports. Examination of the catalyst preparation procedure identified the use of potassium carbonate in the coprecipitation step as a likely source of potassium contamination. The catalysts, nominally "potassium-free", in fact contain up to 2.5% potassium. The system examined in the design therefore contains a great deal more of the basic component (potassium or potassium/cerium) than intended. The "palladium-only" formulation, 10-DAN-54, in actuality contains both palladium and potassium. Some catalysts prepared using a "potassium-free" precipitation step need to be tested to sort out the real effect of potassium (and base) in this system.

Table 1. Catalyst Formulation Designed Set Results

CATALYST SAMPLE	ACTIVITY [1]	SELECTIVITY TO ALCOHOLS [2]	C1 (wt%)	C2 (wt%)	C3 (wt%) [3]	C4 (wt%)[4]
10DAN50	4.79	87.88	55.32	0.00	16.34	16.22
10DAN50R	3.63	70.11	52.14	0.00	11.60	6.37
10DAN57	6.77	93.53	67.32	0.00	3.72	20.09
10DAN57R	6.74	83.99	65.74	0.00	1.76	16.09
3DAN90	10.86	26.00	4.64	3.50	13.50	4.37
11DAN45	5.93	91.44	64.43	0.53	2.65	23.83
11DAN44	0.85	65.00	47.86	0.00	9.09	8.05
10DAN47	3.69	94.78	81.32	1.62	6.55	5.29
10DAN54	6.89	85.59	41.87	1.51	5.08	34.38
10DAN49	0.39	69.78	57.79	0.00	11.99	0.00
10DAN55	7.96	89.93	55.34	1.65	9.32	23.61
10DAN52	3.05	93.62	81.92	0.00	1.97	9.72
10DAN53	4.87	79.28	70.01	0.00	0.00	9.26
10DAN48	4.20	80.80	54.07	0.00	9.22	17.52
10DAN51	6.33	80.51	57.77	0.00	1.85	19.01
10DAN56	5.72	96.31	71.17	0.00	3.46	19.25
10DAN24	3.81	92.61	63.31	0.00	4.43	24.88
10DAN66	6.66	78.43	57.69	0.00	2.00	18.20
10DAN65	4.45	74.61	64.53	0.00	1.82	8.26
10DAN58	2.79	49.67	32.32	0.00	6.46	10.89
10DAN59	5.90	65.06	49.11	0.00	1.73	14.22
10DAN67	3.23	85.95	72.94	0.00	8.23	4.78
<div> <div>[1] ACTIVITY= lbs/ft³-hr</div> <div>[2] SELECTIVITY= wt%</div> <div>[3] product is almost exclusively n-propanol</div> <div>[4] product is almost exclusively Iso-butanol</div> </div>						

Table 2. Design Models from Catalyst Design #2

$$\text{Activity} = 4.59 - 0.127 \cdot K + 0.447 \cdot \text{Pd} - 0.0773 \cdot \text{Ce} \\ \text{(2.5)} \quad \text{(3.3)} \quad \text{(1.9)} \quad R^2 = 0.542$$

Total Alcohols = No Model Found

$$\text{C3+C4 Alcohols} = 38.9 - 0.555 \cdot K + 1.181 \cdot \text{Pd} - 0.48 \cdot \text{Ce} \\ \text{(2.3)} \quad \text{(1.9)} \quad \text{(2.6)} \\ -0.0354 \cdot (\text{Calcination Temperature}) \\ \text{(2.3)} \quad R^2 = 0.561$$

$$\text{C1+C2 Alcohols} = 54.7 + 0.687 \cdot \text{Ce} \\ \text{(2.0)} \quad R^2 = 0.174$$

C3 Alcohol = No Model Found

$$\text{C4 Alcohol} = 27.0 - 0.8 \cdot K + 1.61 \cdot \text{Pd} - 0.378 \cdot \text{Ce} + 11.4 \cdot \text{Mn} \\ \text{(4.1)} \quad \text{(3.2)} \quad \text{(2.5)} \quad \text{(2.2)} \\ -0.029 \cdot (\text{Calcination Temperature}) \\ \text{(2.3)} \quad R^2 = 0.726$$

Figure 1. Product Distribution for 3DAN90 (Spinel Support plus Potassium)

Figure 2. Product Distribution for 10DAN47 (Zn, Cr, Mn Spinel with Excess Zn plus Potassium)

Figure 3. Product Distribution for 10DAN52 (Zn, Cr, Mn Spinel with Excess Zn plus Cerium)

Figure 4. Product Distribution for 10DAN54 (Zn, Cr, Mn Spinel with Excess Zn plus Palladium)

4.2. Task 2 – Engineering Studies

4.2.1. Reaction Engineering

4.2.1.1. Introduction

Task 2 work under this contract involves reaction engineering studies to examine the best catalysts identified in Task 1. New catalysts will be developed and screened in powder form in Task 1. We will develop scaleup and process strategies to make use of the best catalysts found in Task 1 and will develop kinetic models to describe their performance.

Since powders cannot be used commercially in a gas phase reactor (the type which will be used for initial screening studies), we will evaluate different strategies for utilizing new catalysts on an industrial scale. This may include pelletizing or tableting the powdered catalysts for use in gas phase reactors, using powdered catalysts in a gas-liquid-solid slurry reactor, or using solid pellets or powder in other types of three phase reactors, such as trickle bed reactors.

4.2.1.2. Reaction Engineering Activities

The slurry reaction system has been under preparation for catalyst testing. The SOP and necessary safety inspections have been completed and tests will soon begin in the system.

4.2.2. Mathematical Process Development

4.2.2.1. Introduction

Process synthesis work is being performed at Union Carbide to develop mathematical models and process designs for fuel alcohols processes, both under this contract and as part of a subcontract with West Virginia University (DOE Contract DE-AC22-91PC91034). Because of the interrelated nature of these studies, work done to support both contracts is reported here.

The goal of the Task 2 Process Synthesis Study is to determine the most economical process flowsheet for converting coal to fuel alcohols via syngas. The initial phase is to conceptualize the flowsheet and identify design alternatives. West Virginia University has taken the lead role in the definition of the Base Case, and Union Carbide's primary input has been identification of design alternatives. This first phase is now complete, and the second phase, which is the optimization of design conditions, is now underway.

