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March 28, 1996

Mr James Huemmrich
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SUBJECT: **OXYGENATED OCTANE ENHANCERS: SYNGAS TO ISOBUTYLENE**
Contract Number: DE-AC22-91PC90042

Dear Mr. Huemmrich:

Enclosed find copies of the final version of Technical Progress Report No 18. This report has been approved by Dr. Arun Bose. This report contains patentable material which was disclosed in an earlier patent disclosure. Therefore it is marked "patent hold" on the appropriate pages.

If you have any questions concerning this report, please contact me at (847) 391-2038.

Regards,

Terry L. Marker
Sr. Development Specialist

TLM/bls

Enclosures

cc: Document Control Center - U.S. DOE-PETC - MS 921-143
Dr Arun Bose -- DOE PETC - MS 922
Sarla Nanda -- DOE PETC - MS 58-M217
RC/PF: NVD-Syngas to Isobutylene (DOE)
JBaptist, PTBarger, BVVora, TLMarker

CONTRACT TITLE AND NUMBER:
Development of a Catalyst for Conversion of Syngas-Derived Materials to Isobutylene
DE-AC22-91PC90042

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Contract Period: March 15, 1991 to September 14, 1995

QUARTERLY TECHNICAL REPORT

The goals of this project are to develop a catalyst and process for the conversion of syngas to isobutanol. The research will identify and optimize key catalyst and process characteristics. In addition, the commercial potential of the new process will be evaluated by an economic analysis.

The combination of the best conditions from independent process variable studies has afforded the best performance to date with the 2% Pt on Zn/Mn/Zr oxide catalyst. At 325°C, 300 psig, 7/1 MeOH/EtOH molar feed ratio and 1 hr^{-1} MeOH WHSV, 22.2% selectivity to isobutanol is obtained with 55 and 97% conversions of methanol and ethanol, respectively. The results of this run will be used as a basis for the economic evaluation of a higher alcohols process.

The ability of the Pt on Zn/Mn/Zr oxide catalyst to produce isobutanol in the presence of high partial pressures of H_2 has been investigated. Such operation could allow the integration of a higher alcohols process with a conventional methanol synthesis plant by placing it within the methanol synthesis recycle loop. However, higher alcohol yields are severely suppressed by a large H_2 cofeed, even at pressures as low as 50 psig. Elimination of the H_2 co-feed did not restore the performance of the catalyst to expected levels, suggesting that the high H_2 partial pressure has caused degradation of the catalyst. No further testing of high H_2 conditions is planned.

The commercial system has been modeled using the product slate obtained from the 'best case' pilot plant conditions combined with the assumption of equilibrium CO, H_2O, CO_2 and H_2 makes. A stand-alone isobutanol plant processing 500 MT/D synthesis gas-derived methanol can yield 92 MT/D isobutanol and possibly an additional 20 MT/D assuming complete hydrogenation of isobutyraldehyde which accumulates in the liquid recycle loop. The economic and product cost sensitivity analyses of this system are pending. Also, the effect of separator temperature on product losses will be examined in more detail.

EXPERIMENTAL

Catalyst

The preparation of the 2% Pt on Zn/Mn/Zr (60/20/20) oxide catalyst by co-precipitation of an aqueous solution of metal nitrates with KOH at pH 11, followed by impregnation of the calcined support with an aqueous Pt chloride solution has been described previously.[1,2]

Catalytic Testing Procedure

The pilot plant testing of catalysts for the conversion of a methanol/ethanol blend to isoalcohols was accomplished as follows. The catalyst, as 20-40 mesh granules, was loaded into a 1/2" I.D. stainless steel reactor. The reactor was purged N_2 at 250 °C, 10 psig, 0.5 scf/hr for 1 hour then pressure tested with N_2 at 250 °C, 500 psig for 1 hour. After restarting the N_2 purge, temperature and pressure were adjusted to the desired conditions. After 2 hours, the methanol/ethanol blend (10/1 molar) was cut into the plant at the desired rate. Product analyses were obtained using two on-line GCs to analyze the total hydrocarbon/oxygenate product and the overhead gas. Conversions, selectivities and productivities (including CO and CO_2) are based on moles of carbon. The H_2 co-feed in Run 926 was added using an independent feed system that was manifolded with the N_2 and methanol/ethanol feed systems immediately before the reactor inlet. The H_2 feed was established with the N_2 purge for 2 hours prior to the addition of the methanol/ethanol blend. A listing of the pilot plant runs included in this report is given in Table 1.

