# APPENDIX C

# LPMEOH AND LPHBOH MASS BALANCES AND LIQUID ANALYSES

**RUN NO:** AF-R9.1b **TITLE: LPMEOH over BASF S3-86 CATALYST with TEXACO GAS : SV=6700**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 3/22/94 | 3:00 |
| End Date | 3/22/94 | 21:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 62.00 |
| End | 80.00 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 476 |
| Pressure (psig) | 750 |
| Space Velocity (sL/kg-hr) | 6832 |
| Vg (inlet) | 0.85 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1250 |
| Slurry Concentration (wt %) | 45.4 |
| Slurry Level (%) | 92 |
| Gas Holdup (vol %) | 47.2 |

**Performance Results**

| | |
|---|---|
| CO Conversion to H2 (%) | -0.6 |
| CO Conversion to MeOH (%) | 14.5 |
| CO Conversion to MeOH (%) | 14.5 |
| Theoretical Conversion % (1 CSTR) | 14.5 |
| Alcohol Production (Ton/day) | 11.1 |

**Atom Balance Closure (% of inlet)**

| | |
|---|---|
| C | 0.70 |
| H | -1.31 |
| H | -1.31 |
| O | 0.59 |
| N | -0.40 |

| | | Sample# 10:15 | Sample# 17:00 | Sample# 21:02 | Sample# | Sample# | Sample# |
|---|---|---|---|---|---|---|---|
| **Liquid Product Analysis (wt%)** | Methanol | 95.877 | 95.981 | 96.114 | | | |
| | Ethanol | 0.833 | 0.833 | 0.783 | | | |
| | 1-Propanol | 0.334 | 0.329 | 0.318 | | | |
| | iso-Propanol | 0.021 | 0.028 | 0.016 | | | |
| | 1-Butanol | 0.162 | 0.163 | 0.155 | | | |
| | 2-Butanol | 0.058 | 0.058 | 0.053 | | | |
| | iso-Butanol | 0.053 | 0.042 | 0.044 | | | |
| | 2-Methyl-1-Butanol | 0.046 | 0.045 | 0.044 | | | |
| | 1-Pentanol | 0.115 | 0.112 | 0.107 | | | |
| | 2-Methyl-1-Pentanol | 0.000 | 0.000 | 0.000 | | | |
| | 1-Hexanol | 0.036 | 0.043 | 0.042 | | | |
| | 2-Methyl-1-Isobutyrate | 0.000 | 0.000 | 0.000 | | | |
| | Methyl Acetate | 0.218 | 0.210 | 0.193 | | | |
| | Ethyl Acetate | 0.000 | 0.000 | 0.000 | | | |
| | Methyl Formate | 0.915 | 0.870 | 0.853 | | | |
| | DME | 0.085 | 0.074 | 0.070 | | | |
| | CO2 | 0.000 | 0.000 | 0.000 | | | |
| | Water | 1.026 | 1.016 | 1.022 | | | |
| | Oil | 0.243 | 0.261 | 0.225 | | | |
| | Total | 100.022 | 100.065 | 100.039 | | | |