4.2.2.2 Base Case Description and Investment

The Base Case Process for converting coal to fuel alcohols via syngas is completed. The Base Case was developed by West Virginia University with input from Union Carbide. A simplified flow diagram is shown in Figure 1.

The coal is converted to syngas in a Texaco Gasifier. The H_2/CO ratio is increased by adding a steam/natural gas reformer in parallel with the gasifier. The heat is recovered from

the syngas and is then sent to a Rectisol Unit for acid gas removal. The H_2S is selectively removed from the CO_2 and the H_2S is further processed in a Claus Unit to recover the sulfur.

The cleaned syngas is compressed and fed to the alcohol synthesis reactor. The product from the reactor is separated into the fuel alcohol product and a recycle gas. A second acid gas removal system is used to remove the generated CO_2 in the recycle gas. A purge from the recycle gas stream is sent to a power generating unit.

The investment for a 1,500 metric tonne/day Fuel Alcohol Unit is \$473 MM. A breakdown of the estimate by individual processing steps is shown in Table 1, which indicates that the coal to syngas portion of the process is the largest single item at 40% of the total. This dominance suggests that alternative gasification technologies, such as the Shell Gasifier, will need to be evaluated. It should also be noted that the methane to syngas step is only 4% of the total investment and could be eliminated to arrive at a coal-only facility by utilizing a sour gas shift converter downstream of the optimum gasifier.

4.2.2.3 Design Alternatives

In the Base Case, water removal from the fuel alcohol product is attained by controlling the water gas shift reaction in the alcohol synthesis reactor to minimize water. Since experimentation is ongoing, the exact water content is unknown. If the water content is found to be over the allowable limit, water removal alternatives will be considered. These include azeotropic distillation and molecular sieves.

Alternatives to acid gas removal for Rectisol include Selexol and Ucarsol solvents. Both solvents are Union Carbide products, and a more detailed economic comparison is currently underway.

4.2.2.4 Optimization

The optimization can be viewed as two problems consisting of syngas generation and the alcohol synthesis loop. The optimization technique of simulated annealing will be used to optimize the design variables as well as the choice of design alternatives. Initially, the optimizer will be based on simplified models, and more rigor will be added as needed. The alcohol synthesis reaction variables for optimization will include the H_2/CO ratio, conversion, pressure, CO_2 recycle and methanol recycle.

4.2.3. Task 2 Conclusions

The Base Case for production of fuel alcohols from coal is completed, and process design alternatives have been identified. The next phase is to develop simplified models which will be used to optimize operating conditions and design choices.

FIGURE 1
Coal to Fuel Alcohols

Table 1. Coal to Fuel Alcohols Investment

	<u>\$MM</u>	<u>%</u>
Coal Gasification and Processing	185	40
Oxygen Production	82	17
Steam/Power Generation & Heat Recovery	73	15
Alcohol Synthesis Loop	67	14
Acid Gas Removal	33	7
Syn Gas via Methane	20	4
Sulfur Recovery	<u>13</u>	<u>3</u>
Total	473	100

1,500 metric tonne/day Fuel Alcohols

5. Appendix A — Catalyst Tests

[illegible]

[illegible]

[illegible]

CATALYST NAME = 10DAN48		REFERENCE # = PR322		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 211.00	
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.11		TIME PERIOD (hr) = 6.00	
CATALYST VOLUME (ml) = 0.90		CO (mole %) = 47.60		% WATER COLLECTED = 0.00			
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.60					
PRESSURE (psig) = 1100.00		N2 (mole %) = 4.80					
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT	
						mole % w/ CO2	wt % w/o CO2
1	H2	2.02	2952.43	6.36	45.95		
2	N2	28.00	31.23	0.77	5.58		
3	CO	28.10	292.38	6.50	47.00		
4	CO2	44.01	8.67	0.15	1.05	76.36	71.39
5	CH4	16.04	129.88	0.01	0.09	2.39	6.12
6	C2H6	30.07	48.52	0.00	0.02	0.90	1.23
7	C3H8	44.10	41.42	0.06	0.01	0.75	0.70
9	CH3OH	32.04	272.77	1.07	0.24	12.78	16.41
8	C4H10	58.12	27.12	0.04	0.01	0.50	0.35
10	C2H5OH	46.07	0.00	0.00	0.00	0.00	0.00
12	i-C3H7OH	60.10	0.00	0.00	0.00	0.00	0.00
11	n-C3H7OH	60.10	90.02	0.18	0.02	2.18	1.49
15	sec-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00
14	i-C4H9OH	74.12	155.85	0.29	0.03	3.46	1.92
13	n-C4H9OH	74.12	27.62	0.06	0.01	0.69	0.38
16	Me-2-Butanol	88.15	0.00	0.00	0.00	0.00	0.00
REACTANT GASES 1-3 =		217.17		13.63		CO MOLAR CONVERSION (N2 BASIS) = 15.02	
PRODUCT GASES 4-17 w/ CO2 =		8.39		0.20		H2 MOLAR CONVERSION (N2 BASIS) = 16.91	
PRODUCT GASES 5-17 w/o CO2 =		1.98		0.06			
TOTAL HYDROCARBONS =		0.38		0.02		4.54	
C2+ HYDROCARBONS =		0.18		0.00		2.15	
TOTAL ROH/TOTAL HC =		4.21		2.40			
TOTAL ALCOHOLS =		1.60		0.04		19.10	
C1-C2 ALCOHOLS =		1.07		0.03		12.78	
C3 ALCOHOLS =		0.18		0.00		2.18	
C4 ALCOHOLS =		0.35		0.00		4.14	
C3-C4 ROH/TOTAL ROH =		0.33		0.19			
N/B C3-C4 ALCOHOLS =		0.83		0.98			
ROH ACTIVITY (OFFGAS BASIS) =		0.061		g/g cat/hr		lb/lb3/hr	
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.057		g/g cat/hr		lb/lb3/hr	
HIC ACTIVITY (OFFGAS BASIS) =		0.014		g/g cat/hr		lb/lb3/hr	
				4.20		CARBON MASS BALANCE (%) = 107.87	
				4.20		HYDROGEN MASS BALANCE (%) = 104.16	
				1.00		OXYGEN MASS BALANCE (%) = 109.50	

