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HETEROGENEOUS CATALYTIC PROCESS FOR ALCOHOL FUELS FROM SYNGAS

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Table of Contents

1. Executive Summary.....	1
2. Project Objectives	2
3. Project Organization.....	2
4. Technical Progress	3
4.1. Task 1 – Catalyst Studies.....	3
4.1.1. Catalyst Synthesis.....	3
4.1.1.1. Introduction	3
4.1.1.2. Catalyst Synthesis Results	3
4.1.2. Catalyst Evaluation.....	4
4.1.2.1. Introduction	4
4.1.2.4. Catalyst Tests	5
4.1.2.5. Data Handling.....	5
4.1.3. Task 1 Conclusions.....	6
4.2. Task 2 – Engineering Studies	10
4.2.1. Reaction Engineering	10
4.2.1.1. Introduction	10
4.2.1.2. Reaction Engineering Activities.....	10
4.2.2. Mathematical Process Development.....	10
4.2.2.1. Introduction	10
4.2.2.2. Acid Gas Removal	11
4.2.2.3. Options for Varying Syngas Ratio	11
4.2.2.4. Water Removal from the Alcohol Product.....	11
4.2.3. Task 2 Conclusions	11
5. Appendix A — Catalyst Tests	13

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, increase rates to 20 lb/ft³/hr (ca. 350 g/kg-hr), and have conversions of greater than 20%. Earlier work in this organization has shown that a potassium-modified Zn-Cr-Mn-O based catalyst system had alcohol selectivities as high as 70-80 wt%, but the overall alcohol rate was only 11 lb/ft³/hr (ca. 190 g/kg-hr).

To investigate a number of aspects involved in the composition and preparation of these catalysts, a statistically designed set of experiments has been planned. The nineteen catalysts for this fractional factorial designed experiment have been prepared and are currently undergoing testing. Preliminary catalytic performances look quite promising, with some catalysts having selectivities to alcohols (excluding CO₂) as high as 95 wt% and alcohol activities of 4.5 lb/ft³/hr (ca. 65 g/kg-hr). Isobutanol selectivities as high as 34% are seen. The relatively high yield of isobutanol is believed to be formed because the synthesis proceeds predominately via an aldol condensation mechanism over the promoted spinel oxide catalysts. The condensation occurs via beta-addition; thus, the reaction terminates at the branched 2-methyl-1-propanol (iso-butanol) product.

A new data handling system has been installed and is operating. Data collected on the CALS system is transferred over EtherNet to a Macintosh Quadra 700, where a newly devised Excel spreadsheet has made data reduction faster, more reliable, and more flexible.

When testing of the current designed set is completed, an evaluation of the effects of process variables such as pressure, temperature, syngas ratio, etc., will be conducted on the most promising formulations.

Future work will include copper-based catalysts, dealing with different aspects of the support, the impregnation of the metals, and choice of promoters.

The slurry reaction system has been under preparation for catalyst testing. The SOP and necessary safety inspections have been completed and the shakedown of the system is almost complete. When the analytical system is brought up to operating condition, a standard methanol catalyst will be tested in the slurry phase.

Process synthesis work is proceeding toward the development of a computer model which uses simulated annealing to optimize the flowsheet variables. The first phase of the effort, development of a base case flowsheet with a material and energy balance, is nearing completion. The work has focused on three areas; acid gas removal, options for varying the H_2/CO ratio, and water removal from the alcohol product. The requirement of the acid gas removal process is to selectively remove H_2S/COS and CO_2 from syngas. Numerous solvents were considered, and the main contenders for coal generated synthesis gas are Rectisol and Selexol. To incorporate flexibility into the H_2/CO ratio, the base case design consists of a coal gasifier in parallel with a steam/natural gas reformer. Molecular sieves provide an option for water removal from the product, but before continuing work in this area, research on the acceptable water specification will be conducted.

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) C_1-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.

Previous work at UCC on a methanol-isobutanol catalyst used consecutive Hyper-Greco-Latin Squares to identify and bracket levels of important variables in catalyst formulation and preparation. Catalysts with alcohol selectivities as high as 70-80 wt% were developed, but the overall alcohol rate was only 11 lb/ft³/hr (ca. 190 g/kg-hr). It was shown that catalyst performance is more dependent on the catalyst formulation than the catalyst preparation techniques.

A 16-run, 8-variable fractional factorial design had been set up to study the variables in the catalyst formulation and preparation of the methanol-isobutanol catalyst. Several difficulties in the preparation were discovered and solutions were found. We report the current progress of the designed set and other laboratory changes that have improved our ability to effectively screen catalysts.

4.1.1.2. Catalyst Synthesis Results

The nineteen catalysts for the fractional factorial design experiment have been prepared and are currently undergoing testing. Early tests are quite promising with some catalysts having selectivities to alcohols (excluding CO₂) as high as 95 wt% and alcohol activities (offgas basis) of 4.5 lb/ft³/hr (ca. 65 g/kg-hr).

We also have started preparation of a copper-based low-temperature higher alcohol catalyst. We have prepared the spinel oxide, Co_xCu_{1-x}Cr₂O₄, where x ranges from 0 to 1, using a coprecipitation method. It is hypothesized that the introduction of a Fischer-Tropsch metal such as Co to the Cu 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 or by modifying 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 in our isobutanol catalyst.

4.1.2. Catalyst Evaluation

4.1.2.1. Introduction

Project goals are to produce a catalyst for the production of higher alcohols (C_2 and greater) from syngas that has selectivities to oxygenates $> 90\%$ and with activities > 20 lb/ft³/hr (ca. 350 g/kg-hr). This catalyst would be utilized for synthesizing higher alcohols for use as a gasoline additive and octane enhancer.

Previously known catalysts for Higher Alcohol Synthesis (HAS) can be divided into the following classes based on the alcohol product distribution.

Modified Fischer-Tropsch (FT) and Group VIII Metal-Based Catalysts. Traditional Fischer-Tropsch catalysts can be made to produce appreciable amounts of oxygenates (alcohols, aldehydes, acids, ketones and esters) by addition of alkali. Typical FT metals include Fe, Co, Ni, and Ru. The products observed follow an Anderson-Schulz-Flory (ASF) distribution, characteristic of the linear condensation polymerization mechanism. Molybdenum sulfide catalysts promoted with alkali also produce the ASF product distribution. Rh-based catalysts are similar, but produce more C_{2+} oxygenates.

Modified Methanol or Iso-Alcohol Catalysts. These consist of Methanol Synthesis catalysts modified with alkali promoters, forming significant quantities of branched primary alcohols. These can be divided into two classes:

(a) The "high-temperature" ($\sim 400^\circ\text{C}$ operating temperature) catalysts, which are essentially alkali-modified ZnCrO and ZnMnCrO systems. The major products are methanol and iso-butanol, but small amounts of ketones, secondary alcohols, ethers and hydrocarbons are also observed. The formation of higher alcohols is maximized by operating under hydrogen lean conditions (syngas ratio of $H_2/CO = 1$).

The operating catalyst is thought to consist of a microcrystalline $ZnCr_2O_4$ spinel oxide phase. Manganese can be substituted for chromium to reduce the acidity of the spinel, thus decreasing the amounts of ethers and hydrocarbons formed. The presence of alkali is thought to be essential to promote HAS.

The reaction is believed to proceed by a combination of hydrogenation and carbon-carbon bond formation via aldol condensation. This should be contrasted with the modified FT

catalysts which proceed by a classical CO insertion/hydrogenation mechanism. The result of this is the formation of branched alcohols with a non-ASF product distribution.

Our research in this quarter has concentrated on the high-temperature modified methanol synthesis catalysts and the updating of the laboratory computer, system software and the network interface capabilities.