RUN NO: AF-R9.1b TITLE: LPMEOH over BASF S3-86 CATALYST with TEXACO GAS : SV=6700

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 303.4 | 140.9 | 79.8 | 310.4 | | 295.3 | 468.9 | 100.0 | 85.1 | 69.2 | | 80.0 |
| P | psig | 844.2 | 871.5 | 822.4 | 793.4 | | 793.4 | 750.1 | 12.6 | 622.8 | 34.8 | | 1.0 |
| Comp | H2 | 16.23 | 25.13 | 100.00 | 34.49 | | 34.49 | 21.76 | 25.14 | 25.13 | 30.49 | | 0.00 |
| | CO | 77.75 | 57.50 | 0.00 | 52.27 | | 52.27 | 52.77 | 57.53 | 57.50 | 62.17 | | 0.00 |
| | N2 | 0.42 | 1.18 | 0.00 | 0.90 | | 0.90 | 1.08 | 1.18 | 1.18 | 1.59 | | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | CO2 | 5.61 | 16.08 | 0.00 | 12.33 | | 12.33 | 14.75 | 16.09 | 16.08 | 5.74 | | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.05 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.09 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.09 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.47 |
| | MeOH | 0.00 | 0.11 | 0.00 | 0.00 | | 0.00 | 9.11 | 0.00 | 0.11 | 0.00 | | 96.59 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.38 | 0.06 | 0.00 | 0.01 | | 1.83 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.57 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.18 |
| | iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.07 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.04 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | 2-Methyl 1-isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.14 | 0.00 | 0.00 | 0.00 | | 0.03 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 |
| Mole Wt | lb/lb mole | 24.689 | 24.057 | 2.020 | 21.018 | | 21.018 | 25.093 | 24.044 | 24.057 | 21.004 | | 32.191 |
| Flow | SCFH | 19568 | 106283 | 21470 | 147321 | | 147321 | 122930 | 112202 | 6317 | 462 | | 11537 |
| | lb mole/hr | 50.61 | 274.88 | 55.53 | 381.02 | | 381.02 | 317.94 | 290.19 | 16.34 | 1.19 | | 29.84 |
| | lb/hr | 1249.5 | 6612.8 | 112.2 | 8008.3 | | 8008.3 | 7978.1 | 6977.3 | 393.0 | 25.1 | | 960.5 |

**RUN NO:** AF-R9.2 **TITLE: LPMEOH over BASF S3-86 CATALYST with KINGSPORT SYNGAS : SV=4000**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 3/23/94 | 12:00 |
| End Date | 3/24/94 | 9:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 95.00 |
| End | 116.00 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 483 |
| Pressure (psig) | 739 |
| Space Velocity (sL/kg-hr) | 4020 |
| Vg (inlet) | 0.51 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1250 |
| Slurry Concentration (wt %) | 39.4 |
| Slurry Level (%) | 92 |
| Gas Holdup (vol %) | 33.5 |

**Performance Results**

| | |
|---|---|
| CO Conversion to H2 (%) | -4.4 |
| CO Conversion to MeOH (%) | 46.5 |
| CO Conversion to MeOH (%) | 46.5 |
| Theoretical Conversion % (3 CSTR's) | 46.9 |
| Alcohol Production (Ton/day) | 10.8 |

**Atom Balance Closure (% of inlet)**

| | |
|---|---|
| C | 0.12 |
| H | -1.81 |
| H | -1.81 |
| O | 0.61 |
| N | -0.29 |

**Liquid Product Analysis (wt%)**

| | Sample# 16:50 | Sample# 22:00 | Sample# 04:00 | Sample# 08:30 | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 97.511 | 97.442 | 97.596 | 97.624 | | |
| Ethanol | 0.275 | 0.309 | 0.223 | 0.224 | | |
| 1-Propanol | 0.101 | 0.115 | 0.099 | 0.098 | | |
| iso-Propanol | 0.014 | 0.010 | 0.008 | 0.029 | | |
| 1-Butanol | 0.048 | 0.056 | 0.039 | 0.040 | | |
| 2-Butanol | 0.034 | 0.036 | 0.032 | 0.030 | | |
| iso-Butanol | 0.017 | 0.021 | 0.015 | 0.015 | | |
| 2-Methyl-1-Butanol | 0.015 | 0.018 | 0.016 | 0.014 | | |
| 1-Pentanol | 0.042 | 0.049 | 0.027 | 0.029 | | |
| 2-Methyl-1-Pentanol | 0.000 | 0.000 | 0.000 | 0.000 | | |
| 1-Hexanol | 0.013 | 0.018 | 0.011 | 0.010 | | |
| 2-Methyl-1-Isobutyrate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Methyl Acetate | 0.047 | 0.063 | 0.035 | 0.044 | | |
| Ethyl Acetate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Methyl Formate | 0.470 | 0.518 | 0.433 | 0.432 | | |
| DME | 0.069 | 0.065 | 0.067 | 0.069 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 1.325 | 1.232 | 1.401 | 1.344 | | |
| Oil | 0.125 | 0.141 | 0.125 | 0.101 | | |
| Total | 100.106 | 100.093 | 100.127 | 100.103 | | |