CATALYST NAME = 10DAN49		REFERENCE # = PR224		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 212.00	
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00		LIQUID COLLECTED (gm) = 0.00	
CATALYST VOLUME (ml) = 0.80		CO (mole %) = 47.43		% WATER COLLECTED = 0.00		% WATER COLLECTED = 0.00	
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56		TIME PERIOD (hr) = 24.00		TIME PERIOD (hr) = 24.00	
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.01					
				</			

CATALYST NAME = 10DAN50		FEED RATE (scfm) = 200.00		OFFGAS RATE (scfm) = 217.00								
REFERENCE # = PR249		H12/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.06								
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.60		% WATER COLLECTED = 0.00								
CATALYST VOLUME (ml) = 0.90		H12 (mole %) = 47.60		TIME PERIOD (hr) = 4.50								
TEMPERATURE (°C) = 400.00		N2 (mole %) = 4.80										
PRESSURE (psig) = 1100.00												
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT wt % w/ CO2	PRODUCT mole % w/ CO2	PRODUCT wt % w/o CO2	PRODUCT mole % w/o CO2	PRODUCT w1 % ROI only	PRODUCT mole % ROI only	N/B mole %
1	H2	2.02	12.75	6.31	45.86							
2	N2	28.00	21.36	0.76	5.55							
3	CO	28.10	181.99	6.48	47.07							
4	CO2	44.01	6.80	0.15	1.12	77.20	74.06					
5	CH4	16.04	63.54	0.10	0.04	1.11	2.92	4.87	11.27			
6	C2H6	30.07	29.43	0.05	0.01	0.52	0.73	2.29	2.82			
7	C3H8	44.10	29.97	0.05	0.01	0.52	0.49	2.27	1.91			
9	CH3OH	32.04	282.78	1.11	0.03	12.61	16.62	55.32	64.07	62.95	77.87	
8	C4H10	58.12	34.89	0.05	0.00	0.61	0.45	2.69	1.72			
10	C2H5OH	46.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
12	i-C3H7OH	60.10	39.20	0.09	0.00	1.08	0.76	4.72	2.92	5.37	3.54	
11	n-C3H7OH	60.10	114.99	0.23	0.00	2.65	1.86	11.62	7.17	13.22	8.72	2.5
15	sec-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
14	i-C4H9OH	74.12	150.82	0.28	0.00	3.18	1.81	13.96	6.99	15.89	8.50	
13	n-C4H9OH	74.12	21.79	0.05	0.00	0.51	0.29	2.26	1.13	2.57	1.37	0.2
16	Me-2-Butanol	88.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
REACTANT GASES 1-3 =		216.10		13.55				CO MOLAR CONVERSION (N2 BASIS) =		14.40		
PRODUCT GASES 4-17 w/ CO2 =		8.81		0.21				H12 MOLAR CONVERSION (N2 BASIS) =		16.60		
PRODUCT GASES 5-17 w/o CO2 =		2.01		0.05								
TOTAL HYDROCARBONS =		0.24		0.01		2.76		4.60		12.12		17.72
C2+ HYDROCARBONS =		0.15		0.00		1.65		1.67		7.25		6.45
TOTAL ROH/TOTAL HC =		7.25		4.64								
TOTAL ALCOHOLS =		1.77		0.04		20.04		21.34		87.88		82.28
C1-C2 ALCOHOLS =		1.11		0.03		12.61		16.62		55.32		64.07
C3 ALCOHOLS =		0.33		0.01		3.73		2.62		16.34		10.09
C4 ALCOHOLS =		0.33		0.00		3.70		2.11		16.22		8.12
C3-C4 ROH/TOTAL ROH =		0.37		0.22								
N/B C3-C4 ALCOHOLS =		0.74		0.84								
ROI ACTIVITY (OFFGAS BASIS) =		0.069		g/g cat/hr		4.79		lb/l3/hr		CARBON MASS BALANCE (%) =		111.27
ROI ACTIVITY (CO FEEDGAS BASIS) =		0.064		g/g cat/hr		4.79		lb/l3/hr		HYDROGEN MASS BALANCE (%) =		106.84
HIC ACTIVITY (OFFGAS BASIS) =		0.010		g/g cat/hr		0.66		lb/l3/hr		OXYGEN MASS BALANCE (%) =		113.18
OFFGAS BASIS												

CATALYST NAME = 10DAN50R											
REFERENCE # = PR424											
CATALYST WEIGHT (gm) = 1.00											
CATALYST VOLUME (ml) = 0.95											
TEMPERATURE (°C) = 400.00											
PRESSURE (psig) = 1100.00											
GASES		Molecular Weight	GC AREA	OFFGAS weight	OFFGAS molar	OFFGAS mole %	PRODUCT wt %	PRODUCT mole %	PRODUCT wt %	PRODUCT mole %	PRODUCT
		g/m		ugrams	umoles	total	w/ CO2	w/ CO2	w/o CO2	w/o CO2	ROH only
1	H2	2.02	3042.73	13.24	6.55	45.40					
2	N2	28.00	41.32	28.59	1.02	7.07					
3	CO	28.10	297.40	185.86	6.61	45.83					
4	CO2	44.01	10.47	7.73	0.18	1.22	77.89	71.59			
5	CH4	16.04	198.81	0.31	0.02	0.13	3.09	7.78	13.95	27.38	
6	C2H6	30.07	85.15	0.13	0.00	0.03	1.34	1.80	6.05	6.34	
7	C3H8	44.10	77.23	0.12	0.00	0.02	1.18	1.09	5.35	3.82	
9	CH3OH	32.04	291.09	1.14	0.04	0.25	11.53	14.55	52.14	51.22	74.37
8	C4H10	58.12	64.21	0.10	0.00	0.01	1.00	0.70	4.54	2.46	
10	C2H5OH	46.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	i-C3H7OH	60.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	n-C3H7OH	60.10	125.39	0.25	0.00	0.03	2.57	1.73	11.60	6.08	16.55
15	sec-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	i-C4H9OH	74.12	75.16	0.14	0.00	0.01	1.41	0.77	6.37	2.71	9.09
13	n-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	Me-2-Butanol	88.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
REACTANT GASES 1-3 =				227.69		14.19		CO MOLAR CONVERSION (N2 BASIS) =		34.67	
PRODUCT GASES 4-17 w/ CO2 =				9.92		0.25		H2 MOLAR CONVERSION (N2 BASIS) =		35.28	
PRODUCT GASES 5-17 w/o CO2 =				2.19		0.07					
TOTAL HYDROCARBONS =				0.66		0.03		11.36		29.89	
C2+ HYDROCARBONS =				0.35		0.01		3.58		15.94	
TOTAL ROH/TOTAL HC =				2.35		1.50					
TOTAL ALCOHOLS =				1.54		0.04		17.05		60.00	
C1-C2 ALCOHOLS =				1.14		0.04		14.55		52.14	
C3 ALCOHOLS =				0.25		0.00		1.73		11.60	
C4 ALCOHOLS =				0.14		0.00		0.77		6.37	
C3-C4 ROH/TOTAL ROH =				0.26		0.15					
N/B C3-C4 ALCOHOLS =				1.82		2.25					
ROH ACTIVITY (OFFGAS BASIS) =				0.055		g/g cat/hr		3.63		lb/n3/hr	
ROH ACTIVITY (CO FEEDGAS BASIS) =				0.053		g/g cat/hr		3.63		lb/n3/hr	
HC ACTIVITY (OFFGAS BASIS) =				0.024		g/g cat/hr		1.55		lb/n3/hr	
OFFGAS BASIS											
								CARBON MASS BALANCE (%) =		104.78	
								HYDROGEN MASS BALANCE (%) =		102.23	
								OXYGEN MASS BALANCE (%) =		106.61	