4.1.2.4. Catalyst Tests

We are now in the process of testing the catalyst designed set based on promoted zinc-chromium spinel oxides. These materials were the catalysts of choice for methanol synthesis until the introduction of syngas desulfurization techniques allowed the use the more active copper-based catalysts. Alkalization of both the Cu metal and the Zn/Cr spinels is known to promote higher alcohol synthesis (HAS)

The designed set was constructed to investigate a number of variables affecting catalyst composition and synthesis. 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.

Initial results look promising (see Table 1): a number of the catalysts tested are highly selective to alcohols (85-95%) with between 25 - 40% of the alcohols being C₂'s or higher. Isobutanol selectivities between 19-34% are common. The activities are a respectable 4-6 lbs/ft³-hr (60-75 g/kg-hr). Data on the compositions and preparation procedures for these catalysts are listed in Tables 2 and 3. Individual data sheets for each catalyst run are included in Appendix A.

The alcohols produced are almost exclusively methanol and isobutanol. The isobutanol is believed to be formed because the HAS proceeds predominately via an aldol condensation mechanism over the promoted spinel oxide catalysts. The condensation occurs via beta-addition; thus the reaction terminates at the branched 2-methyl-1-propanol (isobutanol) product.

4.1.2.5. Data Handling

An Excel spreadsheet has been incorporated into the data reduction system on a Macintosh Quadra 700 platform, replacing a slow and cumbersome Fortran program residing on the VAX system. Removal of the VAX system from the data reduction equation has also eliminated the communications link previously required between the CALS (data acquisition system) and the VAX system. The Quadra is linked to the CALS via an EtherNet network.

A new program, designated SUMTP, was developed and specifically customized to accumulate, combine and report analytical data generated by the fuel alcohols GC. All run data are systematically deposited into an Excel data file in sequential order. Simple cut and

paste operations allow rapid and precise data transfer from the Excel data file to the "DOE Results" spreadsheet. Another feature of the SUMTP program is the ability to easily graph and/or chart the data in a variety of formats. The fast and easy data reduction will also facilitate catalyst testing since the technician will be able to see the catalytic results before the catalyst test is finished and decide whether additional testing is required.

4.1.3. Task 1 Conclusions

The synthesis of the new set of methanol-isobutanol catalysts has been completed. Testing is ongoing. Another set of experiments based upon the catalytic results will be planned to further optimize the catalyst with regard to activity and selectivity.

Initial results from the isobutanol catalyst designed set appear to be promising. A number of the catalysts tested are highly selective to alcohols (85-95%) with between 25 - 40% of the alcohols being C₂'s or higher. Isobutanol selectivities between 19-34% are common. The activities are in the range of 4-6 lbs/ft³-hr (60-75 g/kg-hr).

The relatively high yield of isobutanol is believed to be formed because the HAS proceeds predominately via an aldol condensation mechanism over the promoted spinel oxide catalysts. The condensation occurs via beta-addition; thus, the reaction terminates at the branched 2-methyl-1-propanol (iso-butanol) product

A new data handling system has been installed and is operating. Data collected on the CALS system is transferred over EtherNet to a Macintosh Quadra 700, where a newly devised Excel spreadsheet has made data reduction faster, more reliable, and more flexible.

When testing of the current designed set is completed, an evaluation of the effects of process variables such as pressure, temperature, syngas ratio, etc., will be conducted on the most promising formulations.

Future work will include copper-based catalysts, dealing with different aspects of the support, the impregnation of the metals, and choice of promoters. We have finished preparing Co_xCu_{1-x}Cr₂O₄, where x ranges from 0, 0.25, 0.5, 0.75, and 1, for use in our copper-based low temperature higher alcohol catalysts.

Table 1. Summary of Catalyst Tests

CATALYST SAMPLE	ACTIVITY [1]	SELECTIVITY TO ALCOHOLS [2]				C3 (wt%)[3]	C4 (wt%)[4]	COMMENTS
		C1 (wt%)	C2 (wt%)	C3 (wt%)[3]	C4 (wt%)[4]			
10DAN50	4.38	87.88	55.32	0.00	16.34	16.22	CENTER POINT	
10DAN50R	3.33	70.11	52.14	0.00	11.60	6.37	CENTER POINT	
10DAN57	6.20	93.53	67.32	0.00	3.72	20.09	CENTER POINT	
10DAN57R	6.18	83.99	65.74	0.00	1.76	16.09	CENTER POINT	
3DAN90	9.78	26.00	4.64	3.50	13.50	4.37		
11DAN45	5.44	91.44	64.43	0.53	2.65	23.83		
11DAN44	0.78	65.00	47.86	0.00	9.09	8.05		
10DAN47	3.38	94.78	81.32	1.62	6.55	5.29		
10DAN54	6.30	85.59	41.87	1.51	5.08	34.38		
10DAN49	0.36	69.78	57.79	0.00	11.99	0.00		
10DAN55	7.30	89.93	55.34	1.65	9.32	23.61		
10DAN52	2.79	93.62	81.92	0.00	1.97	9.72		
10DAN53	4.47	79.28	70.01	0.00	0.00	9.26		
10DAN48	3.85	80.80	54.07	0.00	9.22	17.52		
10DAN51	5.80	80.51	57.77	0.00	1.85	19.01		
10DAN56	5.25	96.31	71.17	0.00	3.46	19.25		
10DAN24	3.50	92.61	63.31	0.00	4.43	24.88		

[1] ACTIVITY= lbs/ft³-hr

[3] product is almost exclusively n-propanol

[2] SELECTIVITY= wt%

[4] product is almost exclusively iso-butanol

Table 2. Catalyst Support Compositions

Chemical Formula of Support	Sample Reference (pH/Temp./°C/Time.Hr)	Zn	Mn	Cr	O	Zn Mn+Cr	Mn Cr	pH	Temp (°C)	Time (hr)	BET S.A. (m ² /g)	Pore Volume (cc/g)	Pore Diameter (nm)
Zn ₂ 0Mn _{0.33} Cr _{0.67} O _{3.5}	10DAN60(9.0/400/11)	2	0.33	0.67	3.5	2.00	0.49	9.0	400.0	11.0	79.9	--	--
Zn ₃ 0Mn _{0.50} Cr _{0.50} O _{4.5}	3DAN134(9.0/500/18)	3	0.5	0.5	4.5	3.00	1.00	9.0	500.0	18.0	35.6	0.250	24.4
	10DAN19(9.0/500/4)	3	0.5	0.5	4.5	3.00	1.00	9.0	500.0	4.0	55.3		
	10DAN19(9.0/300/18)	3	0.5	0.5	4.5	3.00	1.00	9.0	300.0	18.0	112.4		
	3DAN134(9.0/300/4)	3	0.5	0.5	4.5	3.00	1.00	9.0	300.0	4.0	69.4	0.460	18.0
Zn ₃ 0Cr _{1.00} O _{4.5}	10DAN22(9.0/500/18)	3	0	1	4.5	3.00	0.00	9.0	500.0	18.0	39.0	0.097	26.1
	10DAN22(9.0/500/4)	3	0	1	4.5	3.00	0.00	9.0	500.0	4.0	43.0		
	10DAN22(9.0/300/18)	3	0	1	4.5	3.00	0.00	9.0	300.0	18.0	90.2		
	10DAN22(9.0/300/4)	3	0	1	4.5	3.00	0.00	9.0	300.0	4.0	127.6	0.234	16.0
Zn ₂ 0Mn _{0.33} Cr _{0.67} O _{3.5}	3DAN132(9.0/400/11)	2	0.33	0.67	3.5	2.00	0.49	9.0	400.0	11.0	80.1		
Zn ₁ 0Mn _{0.50} Cr _{0.50} O _{4.5}	10DAN24(9.0/500/18)	1	0.5	0.5	4.5	1.00	1.00	9.0	500.0	18.0	35.3	0.243	26.8
	3DAN127(9.0/500/4)	1	0.5	0.5	4.5	1.00	1.00	9.0	500.0	4.0	43.6		
	3DAN127(9.0/300/18)	1	0.5	0.5	4.5	1.00	1.00	9.0	300.0	18.0	96.2		
	10DAN24(9.0/300/4)	1	0.5	0.5	4.5	1.00	1.00	9.0	300.0	4.0	114.1	0.240	8.5
Zn ₁ 0Cr _{1.00} O _{2.5}	11DAN42(9.0/500/18)	1	0	1	2.5	1.00	0.00	9.0	500.0	18.0	1.6	0.005	11.7
	11DAN42(9.0/500/4)	1	0	1	2.5	1.00	0.00	9.0	500.0	4.0	3.3		
	10DAN26(9.0/300/18)	1	0	1	2.5	1.00	0.00	9.0	300.0	18.0	63.7		
	10DAN26(9.0/300/4)	1	0	1	2.5	1.00	0.00	9.0	300.0	4.0	77.4	0.027	5.4
Zn ₂ 0Mn _{0.33} Cr _{0.67} O _{3.5}	10DAN28(9.0/400/11)	2	0.33	0.67	3.5	2.00	0.49	9.0	400.0	11.0	77.1		