RESULTS AND DISCUSSION

Process Variable Studies for Methanol/Ethanol Conversion - Optimum Conditions Test

The previous report in this project described the independent effects of temperature, pressure and methanol/ethanol molar feed ratio on the performance of the 2% Pt on Zn/Mn/Zr oxide catalyst.[2] The highest selectivities to the desired iC_4 oxygenates were obtained at the lowest temperature (325°C), highest pressure (300 psig) and moderate methanol/ethanol feed ratio (7/1 molar). These results are summarized in Table 2. In view of these results, an optimized run has been conducted using this combination of conditions. In addition, methanol space velocity was decreased from 2 hr^{-1} to 1 hr^{-1} by doubling the catalyst loading in order to obtain 50-60% methanol conversion at this lower temperature. The last column of Table 2 shows the results of this test. The methanol conversion was within the targeted range and the isobutanol selectivity

(22.2%) is the highest obtained in any testing in this program. While isobutyraldehyde is reduced (due to the high pressure), the formation of methyl isobutyrate ester is higher than expected. Methyl acetate formation is also high, which is consistent with the earlier testing at 325°C. This suggests that the Cannizzaro reaction becomes more competitive as the aldol condensation step slows. The lower temperature also reduces the formation of light hydrocarbons, CO and CO_2 to the lowest levels observed to date with this catalyst.

In view of the superior selectivities, compared with other conditions, the results of this run will be used as a basis for the economic evaluation of a higher alcohols process using this catalyst. This work is being done as a part of Task 5 of the program.

Methanol/Ethanol Conversion with High H_2 Co-feed

One process concept for the integration of a high alcohols process with a conventional methanol synthesis plant is to place the process immediately after the methanol synthesis reactor using imported ethanol. One advantage of this configuration is that any CO and CO_2 formed in the higher alcohol synthesis reactor can be easily recycled to the methanol synthesis reactor for conversion to additional methanol using the existing recycle loop. In addition, unconverted methanol can be recovered and used for the production of MTBE from the isobutanol in a separate step.

In order for this configuration to be feasible the higher alcohol condensation catalyst must be able to operate in the presence of high H_2 concentrations. The effluent from the methanol synthesis reactor typically contains about 70-80 mole% H_2 as well as some N_2, CO and CO_2. It is also desirable that this process operate at the high pressure of the methanol synthesis reactor (1000-1500 psig) so that the efficiency of the $H_2/CO/CO_2$ separation on the recycle loop is not reduced. Previous results have indicated that co-feeding H_2 at a low level (2/1 H_2/MeOH molar feed ratio) has very little effect on the performance of the Pt on Zn/Mn/Zr oxide catalyst. Methanol conversion is slightly increased and selectivity shifts from isobutyraldehyde to isobutanol with H_2 giving an overall slightly higher productivity for isobutanol. Therefore, a pilot plant test has been conducted to determine the performance of the 2% Pt on Zn/Mn/Zr oxide catalyst at conditions comparable to those inside the methanol synthesis recycle loop.

Table 3 summarizes the results of the pilot plant test of the 2% Pt on Zn/Mn/Zr oxide catalyst at high H_2 partial pressures. At the initial conditions (1200 psig total, 15/1 H_2/MeOH) both methanol and ethanol conversion were very low with only small amount of isobutanol formed. Surprisingly, isobutyraldehyde selectivity was high which is inconsistent with the expected level of product hydrogenation that should be occurring at these conditions. Decreasing pressure to 300 psig and then 50 psig also with a decrease in space velocity) increased conversion and isobutanol selectivity, but it remained far below levels observed previously at lower H_2 levels. Again the isobutyraldehyde selectivity responded in an opposite manner from that expected, decreasing as H_2 content decreased. Elimination of the H_2 co-feed did not restore the performance of the catalyst to expected levels either at 50 psig or 300 psig. This suggests that the high H_2 partial pressure has caused degradation of the catalyst. In view of the poor results obtained in this test, no further testing of high H_2 conditions will be done.

Modeling of a Commercial Isobutanol Synthesis Plant for Economic Analysis

Since experiments using the high H_2 partial pressures typically encountered in the methanol synthesis recycle gas loop showed little promise, a stand-alone isobutanol production plant is being considered for economic evaluation. Under the best-case conditions (300 psig, 320°C, 1 hr^{-1} WHSV) tested in the pilot plant, methanol and ethanol conversions were 55% and 97%, respectively, with 22% selectivity to isobutanol. These performance criteria, along with the product slate obtained, are being used to model the commercial system.