CATALYST NAME = 10DAN51													
REFERENCE # = PR323													
CATALYST WEIGHT (gm) = 1.00													
CATALYST VOLUME (ml) = 0.80													
TEMPERATURE (°C) = 400.00													
PRESSURE (psig) = 1100.00													
GASES		Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT wt % w/ CO2	PRODUCT mole % w/ CO2	PRODUCT wt % w/o CO2	PRODUCT mole % w/o CO2	PRODUCT wt % ROH only	PRODUCT mole % ROH only	N/B mole %
1	H2	2.02	3213.32	13.98	6.92	43.62							
2	N2	28.00	48.83	33.78	1.21	7.61							
3	CO	28.10	338.24	211.38	7.52	47.42							
4	CO2	44.01	7.38	5.45	0.12	0.78	63.73	57.58					
5	CH4	16.04	172.49	0.27	0.02	0.10	3.11	7.70	8.56	18.15			
6	C2H6	30.07	103.08	0.16	0.01	0.03	1.88	2.49	5.18	5.86			
7	C3H8	44.10	73.19	0.11	0.00	0.02	1.30	1.17	3.59	2.77			
9	CH3OH	32.04	456.12	1.79	0.06	0.35	20.96	26.01	57.77	61.33	71.76	85.23	
8	C4H10	58.12	43.34	0.07	0.00	0.01	0.79	0.54	2.16	1.27			
10	C2H5OH	46.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
12	i-C3H7OH	60.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
11	n-C3H7OH	60.10	28.20	0.06	0.00	0.01	0.67	0.44	1.85	1.04	2.29	1.45	#DIV/0!
15	sec-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
14	i-C4H9OH	74.12	317.04	0.59	0.01	0.05	6.89	3.70	19.01	8.72	23.61	12.12	
13	n-C4H9OH	74.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
16	Me-2-Butanol	88.15	29.75	0.06	0.00	0.00	0.68	0.37	1.88	0.86	2.34	1.20	
REACTANT GASES 1-3 =				259.14	15.65								
PRODUCT GASES 4-17 w/ CO2 =				8.55	0.22								37.12
PRODUCT GASES 5-17 w/o CO2 =				3.10	0.09								42.16
TOTAL HYDROCARBONS =				0.60	0.03	0.16	7.07	11.90	19.49	28.05			
C2+ HYDROCARBONS =				0.34	0.01	0.06	3.97	4.20	10.93	9.89			
TOTAL ROH/TOTAL HC =				4.13	2.57								
TOTAL ALCOHOLS =				2.50	0.07	0.41	29.20	30.52	80.51	71.95	100.00	100.00	
C1-C2 ALCOHOLS =				1.79	0.06	0.35	20.96	26.01	57.77	61.33	71.76	85.23	
C3 ALCOHOLS =				0.06	0.00	0.01	0.67	0.44	1.85	1.04	2.29	1.45	
C4 ALCOHOLS =				0.59	0.01	0.05	6.89	3.70	19.01	8.72	23.61	12.12	
C3-C4 ROH/TOTAL ROH =				0.28	0.15								
N/B C3-C4 ALCOHOLS =				0.10	0.12								
ROH ACTIVITY (OFFGAS BASIS) =				0.081	g/g cat/hr	6.33	lb/lb3/hr	OFFGAS BASIS					
ROH ACTIVITY (CO FEEDGAS BASIS) =				0.078	g/g cat/hr	6.33	lb/lb3/hr	C2+ RBON MASS BALANCE (%) =					106.64
HIC ACTIVITY (OFFGAS BASIS) =				0.020	g/g cat/hr	1.53	lb/lb3/hr	HYDROGEN MASS BALANCE (%) =					97.94
								OXYGEN MASS BALANCE (%) =					107.42

	CATALYST NAME = 10DAN52																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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CATALYST NAME = 10DAN53		REFERENCE # = PR294		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 209.00	
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00		LIQUID COLLECTED (gm) = 0.00	
CATALYST VOLUME (ml) = 0.80		CO (mole %) = 47.60		% WATER COLLECTED = 0.00		% WATER COLLECTED = 0.00	
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.60		TIME PERIOD (hr) = 18.00		TIME PERIOD (hr) = 18.00	
PRESSURE (psig) = 1100.00		N2 (mole %) = 4.80					

CATALYST NAME = 10DANS4		FEED RATE (scmm) = 200.00		OFFGAS RATE (scmm) = 198.00	
REFERENCE # = PR174		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.22	
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.43		% WATER COLLECTED = 0.00	
CATALYST VOLUME (ml) = 0.80		H2 (mole %) = 47.56		TIME PERIOD (hr) = 5.00	
TEMPERATURE (°C) = 400.00		N2 (mole %) = 5.01			
PRESSURE (psig) = 1100.00					