Table 3. Catalyst Composition and Metal Loadings

Catalyst Reference	Chemical Formula of Support	Support Reference (pH/Temp. °C/Time.Hr)	K Loading (umole/m2)	KNO3 (g/kg cat)	Pd Loading (umole/m2)	Pd(NH3)(NO3)2 (g/kg cat)	Ce Loading (umole/m2)	Ce(NO3)3 (g/kg cat)	Reduction Temp
10DAN66	Zn2.0Mn.33Cr.67O3.5	10DAN60(9.0/400/11)	6.65	0.26872	2.5	0.29827	8.3	1.44038	450
10DAN53	Zn3.0Mn0.50Cr0.50O4.5	3DAN134 (9.0/500/18)	13.3	0.23957	5	0.26592	16.6	1.28414	600
10DAN47		10DAN19(9.0/500/4)	13.3	0.37179	0	0.00000	0	0.00000	300
10DAN54		10DAN19(9.0/300/18)	0	0.00000	5	0.83887	0	0.00000	300
10DAN52		3DAN134 (9.0/300/4)	0	0.00000	0	0.00000	16.6	2.50197	600
10DAN65	Zn3.0Cr1.0O4.5	10DAN22 (9.0/500/18)	0	0.00000	5	0.29098	16.6	1.40520	300
10DAN58		10DAN22(9.0/500/4)	0	0.00000	0	0.00000	0	0.00000	600
10DAN48		10DAN22(9.0/300/18)	13.3	0.60653	5	0.67323	0	0.00000	600
10DAN49		10DAN22 (9.0/300/4)	13.3	0.85776	0	0.00000	16.6	4.59776	300
10DAN50	Zn2.0Mn.33Cr.67O3.5	3DAN132(9.0/400/11)	6.65	0.26918	2.5	0.29878	8.3	1.44285	450
10DAN59	Zn1.0Mn.50Cr.50O4.5	10DAN24 (9.0/500/18)	0	0.00000	0	0.00000	0	0.00000	600
11DAN45		3DAN127(9.0/500/4)	0	0.00000	5	0.32540	16.6	1.57139	300
11DAN44		3DAN127(9.0/300/18)	13.3	0.64649	0	0.00000	16.6	3.46535	300
10DAN51		10DAN24 (9.0/300/4)	13.3	0.76746	5	0.85186	0	0.00000	600
3DAN90	Zn1.0Cr1.0O2.5	11DAN42 (9.0/500/18)	13.3	0.01076	0	0.00000	0	0.00000	300
10DAN67		11DAN42(9.0/500/4)	13.3	0.02190	5	0.02431	16.6	0.11739	600
10DAN56		10DAN26(9.0/300/18)	0	0.00000	0	0.00000	16.6	2.29582	600
10DAN55		10DAN26 (9.0/300/4)	0	0.00000	5	0.57766	0	0.00000	300
10DAN57	Zn2.0Mn.33Cr.67O3.5	10DAN28 (9.0/400/11)	6.65	0.21565	2.5	0.28771	8.3	1.38938	450

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 the shakedown of the system is almost complete. The system has been pressure-tested, but there have been many problems with the GC which are still under investigation. In the near future we will be running Dowtherm, the solvent of choice at the present time, through the system. These tests will be used to: 1) determine the actual temperature capabilities of the reactor (we are limited by an o-ring slightly removed from the reactor), and 2) become familiar with the capabilities and handling of Dowtherm. Once the GC is fixed we will be running a standard methanol catalyst in the slurry phase for the initial testing of the system.

A nonlinear regression program has been written to be used in fitting kinetics to the reaction data.

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 eventual goal of the Task 2 Process Synthesis work is the development of a computer model which uses simulated annealing to optimize the flowsheet variables. The first phase of the effort, development of a base case flowsheet with a material and energy balance, is nearing completion. The flowsheet is being developed by WVU with input from UCC. In addition to the base case, we have determined options for future case studies. The UCC

work has focused on three areas; acid gas removal, options for varying the H_2/CO ratio, and water removal from the alcohol product.

4.2.2.2. Acid Gas Removal

The requirement of the acid gas removal process is to selectively remove H_2S/COS and CO_2 from syngas. Numerous solvents were considered, and the main contenders for coal generated synthesis gas are Rectisol and Selexol. Both solvents have a large number of commercial installations in comparison to other potential solvents. Also, design information is more readily obtainable.

The tradeoff between Rectisol and Selexol is the selectivity. An economic comparison between the solvents was found in a DOE report (Houston Area Medium Btu Coal Gasification Project, Union Carbide, June 1982), and Rectisol was found to be more economical than Selexol. However, there are differences in the coal as well as the flowsheet, and next quarter we will do an economic evaluation using our conditions.

4.2.2.3. Options for Varying Syngas Ratio

As part of the energy park concept, we need to incorporate flexibility into the H_2/CO ratio. The base case design consists of a coal gasifier in parallel with a steam/natural gas reformer. Based on literature sources and discussions with Texaco, we will consider the following design options:

- Coal gasifier followed by a sour shift converter
- Partial oxidation of natural gas

4.2.2.4. Water Removal from the Alcohol Product

Molecular sieves are being considered for removing water from the alcohol product. Since the amount of water in the feed to the sieve bed is a function of reactor operating conditions, a study was done containing varying amounts of water in the feed. The results indicate molecular sieves can be used to dry the product, but the water specification in the final product has significant impact on the economics. Therefore, before continuing work on the molecular sieve unit, research on the acceptable water specification will be conducted. Optimistically, the water specification may be achievable by operating the reactor to minimize the water content; and thus, eliminating water removal equipment.

4.2.3. Task 2 Conclusions

The slurry reaction system has been under preparation for catalyst testing. The SOP and necessary safety inspections have been completed and the shakedown of the system is almost complete. When the analytical system is brought up to operating condition, a standard methanol catalyst will be tested in the slurry phase.

Process synthesis work is proceeding toward the development of a computer model which uses simulated annealing to optimize the flowsheet variables. The first phase of the effort, development of a base case flowsheet with a material and energy balance, is nearing completion. The work has focused on three areas; acid gas removal, options for varying the H_2/CO ratio, and water removal from the alcohol product. The requirement of the acid gas removal process is to selectively remove H_2S/COS and CO_2 from syngas. Numerous solvents were considered, and the main contenders for coal generated synthesis gas are Rectisol and Selexol. To incorporate flexibility into the H_2/CO ratio, the base case design consists of a coal gasifier in parallel with a steam/natural gas reformer. Molecular sieves provide an option for water removal from the product, but before continuing work in this area, research on the acceptable water specification will be conducted.