It was assumed that methanol alone contributes to the formation of all single-carbon species (CO, CO_2), all C_1-C_5 hydrocarbons, and the methyl groups of dimethyl ether, methyl formate, methyl acetate, methyl butyl ether, and methyl isobutyrate. Furthermore, one carbon of the side products isopropanol and isopentanol was considered to originate from methanol. The smaller amounts of ethanol (12.5 mol-% of the liquid feed) charged were assumed to participate in producing all 2- and 4-carbon groups in the same ratios as shown in the yield data generated from pilot plant run 325. The remaining carbon needed to generate the product slate (after conversion of 97% of the ethanol) was presumed to stem from the feed methanol. Generation of water and hydrogen was observed experimentally, and yields of these products were in accordance with 100% elemental O and H balances. The water gas shift reaction was also modeled and assumed to achieve equilibrium at reaction temperature. A comparison of actual measured and theoretical gas yields, as well as a summary of the conditions and reaction coefficients used in modeling, is provided in Table 4.

A feed rate of 500 MT/day (4000 bbl/day) methanol, supplied from a methanol synthesis plant, was the basis for the commercial simulation. Hyprotech Hysim v2.50 process simulation software was used with the NRTL activity property package (recommended for non-ideal components) to model the system. The flow scheme is depicted in Figure 1. Methanol and the ethanol co-feed are mixed and combined with recycle gas (CO, CO_2, and H_2) and then recycle liquid before being heated to the reactor inlet temperature. Although three reactors are illustrated to model methanol conversion, ethanol conversion and the water gas shift reaction, only one reactor would be used commercially. The reaction product is cooled to 100°F and phase-separated. A significant portion of the separator gas is vented to prevent >25 psia hydrogen partial pressure in the combined reactor feed, since this condition gave poorer selectivity experimentally.

The separator liquid, containing isobutanol, unconverted methanol and ethanol, as well as a number of byproducts, is charged to a distillation column. Excess of 99% of the isobutanol is recoverable in the bottoms product with negligible losses of methanol and ethanol. The byproduct isobutyraldehyde is recovered in the overhead product. The extent of buildup of this species in the liquid recycle loop is difficult to estimate from experimental data, since hydrogenation of this material to isobutanol would eventually occur, improving the alcohol yield. Nevertheless, a liquid purge is required to reject primarily alkane and ester side products, with some corresponding loss of methanol and ethanol.

With liquid recycle, the overall carbon conversion is 98% with 22% selectivity to isobutanol. The expected production of isobutanol is 92 MT/day from 500 MT/day of methanol feed. Results of the simulation. including mass and elemental balances as well as product yields, are given in Table 5. Currently a cost estimate of this process is being performed to examine its economic viability. The improved scenario in which isobutyraldehyde is completely converted to isobutanol will also be considered in the study. Also, the effect of separator temperature on product losses will be examined in more detail.

CONCLUSIONS

The combination of the best conditions from independent process varaible studies has afforded the best performance to date with the 2% Pt on Zn/Mn/Zr oxide catalyst. At 325°C, 300 psig, 7/1 MeOH/EtOH molar feed ratio and 1 hr^{-1} MeOH WHSV, 22.2% slectivity to isobutanol is obtained with 55 and 97% conversions of methanol and ethanol, respectively. Selectivity to total iC_4 oxygenates is 36.1%. In view of the superior selectivities at this condition, the results of this run will be used as a basis for the economic evaluation of a higher alcohols process.

The ability of the Pt on Zn/Mn/Zr oxide catalyst to produce isobutanol from methanol and ethanol in the presence of high partial pressures of H_2 has been investigated. Such operation could allow the integration of a high alcohols process with a conventional methanol synthesis plant by placing it within the emthnaol synthesis recycel loop. However, higher alcohol yeilds are severely suppressed by a large H_2 cofeed, even at pressures as low as 50 psig. Elimination of the H_2 co-feed did not restore the performance of the catalyst to expected levels. This suggests that the high H_2 partial pressure has caused degradation of the catalyst. In view of the poor results obtained in this test, no further testing of high H_2 conditions will be done.