RUN NO: AF-R9.2 TITLE: LPMEOH over BASF S3-86 CATALYST with KINGSPORT SYNGAS : SV=4000

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 311.7 | 163.1 | 88.7 | 325.3 | | 306.9 | 462.7 | 100.0 | 86.3 | 77.2 | | 80.0 |
| P | psig | 779.7 | 893.5 | 681.7 | 755.2 | | 755.2 | 738.5 | 627.1 | 627.1 | 34.3 | | 1.0 |
| Comp | H2 | 16.48 | 54.45 | 100.00 | 58.59 | | 58.59 | 42.85 | 54.52 | 54.45 | 10.97 | | 0.00 |
| | CO | 75.50 | 23.21 | 0.00 | 26.85 | | 26.85 | 19.54 | 23.24 | 23.21 | 9.84 | | 0.00 |
| | N2 | 0.54 | 3.82 | 0.00 | 2.35 | | 2.35 | 3.21 | 3.82 | 3.82 | 1.08 | | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | CO2 | 7.48 | 18.39 | 0.00 | 12.21 | | 12.21 | 15.58 | 18.41 | 18.39 | 72.43 | | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.36 | | 0.05 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.25 |
| | MeOH | 0.00 | 0.14 | 0.00 | 0.00 | | 0.00 | 17.10 | 0.00 | 0.14 | 5.30 | | 97.03 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 1.62 | 0.00 | 0.00 | 0.02 | | 2.34 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.18 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.05 |
| | iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.02 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.10 | 0.00 | 0.00 | 0.00 | | 0.01 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 |
| Mole Wt | lb/lb mole | 24.922 | 16.807 | 2.020 | 14.738 | | 14.738 | 19.932 | 16.786 | 16.807 | 37.024 | | 31.873 |
| Flow | SCFH | 14719 | 51488 | 20474 | 86682 | | 86682 | 63344 | 53234 | 1972 | 487 | | 11388 |
| | lb mole/hr | 38.07 | 133.17 | 52.95 | 224.19 | | 224.19 | 163.83 | 137.68 | 5.10 | 1.26 | | 29.45 |
| | lb/hr | 948.8 | 2238.2 | 107.0 | 3304.0 | | 3304.0 | 3265.4 | 2311.1 | 85.7 | 46.6 | | 938.8 |

**RUN NO:** AF-R10.1 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=5000**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 3/29/94 | 21:00 |
| End Date | 3/30/94 | 13:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 45.92 |
| End | 61.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 573 |
| Pressure (psig) | 750 |
| Space Velocity (sL/kg-hr) | 5044 |
| Vg (inlet) | 0.61 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 41.1 |
| Slurry Level (%) | 91 |
| Gas Holdup (vol %) | 42.4 |

***Performance Results***

| | |
|---|---|
| CO Conversion (%) | 12.5 |
| H2 Conversion (%) | 25.4 |
| H2 Conversion (%) | 25.4 |
| Syngas Conversion (%) | 16.6 |
| MeOH Production (g/kg-oxide-hr) | 183.3 |
| IBOH Production (g/kg oxide-hr) | 25.8 |
| C2-C6 OH Production (g/kg oxide-hr) | 70.0 |