5. Appendix A — Catalyst Tests

CAT/LYST NAME = 3DAN90		REFERENCE # = PR868		FEED RATE (scfm) = 200.00		OFFGAS RATE (scfm) = 132.00				
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.31		N2/CO RATIO = 0.31				
CATALYST VOLUME (ml) = 0.55		CO (mole %) = 47.43		% WATER COLLECTED = 0.00		TIME PERIOD (hr) = 19.00				
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56								
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.01								
GASES	Molecular Weight	GC AREA	OFFGAS weight ugrams	OFFGAS molar umoles	OFFGAS mole % total	PRODUCT wt % w/ CO2	PRODUCT mole % w/ CO2	PRODUCT wt % ROH only	PRODUCT mole % ROH only	N/B mole %
1	H2	2.02	11.05	5.47	37.20					
2	N2	28.00	24.14	0.86	5.86					
3	CO	28.10	158.10	5.63	38.27					
4	CO2	44.01	96.48	2.20	14.93	86.64	80.02			
5	CH4	16.04	3382.34	5.21	2.21	4.67	11.84	34.98	59.26	
6	C2H6	30.07	1399.79	2.18	0.49	1.96	2.65	14.66	13.25	
7	C3H8	44.10	1587.33	2.41	0.37	2.16	1.99	16.20	9.98	
9	CH3OH	32.04	175.48	0.69	0.15	0.62	0.78	4.63	3.93	17.81
8	C4H10	58.12	783.1	1.21	0.14	1.09	0.76	8.15	3.81	
10	C2H5OH	46.07	207.86	0.52	0.08	0.47	0.41	3.50	2.07	13.48
12	i-C3H7OH	60.10	452.96	1.10	0.12	0.98	0.66	7.36	3.33	28.31
11	n-C3H7OH	60.10	450.12	0.91	0.10	0.82	0.55	6.14	2.77	23.60
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	i-C4H9OH	74.12	132.77	0.25	0.02	0.22	0.12	1.66	0.61	6.38
13	n-C4H9OH	74.12	193.87	0.40	0.04	0.36	0.20	2.71	0.99	10.42
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 =		193.28		11.96		CO MOLAR CONVERSION (N2 BASIS) =		31.07		
PRODUCT GASES 4-17 w/ CO2 =		111.49		2.74		H2 MOLAR CONVERSION (N2 BASIS) =		33.18		
PRODUCT GASES 5-17 w/o CO2 =		14.89		0.55						
TOTAL HYDROCARBONS =		11.02		0.47		17.24		74.00		86.30
C2+ HYDROCARBONS =		5.81		0.15		5.40		39.02		27.05
TOTAL ROH/TOTAL HC =		0.35		0.16						
TOTAL ALCOHOLS =		3.87		0.08		3.47		26.00		13.70
C1-C2 ALCOHOLS =		1.21		0.03		1.09		8.14		5.99
C3 ALCOHOLS =		2.01		0.03		1.80		13.50		6.10
C4 ALCOHOLS =		0.65		0.01		0.58		4.37		1.60
C3-C4 ROH/TOTAL ROH =		0.69		0.56						
N/B C3-C4 ALCOHOLS =		0.98		0.96						
ROH ACTIVITY (OFFGAS BASIS) =		0.086		g/g cat/hr		9.78		lb/lb3/hr		
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.131		g/g cat/hr		9.78		lb/lb3/hr		
HC ACTIVITY (OFFGAS BASIS) =		0.245		g/g cat/hr		27.84		lb/lb3/hr		

[illegible]

CATALYST NAME = 10DAN47											
REFERENCE # = PRI73		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 220.00							
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00							
CATALYST VOLUME (ml) = 0.90		CO (mole %) = 47.43		% WATER COLLECTED = 0.00							
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.56		TIME PERIOD (hr) = 24.00							
PRESSURE (psig) = 1100.00		N2 (mole %) = 5.1									
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 mole %	PRODUCT N/B mole %
1	H2	2.02	13.76	6.81	39.92						
2	N2	28.00	33.68	1.20	7.05						
3	CO	28.10	335.32	8.89	52.12						
4	CO2	44.01	4.73	0.11	0.63	74.65	69.18				
5	CH4	16.04	24.35	0.04	0.01	0.59	1.50	2.33	4.88		
6	C2H6	30.07	16.25	0.03	0.00	0.40	0.54	1.58	1.76		
7	C3H8	44.10	13.91	0.02	0.00	0.33	0.31	1.31	1.00		
9	CH3OH	32.04	332.68	1.31	0.24	20.61	26.23	81.31	85.13	85.80	92.17
8	C4H10	58.12	0	0.00	0.00	0.00	0.00	0.00	0.00		
10	C2H5OH	46.07	10.4	0.03	0.00	0.41	0.36	1.62	1.18	1.71	1.28
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	51.89	0.11	0.01	1.66	1.13	6.55	3.66	6.91	3.96
15	sec-C4H9OH	74.12	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	#DIV/0!
14	i-C4H9OH	74.12	45.7	0.09	0.01	1.34	0.74	5.29	2.39	5.58	2.59
13	n-C4H9OH	74.12	0	0.00	0.00	0.00	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	0.00	0.00	0.00
REACTANT GASES 1-3 =			297.31	16.90		CO MOLAR CONVERSION (N2 BASIS) = 21.91					
PRODUCT GASES 4-17 w/ CO2 =			6.34	0.16		H2 MOLAR CONVERSION (N2 BASIS) = 40.36					
PRODUCT GASES 5-17 w/o CO2 =			1.61	0.05							
TOTAL HYDROCARBONS =			0.08	0.00	0.02	1.32	2.35	5.22	7.64		
C2+ HYDROCARBONS =			0.05	0.00	0.01	0.73	0.85	2.89	2.76		
TOTAL ROH/TOTAL HC =			18.14	12.10							
TOTAL ALCOHOLS =			1.52	0.04	0.26	24.02	28.46	94.78	92.36	100.00	100.00
C1-C2 ALCOHOLS =			1.33	0.04	0.24	21.02	26.60	82.94	86.31	87.51	93.45
C3 ALCOHOLS =			0.11	0.00	0.01	1.66	1.13	6.55	3.66	6.91	3.96
C4 ALCOHOLS =			0.09	0.00	0.01	1.34	0.74	5.29	2.39	5.58	2.59
C3-C4 ROH/TOTAL ROH =			0.12	0.07							
N/B C3-C4 ALCOHOLS =			1.24	1.53							
ROH ACTIVITY (OFFGAS BASIS) =			0.049	g/g cat/hr	3.38	lb/m3/hr	OFFGAS BASIS				
ROH ACTIVITY (CO FEEDGAS BASIS) =			0.044	g/g cat/hr	3.38	lb/m3/hr	CARBON MASS BALANCE (%) = 123.12				
HC ACTIVITY (OFFGAS BASIS) =			0.003	g/g cat/hr	0.19	lb/m3/hr	HYDROGEN MASS BALANCE (%) = 93.75				
							OXYGEN MASS BALANCE (%) = 124.41				