Because of the unfavorable pilot plant results at high H_2 partial pressures, the economic and cost sensitivity analyses will be based on a stand-alone isobutanol plant processing 500 MT/D of synthesis gas-derived methanol. Currently, Hyprotech Hysim v2.5 software has been used to model the proposed commercial system which includes recycle of some hydrogen by-product as well as unconverted methanol and ethanol. Most likely, the buildup of isobutyraldehyde in the liquid recycle loop would lead to its eventual conversion to desired isobutanol. The yields of isobutanol from 500 MT/D methanol feed would be 92 MT/D or 112 MT/D considering complete hydrogenation of isobutyraldehyde. The economic and product cost sensitivity analyses of this process are pending, as well as a study to examine the effect of separator temperature on product losses.

REFERENCES

1) P. T. Barger and P. R. Kurek, DOE Quarterly Report No. 15, (1995).

2) P. T. Barger and P. R. Kurek, DOE Quarterly Report No. 17, (1995).

DISCLAIMER

Table 1. Run List

RUN	CATALYST A Book #	CATALYST B Book #	CATALYST DESCRIPTION: CATALYST A	CATALYST DESCRIPTION: CATALYST B	HOS	SIZE	LOADING g	CONDITIONS: TEMP (C) INLET	CONDITIONS: TEMP (C) MAX	CONDITIONS: TOTAL PSIG	CONDITIONS: MeOH WHSV	FEED RATIO MeOH/EtOH/N2/Others
325	8265-98		2.0%Pt / Zn/Mn/Zr (60/20/20) Oxide			20-40M	5		325	300	1	1 / 0.14 / 2 N2
326	8265-98		2.0%Pt / Zn/Mn/Zr (60/20/20) Oxide		0-40	20-40M	25		325	1200	1	1 / 0.14 / 3 N2 / 15 H2
					41-56				325	300	1	1 / 0.14 / 3 N2 / 15 H2
					57-88				325	50	0.5	1 / 0.14 / 3 N2 / 15 H2
					89-112				325	50	0.5	1 / 0.14 / 3 N2
					113-160				325	300	1	1 / 0.14 / 3 N2

Table 2. Effect of Process Variables on Performance of Pt on Zn/Mn/Zr Oxide Catalyst for Methanol/Ethanol Conversion

Catalyst	8265-98 2% Pt on Zn/Mn/Zr (60/20/20) Oxide										
Run Number	309	308	310	308	311	312	308	304	307	306	325
Conditions	2 hr^{-1} MeOH WHSV, 2/1 N_2/MeOH (molar)										1 hr^{-1} WHSV
Temperature (°C)	325	350	375	350	350	350	350	350	350	350	325
Pressure (psig)	30	30	30	30	100	300	30	30	30	30	300
MeOH/EtOH (molar)	10/1	10/1	10/1	10/1	10/1	10/1	10/1	7/1	4/1	1/1	7/1
Conversion (%)											
MeOH	39.7	53.4	64.2	53.4	46.0	56.4	53.4	57.4	58.8	65.5	55.2
EtOH	96.6	99.1	98.1	99.1	95.7	97.6	99.1	97.4	93.4	82.8	97.0
Selectivities (mole %)											
nC_3OH	1.2	0.4	1.1	0.4	0.3	0.8	0.4	1.0	2.9	2.0	1.6
nC_4OH	0.1	0.1	0.1	0.1	0.0	0.0	0.1	0.1	0.5	1.2	0.1
iC_4OH	15.6	11.6	5.7	11.6	14.4	20.7	11.6	15.3	9.1	0.3	22.2
iC_4 Aldehyde	16.6	18.0	13.4	18.0	11.2	7.2	18.0	19.0	12.9	1.0	4.8
Me iButyrate	4.9	4.3	2.1	4.3	5.1	5.6	4.3	5.4	4.9	0.2	9.1
Other Oxygenates	3.4	1.5	4.4	1.5	1.8	1.4	1.5	3.9	9.7	3.1	6.8
Others (No ID)	8.5	7.3	8.1	7.3	5.8	2.1	7.3	5.5	13.4	14.1	13.0
C_1-C_2 Oxygenates	7.2	4.1	2.2	4.1	3.3	3.0	4.1	4.1	6.9	66.9	5.7
C_1-C_4 Hydrocarbons	0.7	1.4	3.5	1.4	2.7	2.6	1.4	1.3	0.9	0.7	1.0
CO	14.5	22.3	33.9	22.3	26.2	31.2	22.3	18.1	13.0	5.1	14.6
CO_2	27.5	28.0	25.5	28.0	29.2	25.2	28.0	26.2	25.8	5.6	21.1
Productivities (mole/kg/hr)											
iC_4OH	5.5	5.1	2.9	5.1	5.6	9.5	5.1	8.1	5.9	0.4	5.7
iC_4 Oxygenates	13.0	14.9	10.8	14.9	11.9	15.4	14.9	21.0	17.4	1.8	9.3