**Atom Balance Closure (% of Inlet)**

| | |
|---|---|
| C | -0.08 |
| H | 0.61 |
| H | 0.61 |
| O | -0.95 |
| N | -0.95 |

**Liquid Product Analysis (wt%)**

| | Sample# 5:30 A | Sample# 5:30 B | Sample# 11:10 A | Sample# 11:10 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 62.865 | 62.839 | 63.461 | 63.528 | | |
| Ethanol | 4.182 | 4.189 | 4.213 | 4.228 | | |
| 1-Propanol | 5.261 | 5.245 | 5.253 | 5.237 | | |
| iso-Propanol | 0.055 | 0.055 | 0.054 | 0.056 | | |
| 1-Butanol | 1.312 | 1.321 | 1.294 | 1.290 | | |
| 2-Butanol | 0.402 | 0.407 | 0.403 | 0.391 | | |
| iso-Butanol | 9.104 | 9.077 | 8.906 | 8.868 | | |
| 2-Methyl-1-Butanol | 2.423 | 2.418 | 2.367 | 2.351 | | |
| 1-Pentanol | 0.797 | 0.786 | 0.777 | 0.777 | | |
| 2-Methyl-1-Pentanol | 1.586 | 1.711 | 1.646 | 1.636 | | |
| 1-Hexanol | 0.320 | 0.320 | 0.314 | 0.313 | | |
| 2-Methyl-1-Isobutyrate | 0.718 | 0.720 | 0.687 | 0.688 | | |
| Methyl Acetate | 0.657 | 0.660 | 0.640 | 0.645 | | |
| Ethyl Acetate | 0.029 | 0.027 | 0.026 | 0.027 | | |
| Methyl Formate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.854 | 0.850 | 1.179 | 1.184 | | |
| Oil + Others (*) | 1.693 | 1.693 | 1.693 | 1.693 | | |
| Total | 92.258 | 92.318 | 92.913 | 92.912 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.1 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=5000

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 287.4 | 130.3 | 63.9 | 419.3 | | 397.9 | 559.5 | 72.8 | 63.3 | 61.3 | 97.4 | 80.0 |
| P | psig | 805.1 | 880.3 | 837.7 | 773.1 | | 773.1 | 749.5 | 720.6 | 698.8 | 27.7 | 165.0 | 1.0 |
| Comp | H2 | 45.09 | 26.42 | 100.00 | 30.97 | | 30.97 | 25.81 | 26.00 | 26.42 | 8.23 | 3.64 | 0.00 |
| | CO | 54.67 | 69.03 | 0.00 | 65.53 | | 65.53 | 64.04 | 67.21 | 69.03 | 51.64 | 27.23 | 0.00 |
| | N2 | 0.24 | 0.94 | 0.00 | 0.77 | | 0.77 | 0.86 | 0.91 | 0.94 | 0.50 | 0.26 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.00 | 3.32 | 0.00 | 2.51 | | 2.51 | 5.60 | 5.87 | 3.32 | 36.01 | 67.15 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.15 | 0.23 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.35 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.35 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 2.84 | 0.00 | 0.00 | 3.46 | 1.50 | 78.74 |
| | H2O | 0.00 | 0.29 | 0.00 | 0.22 | | 0.22 | 0.00 | 0.01 | 0.29 | 0.01 | 0.00 | 2.25 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.13 | 0.00 | 0.00 | 0.00 | 0.00 | 3.64 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.12 | 0.00 | 0.00 | 0.00 | 0.00 | 3.49 |
| | Iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.04 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.17 | 0.00 | 0.00 | 0.00 | 0.00 | 4.84 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.70 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.22 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 1.08 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.36 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.64 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 3.21 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.28 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.69 | 0.00 | 0.00 | 0.00 | 0.00 | 0.16 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.37 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 16.290 | 21.645 | 2.020 | 20.341 | | 20.342 | 22.855 | 22.190 | 21.645 | 31.795 | 37.910 | 39.571 |
| Flow | SCFH | 24000 | 71712 | 0 | 95712 | | 95712 | 85709 | 82036 | 5070 | 215 | 3451 | 3286 |
| | lb mole/hr | 62.07 | 185.47 | 0.00 | 247.55 | | 247.55 | 221.67 | 212.17 | 13.11 | 0.56 | 8.93 | 8.50 |
| | lb/hr | 1011.2 | 4014.5 | 0.0 | 5035.4 | | 5035.4 | 5066.5 | 4708.2 | 283.8 | 17.7 | 338.4 | 336.3 |