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 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	12.84	6.36	42.07							
2	N2	28.00	20.91	0.75	4.94							
3	CO	28.10	217.87	7.75	51.30							
4	CO2	44.01	8.68	0.20	1.31	81.41	77.18					
5	CH4	16.04	129.88	0.20	0.08	1.88	4.88	10.09	21.38			
6	C2H6	30.07	48.52	0.08	0.02	0.71	0.98	3.82	4.32			
7	C3H8	44.10	41.42	0.06	0.01	0.59	0.56	3.18	2.45			
9	CH3OH	32.04	272.77	1.07	0.22	10.05	13.09	54.07	57.37	66.91	81.24	
8	C4H10	58.12	27.12	0.04	0.00	0.39	0.28	2.12	1.24			
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	90.02	0.18	0.02	1.71	1.19	9.22	5.21	11.41	7.38	#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	
14	i-C4H9OH	74.12	155.85	0.29	0.03	2.72	1.53	14.62	6.71	18.09	9.50	
13	n-C4H9OH	74.12	27.62	0.06	0.01	0.54	0.30	2.90	1.33	3.59	1.88	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 =		251.62		14.86				CO MOLAR CONVERSION (N2 BASIS) =		-4.71		
PRODUCT GASES 4-17 w/ CO2 =		10.66		0.26				H2 MOLAR CONVERSION (N2 BASIS) =		14.13		
PRODUCT GASES 5-17 w/o CO2 =		1.98		0.06								
TOTAL HYDROCARBONS =		0.38		0.02		0.11		6.71		19.20		29.39
C2+ HYDROCARBONS =		0.18		0.00		0.03		1.83		9.11		8.00
TOTAL ROH/TOTAL HC =		4.21		2.40								
TOTAL ALCOHOLS =		1.60		0.04		0.27		16.11		80.80		70.61
C1-C2 ALCOHOLS =		1.07		0.03		0.22		13.09		54.07		57.37
C3 ALCOHOLS =		0.18		0.00		0.02		1.19		9.22		5.21
C4 ALCOHOLS =		0.35		0.00		0.03		1.83		17.52		8.03
C3-C4 ROH/TOTAL ROH =		0.33		0.19						21.68		11.38
N/B C3-C4 ALCOHOLS =		0.83		0.98								
ROH ACTIVITY (OFFGAS BASIS) =		0.055		g/g cat/hr		3.85				OFFGAS BASIS		
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.053		g/g cat/hr		3.85				CARBON MASS BALANCE (%) =		117.86
HC ACTIVITY (OFFGAS BASIS) =		0.013		g/g cat/hr		0.91				HYDROGEN MASS BALANCE (%) =		95.35
										OXYGEN MASS BALANCE (%) =		120.10

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

CATALYST NAME = 10DANSO		FEED RATE (scfm) = 200.00		OFFGAS RATE (scfm) = 217.00								
REFERENCE # = PR249		H2/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		H2 (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 ROH only	PRODUCT mole % ROH only	N/B mole %
1	H2	2.02	2930.08	6.31	41.97							
2	N2	28.00	30.88	20.67	4.91							
3	CO	28.10	291.21	7.72	51.37							
4	CO2	44.01	9.21	0.21	1.39	82.11	79.47					
5	CH4	16.04	63.54	0.10	0.04	0.87	2.31	4.87	11.27			
6	C2H6	30.07	29.43	0.05	0.01	0.41	0.58	2.29	2.82			
7	C3H8	44.10	29.97	0.05	0.01	0.41	0.39	2.27	1.91			
9	CH3OH	32.04	282.78	1.11	0.03	9.90	13.15	55.32	64.07	62.95	77.87	
8	C4H10	58.12	34.89	0.05	0.01	0.48	0.35	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	0.84	0.60	4.72	2.92	5.37	3.54	
11	n-C3H7OH	60.10	114.99	0.23	0.00	2.08	1.47	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	2.50	1.44	13.96	6.99	15.89	8.50	
13	n-C4H9OH	74.12	21.79	0.05	0.00	0.40	0.23	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 =		250.42	14.77	CO MOLAR CONVERSION (N2 BASIS) = -5.48								
PRODUCT GASES 4-17 w/ CO2 =		11.23	0.26	H2 MOLAR CONVERSION (N2 BASIS) = 13.82								
PRODUCT GASES 5-17 w/o CO2 =		2.01	0.05									
TOTAL HYDROCARBONS =		0.24	0.01	0.06		2.17	3.64	12.12	17.72			
C2+ HYDROCARBONS =		0.15	0.00	0.02		1.30	1.32	7.25	6.45			
TOTAL ROH/TOTAL HC =		7.25	4.64									
TOTAL ALCOHOLS =		1.77	0.04	0.30		15.72	16.89	87.88	82.28	100.00	100.00	
C1-C2 ALCOHOLS =		1.11	0.03	0.23		9.90	13.15	55.32	64.07	62.95	77.87	
C3 ALCOHOLS =		0.33	0.01	0.04		2.92	2.07	16.34	10.09	18.60	12.26	
C4 ALCOHOLS =		0.33	0.00	0.03		2.90	1.67	16.22	8.12	18.46	9.87	
C3-C4 ROH/TOTAL ROH =		0.37	0.22									
N/B C3-C4 ALCOHOLS =		0.74	0.84									
ROH ACTIVITY (OFFGAS BASIS) =		0.063	g/g cat/hr	4.38	lb/n3/hr	OFFGAS BASIS						
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.058	g/g cat/hr	4.38	lb/n3/hr	CARBON MASS BALANCE (%) = 121.54						
HC ACTIVITY (OFFGAS BASIS) =		0.009	g/g cat/hr	0.60	lb/n3/hr	HYDROGEN MASS BALANCE (%) = 97.77						
						OXYGEN MASS BALANCE (%) = 124.13						

	CATALYST NAME = 10DAN50R																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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CATALYST NAME = 10DAN51											
REFERENCE # = PR323											
FEED RATE (cccm) = 200.00											
OFFGAS RATE (cccm) = 207.00											
LIQUID COLLECTED (gm) = 0.06											
% WATER COLLECTED = 0.00											
TIME PERIOD (hr) = 6.00											
TEMPERATURE (°C) = 400.00											
PRESSURE (psig) = 1100.00											
N2 (mole %) = 4.80											
H2/CO RATIO = 1.00											
CO (mole %) = 47.60											
H2 (mole %) = 47.60											
N2 (mole %) = 4.80											
GC AREA											
Molecular Weight											
g/m											
H2											
N2											
CO											
CO2											
CH4											
C2H6											
C3H8											
CH3OH											
C4H10											
C2H5OH											
i-C3H7OH											
n-C3H7OH											
sec-C4H9OH											
i-C4H9OH											
n-C4H9OH											
Me-2-Butanol											
REACTANT GASES 1-3 = 298.71											
PRODUCT GASES 4-17 w/ CO2 = 10.49											
PRODUCT GASES 5-17 w/o CO2 = 3.10											
TOTAL HYDROCARBONS = 0.60											
C2+ HYDROCARBONS = 0.34											
TOTAL ROH/TOTAL HC = 4.13											
TOTAL ALCOHOLS = 2.50											
C1-C2 ALCOHOLS = 1.79											
C3 ALCOHOLS = 0.06											
C4 ALCOHOLS = 0.59											
C3-C4 ROH/TOTAL ROH = 0.28											
N/B C3-C4 ALCOHOLS = 0.10											
ROH ACTIVITY (OFFGAS BASIS) = 0.074											
ROH ACTIVITY (CO FEEDGAS BASIS) = 0.072											
HC ACTIVITY (OFFGAS BASIS) = 0.018											
CARBON MASS BALANCE (%) = 116.42											
HYDROGEN MASS BALANCE (%) = 89.72											
OXYGEN MASS BALANCE (%) = 117.69											