CATALYST NAME = 10DAN55		REFERENCE # = PR223		FEED RATE (scfm) =		200.00		OFFGAS RATE (scfm) =		210.00	
CATALYST WEIGHT (gm) =		1.00		H2/CO RATIO =		1.00		LIQUID COLLECTED (gm) =		0.17	
CATALYST VOLUME (ml) =		0.75		CO (mole %) =		47.43		% WATER COLLECTED =		0.00	
TEMPERATURE (°C) =		400.00		H2 (mole %) =		47.56		TIME PERIOD (hr) =		4.75	
PRESSURE (psig) =		1100.00		N2 (mole %) =		5.01					
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT w/ CO2 wt %	PRODUCT w/ CO2 mole %	PRODUCT w/o CO2 wt %	PRODUCT w/o CO2 mole %	PRODUCT ROH only wt %	PRODUCT ROH only mole %
1	H2		3154.62	13.72	6.79	43.57					
2	N2		49.35	34.14	1.22	7.82					
3	CO		330.58	206.60	7.35	47.16					
4	CO2		8.48	6.26	0.14	0.91	66.28	63.04			
5	CH4		16.04	0.12	0.01	0.05	1.27	3.32	8.97		
6	C2H6		30.07	0.06	0.00	0.01	0.66	0.92	1.97	2.50	
7	C3H8		44.10	0.04	0.00	0.01	0.46	0.43	1.35	1.17	
9	CH3OH		32.04	1.76	0.06	0.35	18.66	24.37	55.34	65.95	77.22
8	C4H10		58.12	0.09	0.00	0.01	1.00	0.72	2.98	1.96	
10	C2H5OH		46.07	0.05	0.00	0.01	0.56	0.51	1.65	1.37	1.60
12	i-C3H7OH		60.10	15.7	0.04	0.00	0.40	0.28	1.19	0.76	0.89
11	n-C3H7OH		127.62	0.26	0.00	0.03	2.74	1.91	8.13	5.17	6.05
15	sec-C4H9OH		71.03	0.13	0.00	0.01	1.40	0.79	4.15	2.14	2.50
14	i-C4H9OH		333.4	0.62	0.01	0.05	6.56	3.71	19.47	10.03	11.74
13	n-C4H9OH		0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	Me-2-Butanol		88.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
REACTANT GASES 1-3 =				254.46	15.36	CO MOLAR CONVERSION (N2 BASIS) = 36.31					
PRODUCT GASES 4-17 w/ CO2 =				9.45	0.23	H2 MOLAR CONVERSION (N2 BASIS) = 41.31					
PRODUCT GASES 5-17 w/o CO2 =				3.19	0.08						
TOTAL HYDROCARBONS =				0.32	0.01	0.08	3.39	5.40	10.07	14.60	
C2+ HYDROCARBONS =				0.20	0.00	0.03	2.12	2.08	6.30	5.63	
TOTAL ROH/TOTAL HC =				8.93	5.85						
TOTAL ALCOHOLS =				2.87	0.07	0.46	30.32	31.57	89.93	85.40	100.00
C1-C2 ALCOHOLS =				1.82	0.06	0.36	19.22	24.88	57.00	67.32	78.82
C3 ALCOHOLS =				0.30	0.00	0.03	3.14	2.19	9.32	5.92	6.94
C4 ALCOHOLS =				0.75	0.01	0.07	7.96	4.50	23.61	12.16	14.24
C3-C4 ROH/TOTAL ROH =				0.37	0.21						
N/B C3-C4 ALCOHOLS =				0.33	0.40						
ROH ACTIVITY (OFFGAS BASIS) =				0.096	g/g cat/hr	7.96	lb/ft3/hr	OFFGAS BASIS			
ROH ACTIVITY (CO FEEDGAS BASIS) =				0.091	g/g cat/hr	7.96	lb/ft3/hr	CARBON MASS BALANCE (%) = 108.32			
HC ACTIVITY (OFFGAS BASIS) =				0.011	g/g cat/hr	0.89	lb/ft3/hr	HYDROGEN MASS BALANCE (%) = 99.28			
								OXYGEN MASS BALANCE (%) = 109.47			