Table 3. Evaluation of Pt on Zn/Mn/Zr Oxide Catalyst for Methanol/Ethanol Conversion at High H_2 Partial Pressures - Plant 700, Run 326

Catalyst	8265-98 2% Pt on Zn/Mn/Zr (60/20/20) Oxide				
Period	5	7	10	13	18
HOS	33-40	49-56	73-80	97-104	137-144
Conditions	325°C, 7/1 MeOH/EtOH (molar), 3/1 N_2/MeOH (molar)				
Pressure (psig)	1200	300	50	50	300
MeOH WHSV (hr^{-1})	1.0	1.0	0.5	0.5	1.0
H_2/MeOH (molar)	15	15	15	0	0
Conversion (%)					
MeOH	15.3	26.3	53.3	61.6	43.9
EtOH	18.9	36.8	78.7	82.8	64.7
Selectivities (mole %)					
nC_3OH	0.2	0.2	0.1	2.0	0.0
nC_4OH	0.1	1.1	1.3	0.8	1.4
iC_4OH	1.1	1.3	3.4	1.9	2.6
iC_4 Aldehyde	9.1	6.6	3.4	1.7	5.2
Me iButyrate	0.1	0.4	0.4	2.5	1.7
Other Oxygenates	13.2	16.8	13.5	6.6	9.2
Others (No ID)	0.3	2.4	11.9	16.2	12.7
C_1-C_2 Oxygenates	4.1	5.1	1.5	9.2	12.4
C_1-C_4 Hydrocarbons	1.4	0.5	0.4	0.5	0.4
CO	32.0	18.6	14.7	16.3	10.3
CO_2	38.4	47.0	49.4	42.3	44.0
Productivities (mole/kg/hr)					
iC_4OH	0.1	0.2	0.4	0.3	0.5
iC_4 Oxygenates	0.7	1.0	0.8	0.7	1.9

Table 4. Reaction Coefficients for Process Modeling

Temperature, °C	325
Pressure, psig	300
MeOH LHSV, hr-1	1
MeOH/EtOH, molar	7
MeOH/N2 (H2), molar	0.5

Assumptions.

1. C5+ Alcohols are treated as C5's
2. "Other" Aldehydes and Ketones are treated as C5's
3. "Other" Esters are treated as C6's
4. "Other" Hydrocarbons are treated as C6's

Ethanol ——→ (MeAcetate, n-C3OH, MeBuEther, Me i-Butyrate, n-C4OH, i-C4OH, C5+ OH, i-C4 Aldehyde, "Other" Aldehydes and Ketones, "Other" Hydrocarbons)

Methanol ——→ (CO, CO2, DME, MeFormate, MeAcetate, C1-C5 HCBN's, n-C3OH, MeBuEther, Me i-Butyrate, i-C4OH, C5+ OH, i-C4 Aldehyde, "Other" Aldehydes and Ketones, "Other" Hydrocarbons)

Methanol Conv, %	55 18
Ethanol Conv, %	96.95

	% Methanol Conversion	100% Conv Basis	% Ethanol Conversion	100% Conv Basis
Unconverted	44.82		3.05	
CO	12.09	21.91		
CO2	17 48	31.68		
n-C3OH	0.44	0.80	3 07	3.17
n-C4OH			0 40	0.41
i-C4OH	7.29	13.21	38 96	40 19
C5+ OH	0.67	1.21	9.40	9.70
DME	0.87	1.58		
MeBuEther	0 01	0.02	0.16	0.17
i-C4 Aldehyde	1.55	2 81	8.47	8.74
"Other" Ald + Ketone	0.19	0 34	2.60	2.68
MeFormate	0 32	0.58		
MeAcetate	1.18	2 14	8.26	8.52
Me i-Butyrate	1.50	2.72	21.01	21.67
"Other" Esters			4.62	4.77
C2	0 61	1.11		
C3	0.20	0 36		
C5	0 01	0.02		
Other HC	10 77	19.52		
Total	100 00	100.00	100 00	100.00