CATALYST NAME = 10DAN52		FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 212.00								
REFERENCE # = PR293		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00								
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.60		% WATER COLLECTED = 0.00								
CATALYST VOLUME (ml) = 0.75		H2 (mole %) = 47.60		TIME PERIOD (hr) = 18.00								
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 ROH only wt %	PRODUCT ROH only mole %	N/B mole %
1	H2	2.02	12.73	6.30	42.41							
2	N2	28.00	20.04	0.72	4.82							
3	CO	28.10	218.02	7.76	52.22							
4	CO2	44.01	2.23	0.05	0.34	68.80	62.15					
5	CH4	16.04	26.75	0.04	0.02	1.27	3.15	4.07	8.31			
6	C2H6	30.07	15.02	0.02	0.01	0.72	0.95	2.31	2.52			
7	C3H8	44.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
9	CH3OH	32.04	211.07	0.83	0.17	25.56	31.71	81.92	83.79	87.50	93.97	
8	C4H10	58.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00			
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	9.85	0.02	0.00	0.62	0.41	1.97	1.08	2.11	1.21	#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	
14	i-C4H9OH	74.12	52.94	0.10	0.01	3.03	1.63	9.72	4.30	10.39	4.82	
13	n-C4H9OH	74.12	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	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
REACTANT GASES 1-3 =		250.79		14.78				CO MOLAR CONVERSION (N2 BASIS) =		-9.30		
PRODUCT GASES 4-17 w/ CO2 =		3.25		0.08				H2 MOLAR CONVERSION (N2 BASIS) =		11.24		
PRODUCT GASES 5-17 w/o CO2 =		1.01		0.03								
TOTAL HYDROCARBONS =		0.06		0.00		0.02		1.99		6.38		10.83
C2+ HYDROCARBONS =		0.02		0.00		0.01		0.72		2.31		2.52
TOTAL ROH/TOTAL HC =		14.67		8.23								
TOTAL ALCOHOLS =		0.95		0.03		0.19		29.21		93.62		99.17
C1-C2 ALCOHOLS =		0.83		0.03		0.17		25.56		81.92		83.79
C3 ALCOHOLS =		0.02		0.00		0.00		0.62		1.97		1.08
C4 ALCOHOLS =		0.10		0.00		0.01		3.03		9.72		4.30
C3-C4 ROH/TOTAL ROH =		0.12		0.06								
N/B C3-C4 ALCOHOLS =		0.20		0.25								
ROH ACTIVITY (OFFGAS BASIS) =		0.034		g/g cat/hr		2.79		lb/ft3/hr		CARBON MASS BALANCE (%) =		117.60
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.032		g/g cat/hr		2.79		lb/ft3/hr		HYDROGEN MASS BALANCE (%) =		95.45
HC ACTIVITY (OFFGAS BASIS) =		0.002		g/g cat/hr		0.19		lb/ft3/hr		OXYGEN MASS BALANCE (%) =		118.23

CATALYST NAME = 10DAN53		REFERENCE # = PR294		FEED RATE (ccm) = 200.00		OFFGAS RATE (ccm) = 200.00		LIQUID COLLECTED (gm) = 0.00		TIME PERIOD (hr) = 18.00	
CATALYST WEIGHT (gm) = 1.00		H2/CO RATIO = 1.00		CO (mole %) = 47.60		wt %		% WATER COLLECTED = 0.00			
CATALYST VOLUME (ml) = 0.80		CO (mole %) = 47.60		H2 (mole %) = 47.60		w/o CO2					
TEMPERATURE (°C) = 400.00		H2 (mole %) = 47.60		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 wt % ROH only	PRODUCT mole % ROH only
1	H2	2.02	13.62	6.74	39.95						
2	N2	28.00	32.53	1.16	6.88						
3	CO	28.10	246.90	8.79	52.06						
4	CO2	44.01	4.74	0.11	0.64	66.82	57.67				
5	CH4	16.04	209.26	0.32	0.12	4.55	10.77	13.70	25.44		
6	C2H6	30.07	58.02	0.09	0.02	1.28	1.61	3.85	3.81		
7	C3H8	44.10	32.96	0.05	0.01	0.71	0.61	2.13	1.44		
9	CH3OH	32.04	418.97	1.65	0.30	23.23	27.54	70.01	65.06	88.31	94.59
8	C4H10	58.12	15.83	0.02	0.00	0.35	0.23	1.04	0.53		
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	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
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	117.14	0.22	0.02	3.07	1.58	9.26	3.72	11.69	5.41
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 =			293.05	16.69						CO MOLAR CONVERSION (N2 BASIS) =	23.75
PRODUCT GASES 4-17 w/ CO2 =			7.09	0.19						H2 MOLAR CONVERSION (N2 BASIS) =	41.48
PRODUCT GASES 5-17 w/o CO2 =			2.35	0.08							
TOTAL HYDROCARBONS =			0.49	0.02	0.15	6.88	13.22	20.72	31.22		
C2+ HYDROCARBONS =			0.17	0.00	0.03	2.33	2.45	7.02	5.78		
TOTAL ROH/TOTAL HC =			3.83	2.20							
TOTAL ALCOHOLS =			1.86	0.05	0.32	26.30	29.12	79.28	68.78	100.00	100.00
C1-C2 ALCOHOLS =			1.65	0.05	0.30	23.23	27.54	70.01	65.06	88.31	94.59
C3 ALCOHOLS =			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C4 ALCOHOLS =			0.22	0.00	0.02	3.07	1.58	9.26	3.72	11.69	5.41
C3-C4 ROH/TOTAL ROH =			0.12	0.05							
N/B C3-C4 ALCOHOLS =			0.00	0.00							
ROH ACTIVITY (OFFGAS BASIS) =			0.057	g/g cat/hr	4.47	lb/lb3/hr				CARBON MASS BALANCE (%) =	116.92
ROH ACTIVITY (CO FEEDGAS BASIS) =			0.055	g/g cat/hr	4.47	lb/lb3/hr				HYDROGEN MASS BALANCE (%) =	89.96
HC ACTIVITY (OFFGAS BASIS) =			0.015	g/g cat/hr	1.17	lb/lb3/hr				OXYGEN MASS BALANCE (%) =	117.80

CATALYST NAME = 18DAN54		FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 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) = 0.30		H2 (mole %) = 47.56		TIME PERIOD (hr) = 5.00								
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 wt % ROH only	PRODUCT mole % ROH only	N/B mole %
1	H2	2.02	2822.99	12.28	6.08	41.75						
2	N2	28.00	30.21	20.22	0.72	4.96						
3	CO	28.10	278.47	207.51	7.38	50.71						
4	CO2	44.01	13.51	13.53	0.31	2.11	82.94	81.87				
5	CH4	16.04	76.19	0.12	0.01	0.05	0.72	1.95	4.22	10.75		
6	C2H6	30.07	80.58	0.13	0.00	0.03	0.77	1.11	4.52	6.14		
7	C3H8	44.10	33.3	0.05	0.00	0.01	0.31	0.31	1.82	1.69		
9	CH3OH	32.04	296.4	1.16	0.04	0.25	7.14	9.68	41.87	53.43	48.92	67.89
8	C4H10	58.12	69.18	0.11	0.00	0.01	0.66	0.49	3.85	2.71		
10	C2H5OH	46.07	16.72	0.04	0.00	0.01	0.26	0.24	1.51	1.34	1.76	1.70
12	i-C3H7OH	60.10	17.42	0.04	0.00	0.00	0.26	0.19	1.52	1.03	1.77	1.31
11	n-C3H7OH	60.10	48.87	0.10	0.00	0.01	0.61	0.44	3.57	2.43	4.17	3.08
15	sec-C4H9OH	74.12	74.16	0.14	0.00	0.01	0.85	0.50	4.96	2.74	5.79	3.47
14	i-C4H9OH	74.12	440.06	0.82	0.01	0.08	5.02	2.94	29.42	16.23	34.37	20.62
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	38.97	0.08	0.00	0.01	0.47	0.27	2.75	1.52	3.21	1.93
REACTANT GASES 1-3 =		240.01		14.19				CO MOLAR CONVERSION (N2 BASIS) =		-8.00		
PRODUCT GASES 4-17 w/ CO2 =		16.31		0.38				H2 MOLAR CONVERSION (N2 BASIS) =		11.34		
PRODUCT GASES 5-17 w/o CO2 =		2.78		0.07								
TOTAL HYDROCARBONS =		0.40		0.01								
C2+ HYDROCARBONS =		0.28		0.01				14.41		21.29		
TOTAL ROH/TOTAL HC =		5.94		3.70				10.19		10.54		
TOTAL ALCOHOLS =		2.38		0.05								
C1-C2 ALCOHOLS =		1.21		0.04				85.59		78.71		100.00
C3 ALCOHOLS =		0.14		0.00				43.38		54.77		50.68
C4 ALCOHOLS =		0.96		0.01				5.08		3.46		5.94
C3-C4 ROH/TOTAL ROH =		0.49		0.30				34.38		18.96		40.17
N/B C3-C4 ALCOHOLS =		0.10		0.12								24.09
ROH ACTIVITY (OFFGAS BASIS) =		0.081		g/g cat/hr		6.30		lb/n3/hr		OFFGAS BASIS		
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.082		g/g cat/hr		6.30		lb/n3/hr		CARBON MASS BALANCE (%) =		112.10
HC ACTIVITY (OFFGAS BASIS) =		0.014		g/g cat/hr		1.05		lb/n3/hr		HYDROGEN MASS BALANCE (%) =		89.72
										OXYGEN MASS BALANCE (%) =		115.46