CATALYST NAME = 10QAN56												
REFERENCE # = PR355			FEED RATE (cccm) = 200.00			OFFGAS RATE (cccm) = 209.00						
CATALYST WEIGHT (gm) = 1.00			H2/CO RATIO = 1.00			LIQUID COLLECTED (gm) = 0.03						
CATALYST VOLUME (ml) = 0.90			CO (mole %) = 47.60			% WATER COLLECTED = 0.00						
TEMPERATURE (°C) = 400.00			H2 (mole %) = 47.60			TIME PERIOD (hr) = 5.50						
PRESSURE (psig) = 1100.00			N2 (mole %) = 4.80									
GASES			Molecular Weight		GC AREA		OFFGAS		OFFGAS		OFFGAS	
			g/m				molar		mole %		PRODUCT	
							umoles		total		wt %	
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CATALYST NAME = 10DAN57R		REFERENCE # = PR423		FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 203.00						
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00								
CATALYST VOLUME (ml) = 0.70		CO (mole %) = 47.43		% WATER COLLECTED = 0.00								
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56		TIME PERIOD (hr) = 25.00								
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.91										
GASES	Molecular Weight	GC AREA	OFFGAS weight	OFFGAS umoles	OFFGAS mole %	PRODUCT wt %	PRODUCT mole %	PRODUCT wt %	PRODUCT mole %	PRODUCT ROH only	PRODUCT ROH only	N/B mole-%
	g/m		ugrams		total	w/ CO2	w/ CO2	w/o CO2	w/o CO2			
1	H2	2.02	3216.925	13.99	6.93	43.43						
2	N2	28.00	52.038	36.00	1.29	8.06						
3	CO	28.10	339.41	212.11	7.55	47.33						
4	CO2	44.01	6.042	4.46	0.10	0.64	54.09					
5	CH4	16.04	149.598	0.23	0.01	0.09	7.66	8.08	16.69			
6	C2H6	30.07	73.388	0.11	0.00	0.02	2.03	4.02	4.42			
7	C3H8	44.10	32.412	0.05	0.00	0.01	0.60	1.73	1.30			
9	CH3OH	32.04	476.995	1.87	0.06	0.37	31.21	65.74	68.00	78.28	89.07	
8	C4H10	58.12	40.314	0.06	0.00	0.01	0.57	2.19	1.25			
10	C2H5OH	46.07	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
12	i-C3H7OH	60.10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
11	n-C3H7OH	60.10	24.785	0.05	0.00	0.01	0.45	1.76	0.97	2.10	1.27	#DIV/0!
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
14	i-C4H9OH	74.12	246.591	0.46	0.01	0.04	3.30	16.09	7.19	19.15	9.42	
13	n-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0
16	Me-2-Butanol	88.15	5.7	0.01	0.00	0.00	0.08	0.39	0.18	0.47	0.23	
REACTANT GASES 1-3 =				262.11	15.76		CO MOLAR CONVERSION (N2 BASIS) = 37.98					
PRODUCT GASES 4-17 w/ CO2 =				7.31	0.19		H2 MOLAR CONVERSION (N2 BASIS) = 43.24					
PRODUCT GASES 5-17 w/o CO2 =				2.85	0.09							
TOTAL HYDROCARBONS =				0.46	0.02	0.13	10.86	16.01	23.66			
C2+ HYDROCARBONS =				0.23	0.01	0.04	3.20	7.93	6.97			
TOTAL ROH/TOTAL HC =				5.24	3.23							
TOTAL ALCOHOLS =				2.39	0.07	0.41	35.04	83.99	76.34	100.00	100.00	
C1-C2 ALCOHOLS =				1.87	0.06	0.37	31.21	65.74	68.00	78.28	89.07	
C3 ALCOHOLS =				0.05	0.00	0.01	0.45	1.76	0.97	2.10	1.27	
C4 ALCOHOLS =				0.46	0.01	0.04	3.30	16.09	7.19	19.15	9.42	
C3-C4 ROH/TOTAL ROH =				0.22	0.11							
N/B C3-C4 ALCOHOLS =				0.11	0.14							
ROH ACTIVITY (OFFGAS BASIS) =				0.076	g/g cat/hr	6.74	OFFGAS BASIS					
ROH ACTIVITY (CO FEEDGAS BASIS) =				0.075	g/g cat/hr	6.74	CARBON MASS BALANCE (%) = 104.20					
HC ACTIVITY (OFFGAS BASIS) =				0.014	g/g cat/hr	1.28	HYDROGEN MASS BALANCE (%) = 95.40					
							OXYGEN MASS BALANCE (%) = 104.90					

CATALYST NAME = 10DAN58		FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 201.00	
REFERENCE # = PK572		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.03	
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.43		% WATER COLLECTED = 0.00	
CATALYST VOLUME (ml) = 1.20		H2 (mole %) = 47.56		TIME PERIOD (hr) = 5.50	
TEMPERATURE (°C) = 400.00		N2 (mole %) = 5.01			
PRESSURE (psig) = 1100.00					

CATALYST NAME = 10DAN59		REFERENCE # = PR571		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 203.00						
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00		LIQUID COLLECTED (gm) = 0.00						
CATALYST VOLUME (ml) = 0.75		CO (mole %) = 47.43		% WATER COLLECTED = 0.00		% WATER COLLECTED = 0.00						
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56		TIME PERIOD (hr) = 21.00		TIME PERIOD (hr) = 21.00						
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.01										
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT		PRODUCT		PRODUCT		N/B mole %
						wt %	w/ CO2	wt %	w/ CO2	wt %	w/ CO2	
1	H2	2.02	3106.433	13.51	6.69	43.26						
2	N2	28.00	50.491	34.93	1.25	8.07						
3	CO	28.10	325.158	203.21	7.23	46.76						
4	CO2	44.01	10.587	7.82	0.18	1.15	70.03					
5	CH4	16.04	500.223	0.77	0.05	0.31	6.90					
6	C2H6	30.07	143.155	0.22	0.01	0.05	2.00					
7	C3H8	44.10	67.648	0.10	0.00	0.02	0.92					
9	CH3OH	32.04	418.254	1.64	0.05	0.33	14.72					
8	C4H10	58.12	47.108	0.07	0.00	0.01	0.65					
10	C2H5OH	46.07	0	0.00	0.00	0.00	0.00					
12	i-C3H7OH	60.10	0	0.00	0.00	0.00	0.00					
11	n-C3H7OH	60.10	28.606	0.06	0.00	0.01	0.52					#DIV/0!
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00	0.00					
14	i-C4H9OH	74.12	255.811	0.48	0.01	0.04	4.26					
13	n-C4H9OH	74.12	0	0.00	0.00	0.00	0.00					0.0
16	Me-2-Butanol	88.15	0	0.00	0.00	0.00	0.00					0.00
REACTANT GASES 1-3 =				251.65	15.17		CO MOLAR CONVERSION (N2 BASIS) = 38.77					
PRODUCT GASES 4-17 w/ CO2 =				11.17	0.30		H2 MOLAR CONVERSION (N2 BASIS) = 43.51					
PRODUCT GASES 5-17 w/o CO2 =				3.35	0.12							
TOTAL HYDROCARBONS =				1.17	0.06	0.38	10.47	19.99	34.94	50.15		
C2+ HYDROCARBONS =				0.40	0.01	0.07	3.57	3.73	11.93	9.36		
TOTAL ROH/TOTAL HC =				1.86	0.99							
TOTAL ALCOHOLS =				2.18	0.06	0.38	19.50	19.87	65.06	49.85	100.00	100.00
C1-C2 ALCOHOLS =				1.64	0.05	0.33	14.72	17.37	49.11	43.58	75.48	87.42
C3 ALCOHOLS =				0.06	0.00	0.01	0.52	0.33	1.73	0.82	2.67	1.65
C4 ALCOHOLS =				0.48	0.01	0.04	4.26	2.17	14.22	5.45	21.85	10.94
C3-C4 ROH/TOTAL ROH =				0.25	0.13							
N/B C3-C4 ALCOHOLS =				0.12	0.15							
ROH ACTIVITY (OFFGAS BASIS) =				0.071	g/g cat/hr	5.90	lb/lb3/hr	OFFGAS BASIS				
ROH ACTIVITY (CO FEEDGAS BASIS) =				0.070	g/g cat/hr	5.90	lb/lb3/hr	CARBON MASS BALANCE (%) = 104.67				
HC ACTIVITY (OFFGAS BASIS) =				0.038	g/g cat/hr	3.17	lb/lb3/hr	HYDROGEN MASS BALANCE (%) = 96.08				
								OXYGEN MASS BALANCE (%) = 105.82				