**RUN NO:** AF-R10.2 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=3000**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 3/31/94 | 0:00 |
| End Date | 3/31/94 | 17:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 72.92 |
| End | 89.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 572 |
| Pressure (psig) | 753 |
| Space Velocity (sL/kg-hr) | 3030 |
| Vg (inlet) | 0.37 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 38.4 |
| Slurry Level (%) | 92 |
| Gas Holdup (vol %) | 36.3 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 13.7 |
| H2 Conversion (%) | 25.4 |
| H2 Conversion (%) | 25.4 |
| Syngas Conversion (%) | 17.3 |
| MeOH Production (g/kg-oxide-hr) | 94.5 |
| IBOH Production (g/kg oxide-hr) | 18.7 |
| C2-C6 OH Production (g/kg oxide-hr) | 45.5 |

**Atom Balance Closure (% of inlet)**

| | |
|---|---|
| C | 0.87 |
| H | 1.65 |
| H | 1.65 |
| O | -0.54 |
| N | -0.45 |

**Liquid Product Analysis (wt%)**

| | Sample# 5:30 A | Sample# 5:30 B | Sample# 14:20 A | Sample# 14:20 B | Sample# 15:50 A | Sample# 15:50 B |
|---|---|---|---|---|---|---|
| Methanol | 55.357 | 55.845 | 55.212 | 55.434 | 54.809 | 55.853 |
| Ethanol | 3.435 | 3.441 | 3.407 | 3.406 | 3.352 | 3.414 |
| 1-Propanol | 5.380 | 5.421 | 5.371 | 5.378 | 5.282 | 5.349 |
| Iso-Propanol | 0.047 | 0.052 | 0.051 | 0.059 | 0.053 | 0.048 |
| 1-Butanol | 1.322 | 1.332 | 1.313 | 1.324 | 1.303 | 1.311 |
| 2-Butanol | 0.380 | 0.380 | 0.377 | 0.382 | 0.375 | 0.377 |
| iso-Butanol | 12.835 | 12.923 | 12.768 | 12.771 | 12.636 | 12.746 |
| 2-Methyl-1-Butanol | 3.271 | 3.094 | 3.230 | 3.052 | 3.190 | 3.040 |
| 1-Pentanol | 0.848 | 0.861 | 0.844 | 0.845 | 0.832 | 0.842 |
| 2-Methyl-1-Pentanol | 2.101 | 1.945 | 2.341 | 2.083 | 2.138 | 2.306 |
| 1-Hexanol | 0.321 | 0.315 | 0.327 | 0.329 | 0.320 | 0.324 |
| 2-Methyl-1-Isobutyrate | 1.061 | 1.072 | 1.049 | 1.052 | 1.035 | 1.051 |
| Methyl Acetate | 0.574 | 0.583 | 0.571 | 0.580 | 0.565 | 0.577 |
| Ethyl Acetate | 0.024 | 0.028 | 0.027 | 0.029 | 0.022 | 0.013 |
| Methyl Formate | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| Water | 0.897 | 0.907 | 1.230 | 1.243 | 1.237 | 1.258 |
| Oil + Others (*) | 1.237 | 1.237 | 1.687 | 1.687 | 1.223 | 1.223 |
| Total | 89.090 | 89.436 | 89.805 | 89.654 | 88.372 | 89.732 |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.2 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=3000