CATALYST NAME =		10DAN55				FEED RATE (cccm) =		200.00				OFFGAS RATE (cccm) =		210.00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
REFERENCE # =		PR223				H2/CO RATIO =		1.00				LIQUID COLLECTED (gm) =		0.17																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
CATALYST WEIGHT (gm) =		1.00				CO (mole %) =		47.43				% WATER COLLECTED =		0.00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
CATALYST VOLUME (ml) =		0.75				H2 (mole %) =		47.56				TIME PERIOD (hr) =		4.75																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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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	PRODUCT wt % ROH only	PRODUCT mole % ROH only	PRODUCT wt % ROH only	PRODUCT mole % ROH only																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

CATALYST NAME =		10DAN56			FEED RATE (cccm) =						OFFGAS RATE (cccm) =			
REFERENCE # =		PR355			H2/CO RATIO =						LIQUID COLLECTED (gm) =		209.00	
CATALYST WEIGHT (gm) =		1.00			CO (mole %) =						% WATER COLLECTED =		0.03	
CATALYST VOLUME (ml) =		0.90			H2 (mole %) =						TIME PERIOD (hr) =		0.00	
TEMPERATURE (°C) =		400.00			N2 (mole %) =								5.50	
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	
1	H2	2.02	3182.15	13.84	6.85	40.06								
2	N2	28.00	50.20	33.61	1.20	7.02								
3	CO	28.10	334.53	249.28	8.87	51.86								
4	CO2	44.01	4.81	4.82	0.11	0.64	65.11	60.67						
5	CH4	16.04	32.10	0.05	0.00	0.02	0.67	1.71	1.92	4.34				
6	C2H6	30.07	29.32	0.05	0.00	0.01	0.62	0.84	1.77	2.14				
7	C3H8	44.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00				
9	CH3OH	32.04	467.28	1.84	0.06	0.34	24.83	31.77	71.17	80.78	73.89	86.38		
8	C4H10	58.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00				
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	43.97	0.09	0.00	0.01	1.21	0.82	3.46	2.09	3.59	2.24	#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	267.01	0.50	0.01	0.04	6.71	3.71	19.25	9.44	19.98	10.10		
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	32.04	0.06	0.00	0.00	0.85	0.47	2.44	1.20	2.53	1.28		
REACTANT GASES 1-3 =		296.73	16.92								CO MOLAR CONVERSION (N2 BASIS) =		25.46	
PRODUCT GASES 4-17 w/ CO2 =		7.40	0.18								H2 MOLAR CONVERSION (N2 BASIS) =		42.42	
PRODUCT GASES 5-17 w/o CO2 =		2.58	0.07											
TOTAL HYDROCARBONS =		0.10	0.00		0.03		1.29		2.55		3.69		6.49	
C2+ HYDROCARBONS =		0.05	0.00		0.01		0.62		0.84		1.77		2.14	
TOTAL ROH/TOTAL HC =		26.11	14.42											
TOTAL ALCOHOLS =		2.49	0.07		0.39		33.60		36.78		96.31		93.51	
C1-C2 ALCOHOLS =		1.84	0.06		0.34		24.83		31.77		71.17		80.78	
C3 ALCOHOLS =		0.09	0.00		0.01		1.21		0.82		3.46		2.09	
C4 ALCOHOLS =		0.50	0.01		0.04		6.71		3.71		19.25		9.44	
C3-C4 ROH/TOTAL ROH =		0.26	0.14											
N/B C3-C4 ALCOHOLS =		0.18	0.22											
ROH ACTIVITY (OFFGAS BASIS) =		0.076	g/g cat/hr		5.25		lb/m3/hr				CARBON MASS BALANCE (%) =		116.54	
ROH ACTIVITY (CO FEEDGAS BASIS) =		0.072	g/g cat/hr		5.25		lb/m3/hr				HYDROGEN MASS BALANCE (%) =		90.14	
HC ACTIVITY (OFFGAS BASIS) =		0.003	g/g cat/hr		0.20		lb/m3/hr				OXYGEN MASS BALANCE (%) =		117.52	

CATALYST NAME = 10DAN57		FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 218.00					
REFERENCE # = PR250		H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00					
CATALYST WEIGHT (gm) = 1.00		CO (mole %) = 47.60		% WATER COLLECTED = 0.00					
CATALYST VOLUME (ml) = 0.70		H2 (mole %) = 47.60		TIME PERIOD (hr) = 4.00					
TEMPERATURE (°C) = 400.00		N2 (mole %) = 4.80							
PRESSURE (psig) = 1100.00									
GASES	Molecular Weight	GC AREA	OFFGAS	OFFGAS	PRODUCT	PRODUCT	PRODUCT	PRODUCT	PRODUCT
			weight	molar	mole %	wt %	mole %	wt %	mole %
			ugrams	umoles	total	w/ CO2	w/o CO2	w/o CO2	ROH only
									N/B
1	H2		2.02	3194.50	13.90	6.88	40.02		
2	N2		28.00	48.56	32.51	1.16	6.75		
3	CO		28.10	337.66	251.61	8.95	52.09		
4	CO2		44.01	5.68		0.13	0.75	66.64	
5	CH4		16.04	41.88		0.06	0.02	2.74	6.22
6	C2H6		30.07	37.18		0.06	0.01	0.72	2.98
7	C3H8		44.10	19.66		0.03	0.00	0.37	1.05
9	CH3OH		32.04	403.17	1.58	0.05	0.29	19.71	71.98
8	C2H5OH		58.12	0.00	0.00	0.00	0.00	0.00	0.00
10	C2H5OH		46.07	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
11	n-C3H7OH		60.10	43.14	0.09	0.00	0.01	1.09	3.72
15	sec-C4H9OH		74.12	0.00	0.00	0.00	0.00	0.00	0.00
14	i-C4H9OH		74.12	254.17	0.47	0.01	0.04	5.88	21.48
13	n-C4H9OH		74.12	0.00	0.00	0.00	0.00	0.00	0.00
16	Me-2-Butanol		88.15	28.75	0.06	0.00	0.00	0.70	1.18
		REACTANT GASES 1-3 =		16.99				CO MOLAR CONVERSION (N2 BASIS) = 22.23	
		PRODUCT GASES 4-17 w/ CO2 =		8.04		0.19		H2 MOLAR CONVERSION (N2 BASIS) = 40.25	
		PRODUCT GASES 5-17 w/o CO2 =		2.35		0.06			
		TOTAL HYDROCARBONS =		0.15		0.01		3.42	
		C2+ HYDROCARBONS =		0.09		0.00		6.47	
		TOTAL ROH/TOTAL HC =		14.45		8.76		10.25	
								3.73	
								4.03	
		TOTAL ALCOHOLS =		2.20		0.06		29.94	
		C1-C2 ALCOHOLS =		1.58		0.05		27.58	
		C3 ALCOHOLS =		0.09		0.00		19.71	
		C4 ALCOHOLS =		0.47		0.01		0.75	
		C3-C4 ROH/TOTAL ROH =		0.28		0.15		0.75	
		N/B C3-C4 ALCOHOLS =		0.19		0.23		3.29	
								20.09	
								9.86	
								21.48	
								10.99	
</									