CATALYST NAME = 10DAN65		FEED RATE (ccm) =		OFFGAS RATE (ccm) =		LIQUID COLLECTED (gm) =		TIME PERIOD (hr) =		216.00	
REFERENCE # = PR520		H2/CO RATIO =		200.00		1.00		47.43		0.00	
CATALYST WEIGHT (gm) =		CO (mole %) =		47.43		47.56		5.01		20.00	
CATALYST VOLUME (ml) =		H2 (mole %) =		47.56		5.01					
TEMPERATURE (°C) =		N2 (mole %) =									
PRESSURE (psig) =											
GASES	Molecular	GC AREA	OFFGAS weight	OFFGAS molar	OFFGAS mole %	PRODUCT wt %	PRODUCT w/CO2	PRODUCT mole %	PRODUCT w/o CO2	PRODUCT mole %	PRODUCT w/o CO2
	Weight		ugrams	umoles	total	w/CO2					
1	H2	3033.15	13.19	6.53	45.90						
2	N2	28.00	26.75	0.96	6.71						
3	CO	28.10	185.25	6.59	46.33						
4	CO2	44.01	3.95	0.09	0.63	68.96		59.87			
5	CH4	16.04	181.912	0.28	0.12	4.89		11.66	15.77	29.04	
6	C2H6	30.07	48.752	0.08	0.02	1.33		1.69	4.28	4.21	
7	C3H8	44.10	23.775	0.04	0.01	0.63		0.55	2.03	1.36	
9	CH3OH	32.04	291.781	1.15	0.25	20.03		23.88	64.53	59.52	93.43
8	C4H10	58.12	37.909	0.06	0.01	1.03		0.67	3.31	1.68	
10	C2H5OH	46.07	0	0.00	0.00	0.00		0.00	0.00	0.00	
12	i-C3H7OH	60.10	0	0.00	0.00	0.00		0.00	0.00	0.00	
11	n-C3H7OH	60.10	15.898	0.03	0.00	0.56		0.36	1.82	0.89	
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00		0.00	0.00	0.00	
14	i-C4H9OH	74.12	78.929	0.15	0.01	2.56		1.32	8.26	3.29	11.07
13	n-C4H9OH	74.12	0	0.00	0.00	0.00		0.00	0.00	0.00	0.00
16	Me-2-Butanol	88.15	0	0.00	0.00	0.00		0.00	0.00	0.00	0.00
REACTANT GASES 1-3 =		225.19	14.08								
PRODUCT GASES 4-17 w/CO2 =		5.73	0.15								
PRODUCT GASES 5-17 w/o CO2 =		1.78	0.06								
TOTAL HYDROCARBONS =		0.45	0.02		0.15	7.88		14.56	25.39	36.29	
C2+ HYDROCARBONS =		0.17	0.00		0.03	2.99		2.91	9.62	7.25	
TOTAL ROH/TOTAL HC =		2.94	1.76								
TOTAL ALCOHOLS =		1.33	0.04		0.27	23.16		25.56	74.61	63.71	100.00
C1-C2 ALCOHOLS =		1.15	0.04		0.25	20.03		23.88	64.53	59.52	93.43
C3 ALCOHOLS =		0.03	0.00		0.00	0.56		0.36	1.82	0.89	1.40
C4 ALCOHOLS =		0.15	0.00		0.01	2.56		1.32	8.26	3.29	11.07
C3-C4 ROH/TOTAL ROH =		0.14	0.07								
N/B C3-C4 ALCOHOLS =		0.22	0.27								
ROH ACTIVITY (OFFGAS BASIS) =		0.050			4.45	1b/lb3/hr					108.12
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.046			4.45	1b/lb3/hr					106.38
HC ACTIVITY (OFFGAS BASIS) =		0.017			1.51	1b/lb3/hr					108.99

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CATALYST NAME = 10DAN67		FEED RATE (sccm) = 200.00		OFFGAS RATE (sccm) = 210.00															
REFERENCE # = PR597		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00															
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.43		% WATER COLLECTED = 0.00															
CATALYST VOLUME (ml) = 0.60		H2 (mole %) = 47.56		TIME PERIOD (hr) = 24.00															
TEMPERATURE (°C) = 400.00		N2 (mole %) = 5.01																	
PRESSURE (psig) = 1100.00																			
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT wt % w/ CO2	PRODUCT mole % w/ CO2	PRODUCT wt % w/o CO2	PRODUCT mole % w/o CO2	PRODUCT ROH only	PRODUCT mole % ROH only	N/B mole %							
1	H2	2.02	13.23	6.55	44.14														
2	N2	28.00	32.33	1.15	7.78														
3	CO	28.10	198.02	7.05	47.48														
4	CO2	44.01	2.41	0.05	0.37	70.09	62.66												
5	CH4	16.04	59.472	0.09	0.04	2.66	6.53	8.90	17.49										
6	C2H6	30.07	18.305	0.03	0.01	0.83	1.09	2.77	2.91										
7	C3H8	44.10	7.522	0.01	0.00	0.33	0.30	1.11	0.79										
9	CH3OH	32.04	191.028	0.75	0.16	21.82	26.80	72.94	71.77	84.86	91.87								
8	C4H10	58.12	8.388	0.01	0.00	0.38	0.26	1.26	0.69										
10	C2H5OH	46.07	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00								
12	i-C3H7OH	60.10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00								
11	n-C3H7OH	60.10	41.728	0.08	0.01	2.46	1.61	8.23	4.32	9.57	5.53	#DIV/0!							
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00								
14	i-C4H9OH	74.12	26.47	0.05	0.00	1.43	0.76	4.78	2.03	5.57	2.60								
13	n-C4H9r	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0							
16	Me-2-Br	88.15	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00								
REACTANT GASES 1-3 = 243.58												CO MOLAR CONVERSION (N2 BASIS) = 35.54							
PRODUCT GASES 4-17 w/ CO2 = 3.44												H2 MOLAR CONVERSION (N2 BASIS) = 40.24							
PRODUCT GASES 5-17 w/o CO2 = 1.03																			
TOTAL HYDROCARBONS = 0.14												8.17		14.05		21.88			
C2+ HYDROCARBONS = 0.05												1.54		5.15		4.39			
TOTAL ROH/TOTAL HC = 6.12																			
TOTAL ALCOHOLS = 0.88												25.71		85.95		78.12		100.00	
C1-C2 ALCOHOLS = 0.75												21.82		72.94		71.77		84.86	
C3 ALCOHOLS = 0.08												2.46		1.61		4.32		9.57	
C4 ALCOHOLS = 0.05												1.43		0.76		2.03		5.57	
C3-C4 ROH/TOTAL ROH = 0.15																			
N/B C3-C4 ALCOHOLS = 1.72																			
ROH ACTIVITY (OFFGAS BASIS) = 0.031												lb/ft3/hr		CARBON MASS BALANCE (%) = 106.53					
ROH ACTIVITY (CO FEEDGAS BASIS) = 0.030												lb/ft3/hr		HYDROGEN MASS BALANCE (%) = 98.53					
HC ACTIVITY (OFFGAS BASIS) = 0.005												lb/ft3/hr		OXYGEN MASS BALANCE (%) = 107.14					