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 274.6 | 135.5 | 71.0 | 343.4 | | 319.1 | 555.3 | 68.1 | 61.5 | 58.2 | 70.9 | 80.0 |
| P | psig | 784.5 | 880.8 | 841.2 | 763.4 | | 763.4 | 752.8 | 745.6 | 730.3 | 27.9 | 165.0 | 1.0 |
| Comp | H2 | 38.34 | 24.49 | 100.00 | 29.31 | | 29.31 | 24.50 | 24.19 | 24.49 | 7.43 | 3.30 | 0.00 |
| | CO | 60.69 | 69.39 | 0.00 | 66.32 | | 66.32 | 64.14 | 67.10 | 69.39 | 48.99 | 25.92 | 0.00 |
| | N2 | 0.88 | 2.01 | 0.00 | 1.63 | | 1.63 | 1.82 | 1.92 | 2.01 | 1.02 | 0.51 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.09 | 3.87 | 0.00 | 2.58 | | 2.58 | 6.52 | 6.78 | 3.87 | 39.43 | 69.26 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.15 | 0.24 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.33 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.33 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 2.45 | 0.00 | 0.00 | 2.95 | 0.78 | 73.66 |
| | H2O | 0.00 | 0.25 | 0.00 | 0.16 | | 0.16 | 0.00 | 0.01 | 0.25 | 0.02 | 0.00 | 2.67 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 3.15 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | 3.80 |
| | iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.04 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.21 | 0.00 | 0.00 | 0.00 | 0.00 | 7.34 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.76 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.22 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.04 | 0.00 | 0.00 | 0.00 | 0.00 | 1.52 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.41 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.90 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 4.57 |
| | 2-Methyl 1-isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.44 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.79 | 0.00 | 0.00 | 0.00 | 0.00 | 0.20 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.77 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 18.059 | 22.239 | 2.020 | 20.788 | | 20.788 | 23.436 | 22.808 | 22.239 | 32.533 | 38.309 | 42.144 |
| Flow | SCFH | 19900 | 37609 | 0 | 57509 | | 57509 | 51305 | 48768 | 8211 | 198 | 2174 | 1791 |
| | lb mole/hr | 51.47 | 97.27 | 0.00 | 148.74 | | 148.74 | 132.69 | 126.13 | 21.24 | 0.51 | 5.62 | 4.63 |
| | lb/hr | 929.4 | 2163.2 | 0.0 | 3092.0 | | 3092.0 | 3109.8 | 2876.8 | 472.3 | 16.6 | 215.4 | 195.2 |

**RUN NO:** AF-R10.3 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 4/1/94 | 4:00 |
| End Date | 4/1/94 | 16:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 100.92 |
| End | 112.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 572 |
| Pressure (psig) | 751 |
| Space Velocity (sL/kg-hr) | 8242 |
| Vg (inlet) | 1.00 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 44.8 |
| Slurry Level (%) | 90 |
| Gas Holdup (vol %) | 50.1 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 7.6 |
| H2 Conversion (%) | 21.0 |
| H2 Conversion (%) | 21.0 |
| Syngas Conversion (%) | 11.7 |
| MeOH Production (g/kg-oxide-hr) | 274.6 |
| IBOH Production (g/kg oxide-hr) | 16.6 |
| C2-C6 OH Production (g/kg oxide-hr) | 50.5 |