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 %) = 5.01												
GASES	Molecular Weight	GC AREA	OFFGAS weight	OFFGAS molar	OFFGAS mole %	PRODUCT wt %	PRODUCT mole %	PRODUCT w/o CO2	PRODUCT w/o CO2	PRODUCT wt %	PRODUCT mole %	ROH only	ROH only	N/B
			ugrams	umoles	total	w/CO2	w/CO2							
1	H2	2.02	3216.925	13.99	39.82									
2	N2	28.00	52.038	34.84	7.15									
3	CO	28.10	339.41	252.92	51.74									
4	CO2	44.01	6.042	6.05	0.14	67.97	61.50							
5	CH4	16.04	149.598	0.23	0.08	2.59	6.43	8.08	16.69					
6	C2H6	30.07	73.388	0.11	0.02	1.29	1.70	4.02	4.42					
7	C3H8	44.10	32.412	0.05	0.01	0.55	0.50	1.73	1.30					
9	CH3OH	32.04	476.995	1.87	0.06	21.06	26.18	65.74	68.00	78.28	89.07			
8	C4H10	58.12	40.314	0.06	0.01	0.70	0.48	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	0.57	0.37	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	5.15	2.77	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	0.13	0.07	0.39	0.18	0.47	0.23			
REACTANT GASES 1-3 = 301.75												CO MOLAR CONVERSION (N2 BASIS) = 23.58		
PRODUCT GASES 4-17 w/CO2 = 8.90												H2 MOLAR CONVERSION (N2 BASIS) = 41.35		
PRODUCT GASES 5-17 w/o CO2 = 2.85														
TOTAL HYDROCARBONS = 0.46														
C2+ HYDROCARBONS = 0.23												5.13 9.11 16.01 23.66		
TOTAL ROH/TOTAL HC = 5.24												2.54 2.68 7.93 6.97		
TOTAL ALCOHOLS = 2.39														
C1-C2 ALCOHOLS = 1.87												83.99 76.34 100.00 100.00		
C3 ALCOHOLS = 0.05												65.74 68.00 78.28 89.07		
C4 ALCOHOLS = 0.46												1.76 0.97 2.10 1.27		
C3-C4 ROH/TOTAL ROH = 0.22												16.09 7.19 19.15 9.42		
N/B C3-C4 ALCOHOLS = 0.11														
ROH ACTIVITY (OFFGAS BASIS) = 0.069												lb/m3/hr		
ROH ACTIVITY (CO FEEDGAS BASIS) = 0.068												lb/m3/hr		113.84
HC ACTIVITY (OFFGAS BASIS) = 0.013												lb/m3/hr		87.47
														114.93
												OFFGAS BASIS		
												CARBON MASS BALANCE (%) =		
												HYDROGEN MASS BALANCE (%) =		
												OXYGEN MASS BALANCE (%) =		

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CATALYST NAME = 11DAN45		REFERENCE # = 125	FEED RATE (cccm) = 200.00		OFFGAS RATE (cccm) = 216.00							
CATALYST WEIGHT (gm) = 1.00			H2/CO RATIO = 1.00		LIQUID COLLECTED (gm) = 0.00							
CATALYST VOLUME (ml) = 0.85			CO (mole %) = 47.43		% WATER COLLECTED = 0.00							
TEMPERATURE (°C) = 400.00			H2 (mole %) = 47.56		TIME PERIOD (hr) = 26.50							
PRESSURE (psig) = 1100.00			N2 (mole %) = 5.91									
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/R mole %
1	H2	2.02	13.75	6.81	40.21							
2	N2	28.00	32.66	1.17	6.89							
3	CO	28.10	329.81	8.75	51.67							
4	CO2	44.01	6.06	0.14	0.81	70.34	66.71					
5	CH4	16.04	41.43	0.06	0.02	0.74	1.92	2.49	5.78			
6	C2H6	30.07	34.01	0.05	0.01	0.62	0.85	2.07	2.56			
7	C3H8	44.10	22.49	0.03	0.00	0.40	0.38	1.34	1.13			
9	CH3OH	32.04	419.48	1.65	0.05	19.11	24.90	64.43	74.80	70.46	84.21	
8	C4H10	58.12	43.9	0.07	0.01	0.79	0.57	2.66	1.70			
10	C2H5OH	46.07	5.43	0.01	0.00	0.16	0.14	0.53	0.43	0.58	0.48	
12	i-C3H7OH	60.10	9.97	0.02	0.00	0.28	0.19	0.94	0.58	1.03	0.66	
11	n-C3H7OH	60.10	21.52	0.04	0.00	0.51	0.35	1.71	1.06	1.87	1.19	1.8
15	sec-C4H9OH	74.12	49.55	0.09	0.01	1.07	0.60	3.60	1.81	3.94	2.03	
14	i-C4H9OH	74.12	278.26	0.52	0.01	6.00	3.38	20.23	10.15	22.12	11.43	
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	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
REACTANT GASES 1-3 =			292.17	16.72		CO MOLAR CONVERSION (N2 BASIS) =		20.79				
PRODUCT GASES 4-17 w/ CO2 =			8.63	0.21		H2 MOLAR CONVERSION (N2 BASIS) =		38.57				
PRODUCT GASES 5-17 w/o CO2 =			2.56	0.07								
TOTAL HYDROCARBONS =			0.22	0.01	0.05	2.54	3.72	8.56	11.18			
C2+ HYDROCARBONS =			0.16	0.00	0.02	1.80	1.80	6.07	5.39			
TOTAL ROH/TOTAL HC =			10.68	7.95								
TOTAL ALCOHOLS =			2.34	0.06	0.36	27.12	29.57	91.44	88.82	100.00	100.00	
C1-C2 ALCOHOLS =			1.66	0.05	0.31	19.27	25.04	64.96	75.23	71.04	84.69	
C3 ALCOHOLS =			0.07	0.00	0.01	0.79	0.55	2.65	1.64	2.90	1.85	
C4 ALCOHOLS =			0.61	0.01	0.05	7.07	3.98	23.83	11.96	26.06	13.46	
C3-C4 ROH/TOTAL ROH =			0.29	0.15								
N/B C3-C4 ALCOHOLS =			0.07	0.08								
ROH ACTIVITY (OFFGAS BASIS) =			0.074	g/g cat/hr	5.44	lb/lb3/hr	OFFGAS BASIS					
ROH ACTIVITY (CO FEEDGAS BASIS) =			0.069	g/g cat/hr	5.44	lb/lb3/hr	CARBON MASS BALANCE (%) =		120.90			
HC ACTIVITY (OFFGAS BASIS) =			0.007	g/g cat/hr	0.51	lb/lb3/hr	HYDROGEN MASS BALANCE (%) =		93.62			
							OXYGEN MASS BALANCE (%) =		122.21			

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