	C	H	O
Methanol	1	4	1
Ethanol	2	6	1
CO	1		1
CO2	1		2
n-C3OH	3	8	1
n-C4OH	4	10	1
i-C4OH	4	10	1
C5+ OH	5	12	1
DME	2	6	1
MeBuEther	5	12	1
i-C4 Aldehyde	4	8	1
i-Pentanal	5	10	1
MeFormate	2	4	2
MeAcetate	3	6	2
Me i-Butyrate	5	10	2
Et i-Butyrate	6	12	2
C2	2	6	
C3	3	8	
C5	5	12	
C6	6	14	

Reaction Coefficients for HYSIM Simulation:

Methanol	-100	
Ethanol		-100
CO	21.91	
CO2	31.68	
n-C3OH	0.27	2 11
n-C4OH		0.21
i-C4OH	3 30	20.09
C5+ OH	0.24	3.88
DME	0.79	
MeBuEther	0.00	0.07
i-C4 Aldehyde	0.70	4.37
i-Pentanal	0.07	1.07
MeFormate	0.29	
MeAcetate	0.71	5.68
Me i-Butyrate	0.54	8.67
Et i-Butyrate		1.59
C2	0.55	
C3	0.12	
C5	0.00	
C6	3.25	
H2	138.8	37.27
H2O	6.26	36.32
C Balance:	100.00	100.02
H Balance.	100.00	100.00
O Balance.	100.00	100.00

Gas Distribution (Molar):

@55 18/96 95 MeOH/EtOH Conversions

	Calc	at Equil	Actual
H2	62.29	67.40	71.30
H2O	21.37	16.26	3.70
CO	6.68	2.11	10.21
CO2	9.66	14.23	14.79
Total	100.00	100.00	100.00

Table 5. Mass Balance and Yields from Process Simulation

	Feed Kg-Moles/hr		Product Kg-Moles/hr					
	Methanol	Ethanol	Recy Vent	Liq Purge	Ovd Vapor	Liq Product	Recy Liq	Recy Gas
Methanol	650		7.7	12.8	0.3		477.4	0.6
Ethanol		156		0.1			4.6	
Isobutanol			0.1			51.9	66.6	

C Conv:	97.8
IC4OH Sel:	21.6

TOTAL IN: PER DAY	Metric Tons	672	TOTAL OUT: PER DAY	Metric Tons	673
	Kg-Moles C	23095		Kg-Moles C	23120
	Kg-Moles H	84884		Kg-Moles H	84925
	Kg-Moles O	19347		Kg-Moles O	19355

	C	H	O					MOLES C	MOLES H	MOLES O
Methanol	1	4	1	5.94	9.83	0.22	0.00	499	1997	499
Ethanol	2	6	1	0.05	0.14	0.00	0.00	8	24	4
Hydrogen		2		49.13	0.00	0.14		0	48884	0
CO	1		1	34.31	0.00	0.11		1230	0	1230
CO2	1		2	298.57	0.61	2.83		6864	0	13728
n-C3OH	3	8	1	0.42	2.23	0.02	4.51	358	956	119
n-C4OH	4	10	1	0.00	0.00		0.58	31	79	8
i-C4OH	4	10	1	0.19	0.02	0.00	92.40	5001	12502	1250
C5+ OH	5	12	1	0.01			15.98	907	2178	181
DME	2	6	1	4.93	0.41	0.08		235	706	118
MeBuEther	5	12	1	0.14	0.16	0.00	0.01	17	41	3
i-C4 Aldehyde	4	8	1	6.72	10.50	0.19	2.46	1103	2206	276
i-Pentanal	5	10	1	0.00			4.35	253	506	51
MeFormate	2	4	2	1.95	0.56	0.04		85	170	85
MeAcetate	3	6	2	14.66	8.55	0.38	0.00	956	1911	637
Me i-Butyrate	5	10	2	0.59	0.46	0.01	41.09	2065	4129	826
Et i-Butyrate	6	12	2	0.04			6.87	357	714	119
C2	2	6		2.48	0.00	0.02		166	499	0
C3	3	8		0.77	0.01	0.01		54	145	0
C5	5	12		0.05	0.01	0.00		4	9	0
C6	6	14		30.15	11.03	0.81	0.00	2926	6827	0
Water	0	2	1	1.13	2.80	0.05		0	442	221
Total				452.22	47.33	4.91	168.25	23120	84925	19355

Figure 1. Process Flow Scheme for Modeling