CATALYST NAME = 11DAN44		REFERENCE # = PRI26		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 214.00			
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.06		LIQUID COLLECTED (gm) = 0.06			
CATALYST VOLUME (ml) = 0.65		CO (mole %) = 47.43		% WATER COLLECTED = 0.00		% WATER COLLECTED = 0.00			
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56		TIME PERIOD (hr) = 5.25		TIME PERIOD (hr) = 5.25			
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.01							
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CATALYST NAME =		I11DAN45		FEED RATE (scfm) =		200.00		OFFGAS RATE (scfm) =		216.00	
REFERENCE # =		125		H2/CO RATIO =		1.00		LIQUID COLLECTED (gm) =		0.00	
CATALYST WEIGHT (gm) =		1.00		CO (mole %) =		47.43		% WATER COLLECTED =		0.00	
CATALYST VOLUME (ml) =		0.85		H2 (mole %) =		47.56		TIME PERIOD (hr) =		26.50	
TEMPERATURE (°C) =		400.00		N2 (mole %) =		5.01					
PRESSURE (psig) =		1100.00									
GASES	Molecular Weight	GC AREA	OFFGAS weight	OFFGAS umoles	OFFGAS mole % total	PRODUCT wt % w/CO2	PRODUCT mole % w/CO2	PRODUCT wt % w/o CO2	PRODUCT mole % w/o CO2	PRODUCT ROH only	PRODUCT N/B mole % ROH only
1	H2	2.02	3160.72	13.75	6.81	43.86					
2	N2	28.00	48.78	33.75	1.21	7.77					
3	CO	28.10	329.81	206.11	7.34	47.27					
4	CO2	44.01	6.06	4.48	0.10	0.66	63.63	59.65			
5	CH4	16.04	41.43	0.06	0.00	0.03	0.91	2.33	2.49	5.78	
6	C2H6	30.07	34.01	0.05	0.00	0.01	0.75	1.03	2.07	2.56	
7	C3H8	44.10	22.49	0.03	0.00	0.00	0.49	0.45	1.34	1.13	
9	CH3OH	32.04	419.48	1.65	0.05	0.33	23.43	30.18	64.43	74.80	84.21
8	C4H10	58.12	43.9	0.07	0.00	0.01	0.97	0.69	2.66	1.70	
10	C2H5OH	46.07	5.43	0.01	0.00	0.00	0.19	0.17	0.53	0.43	0.48
12	i-C3H7OH	60.10	9.97	0.02	0.00	0.00	0.34	0.24	0.94	0.58	0.66
11	n-C3H7OH	60.10	21.52	0.04	0.00	0.00	0.62	0.43	1.71	1.06	1.19
15	sec-C4H9OH	74.12	49.55	0.09	0.00	0.01	1.31	0.73	3.60	1.81	2.03
14	i-C4H9OH	74.12	278.26	0.52	0.01	0.05	7.36	4.10	20.23	10.15	11.43
13	n-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	Me-2-Butanol	88.15	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
REACTANT GASES 1-3 =		253.61		15.35				CO MOLAR CONVERSION (N2 BASIS) =		35.71	
PRODUCT GASES 4-17 w/CO2 =		7.03		0.17				H2 MOLAR CONVERSION (N2 BASIS) =		40.51	
PRODUCT GASES 5-17 w/o CO2 =		2.56		0.07							
TOTAL HYDROCARBONS =		0.22		0.01		0.05		3.11		4.51	
C2+ HYDROCARBONS =		0.16		0.00		0.02		2.21		2.18	
TOTAL ROH/TOTAL HC =		10.68		7.95				6.07		5.39	
TOTAL ALCOHOLS =		2.34		0.06		0.39		33.26		35.84	
C1-C2 ALCOHOLS =		1.66		0.05		0.33		23.63		30.35	
C3 ALCOHOLS =		0.07		0.00		0.01		0.96		0.66	
C4 ALCOHOLS =		0.61		0.01		0.05		8.67		4.83	
C3-C4 ROH/TOTAL ROH =		0.29		0.15							
N/B C3-C4 ALCOHOLS =		0.07		0.08							
ROH ACTIVITY (OFFGAS BASIS) =		0.081		g/g cat/hr		5.93		lb/n3/hr		CARBON MASS BALANCE (%) =	
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.075		g/g cat/hr		5.93		lb/n3/hr		HYDROGEN MASS BALANCE (%) =	
HC ACTIVITY (OFFGAS BASIS) =		0.008		g/g cat/hr		0.56		lb/n3/hr		OXYGEN MASS BALANCE (%) =	

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