**Atom Balance Closure (% of Inlet)**

| | |
|---|---|
| C | -0.93 |
| H | 0.85 |
| H | 0.85 |
| O | -1.41 |
| N | 0.11 |

**Liquid Product Analysis (wt%)**

| | Sample# 7:45 A | Sample# 7:45 B | Sample# 14:15 A | Sample# 14:15 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 73.935 | 74.039 | 75.423 | 75.584 | | |
| Ethanol | 4.142 | 4.079 | 4.050 | 4.050 | | |
| 1-Propanol | 4.416 | 4.402 | 4.355 | 4.318 | | |
| iso-Propanol | 0.050 | 0.043 | 0.049 | 0.047 | | |
| 1-Butanol | 1.025 | 1.027 | 1.002 | 0.991 | | |
| 2-Butanol | 0.352 | 0.358 | 0.352 | 0.347 | | |
| Iso-Butanol | 5.570 | 5.628 | 5.069 | 5.011 | | |
| 2-Methyl-1-Butanol | 1.408 | 1.413 | 1.378 | 1.370 | | |
| 1-Pentanol | 0.602 | 0.599 | 0.580 | 0.575 | | |
| 2-Methyl-1-Pentanol | 0.990 | 1.000 | 0.878 | 0.899 | | |
| 1-Hexanol | 0.232 | 0.233 | 0.226 | 0.223 | | |
| 2-Methyl-1-Isobutyrate | 0.372 | 0.372 | 0.317 | 0.315 | | |
| Methyl Acetate | 0.518 | 0.504 | 0.476 | 0.483 | | |
| Ethyl Acetate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Methyl Formate | 0.215 | 0.226 | 0.217 | 0.221 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.711 | 0.705 | 0.677 | 0.673 | | |
| Oil + Others (*) | 1.540 | 1.540 | 2.573 | 2.573 | | |
| Total | 96.078 | 96.168 | 97.622 | 97.680 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.3 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 296.5 | 138.0 | 76.1 | 431.6 | | 413.8 | 565.9 | 79.4 | 67.7 | 64.4 | 80.1 | 80.0 |
| P | psig | 861.4 | 901.3 | 816.7 | 806.0 | | 806.0 | 751.3 | 664.7 | 619.5 | 30.4 | 165.1 | 1.0 |
| Comp | H2 | 48.18 | 25.49 | 100.00 | 29.46 | | 29.46 | 25.12 | 25.13 | 25.49 | 9.90 | 4.34 | 0.00 |
| (mole%) | CO | 50.95 | 68.97 | 0.00 | 65.85 | | 65.85 | 65.66 | 68.33 | 68.97 | 58.36 | 33.35 | 0.00 |
| | N2 | 0.80 | 2.23 | 0.00 | 1.94 | | 1.94 | 2.09 | 2.15 | 2.23 | 1.39 | 0.71 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.06 | 3.31 | 0.00 | 2.75 | | 2.75 | 4.18 | 4.39 | 3.31 | 26.78 | 60.58 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.09 | 0.24 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.13 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 2.52 | 0.00 | 0.00 | 3.46 | 0.77 | 86.01 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 1.41 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.09 | 0.00 | 0.00 | 0.00 | 0.00 | 3.26 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.07 | 0.00 | 0.00 | 0.00 | 0.00 | 2.68 |
| | Iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.07 | 0.00 | 0.00 | 0.00 | 0.00 | 2.65 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.50 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.18 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.58 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.34 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.43 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.12 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.37 | 0.00 | 0.00 | 0.00 | 0.00 | 0.18 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.18 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 15.497 | 21.914 | 2.020 | 20.793 | | 20.793 | 22.503 | 22.180 | 21.914 | 29.876 | 36.650 | 36.463 |
| Flow | SCFH | 27622 | 128789 | 0 | 156411 | | 156411 | 144910 | 140643 | 9580 | 194 | 1432 | 4471 |
| | lb mole/hr | 71.44 | 333.09 | 0.00 | 404.53 | | 404.54 | 374.79 | 363.75 | 24.78 | 0.50 | 3.70 | 11.56 |
| | lb/hr | 1107.1 | 7299.5 | 0.0 | 8411.6 | | 8411.7 | 8433.9 | 8067.9 | 543.0 | 15.0 | 135.8 | 421.7 |

**RUN NO:** AF-R10.4 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 4/1/94 | 21:00 |
| End Date | 4/2/94 | 7:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 117.92 |
| End | 127.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 573 |
| Pressure (psig) | 1300 |
| Space Velocity (sL/kg-hr) | 8227 |
| Vg (inlet) | 0.58 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 41.9 |
| Slurry Level (%) | 92 |
| Gas Holdup (vol %) | 44.0 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 12.7 |
| H2 Conversion (%) | 34.3 |
| H2 Conversion (%) | 34.3 |
| Syngas Conversion (%) | 19.6 |
| MeOH Production (g/kg-oxide-hr) | 528.0 |
| IBOH Production (g/kg oxide-hr) | 20.8 |
| C2-C6 OH Production (g/kg oxide-hr) | 86.9 |

**Atom Balance Closure (% of Inlet)**

| | |
|---|---|
| C | 0.74 |
| H | -1.26 |
| H | -1.26 |
| O | 0.07 |
| N | -0.24 |

**Liquid Product Analysis (wt%)**

| | Sample# 3:45 A | Sample# 3:45 B | Sample# 6:35 A | Sample# 6:35 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 81.365 | 81.103 | 81.750 | 81.772 | | |
| Ethanol | 3.670 | 3.698 | 3.568 | 3.552 | | |
| 1-Propanol | 3.755 | 3.773 | 3.645 | 3.627 | | |
| iso-Propanol | 0.042 | 0.043 | 0.045 | 0.042 | | |
| 1-Butanol | 0.830 | 0.824 | 0.801 | 0.796 | | |
| 2-Butanol | 0.262 | 0.259 | 0.255 | 0.254 | | |
| iso-Butanol | 2.638 | 2.631 | 2.551 | 2.533 | | |
| 2-Methyl-1-Butanol | 0.770 | 0.776 | 0.748 | 0.740 | | |
| 1-Pentanol | 0.442 | 0.439 | 0.428 | 0.423 | | |
| 2-Methyl-1-Pentanol | 0.449 | 0.451 | 0.438 | 0.433 | | |
| 1-Hexanol | 0.178 | 0.176 | 0.171 | 0.173 | | |
| 2-Methyl-1-Isobutyrate | 0.212 | 0.214 | 0.206 | 0.205 | | |
| Methyl Acetate | 0.873 | 0.865 | 0.830 | 0.839 | | |
| Ethyl Acetate | 0.000 | 0.022 | 0.019 | 0.009 | | |
| Methyl Formate | 0.619 | 0.845 | 0.851 | 0.851 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.257 | 0.273 | 0.284 | 0.273 | | |
| Oil + Others (*) | 0.709 | 0.709 | 0.575 | 0.575 | | |
| Total | 97.071 | 97.101 | 97.165 | 97.097 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.4 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 293.2 | 118.7 | 78.4 | 376.4 | | 360.1 | 556.9 | 86.6 | 73.6 | 61.8 | 163.4 | 80.0 |
| P | psig | 782.0 | 816.1 | 814.4 | 1323.3 | | 1323.3 | 1300.1 | 696.5 | 658.0 | 31.5 | 165.1 | 1.0 |
| Comp | H2 | 6.85 | 21.48 | 100.00 | 30.25 | | 30.25 | 22.64 | 22.27 | 21.48 | 7.25 | 3.13 | 0.00 |
| | CO | 91.93 | 72.56 | 0.00 | 65.46 | | 65.46 | 65.11 | 70.36 | 72.56 | 51.92 | 30.09 | 0.00 |
| | N2 | 1.13 | 2.11 | 0.00 | 1.62 | | 1.62 | 1.85 | 2.03 | 2.11 | 1.08 | 0.58 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.10 | 3.85 | 0.00 | 2.67 | | 2.67 | 5.10 | 5.33 | 3.85 | 29.13 | 59.25 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.28 | 0.43 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.41 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.41 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.47 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 5.12 | 0.00 | 0.00 | 10.34 | 6.52 | 90.02 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.53 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.16 | 0.00 | 0.00 | 0.00 | 0.00 | 2.78 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.13 | 0.00 | 0.00 | 0.00 | 0.00 | 2.18 |
| | Iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.09 | 0.00 | 0.00 | 0.00 | 0.00 | 1.24 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.39 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.12 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.30 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.17 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.15 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.06 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.07 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.54 | 0.00 | 0.00 | 0.00 | 0.00 | 0.08 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.79 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 26.246 | 23.042 | 2.020 | 20.576 | | 20.576 | 23.547 | 23.075 | 23.042 | 31.252 | 37.018 | 35.212 |
| Flow | SCFH | 25279 | 108627 | 22219 | 156125 | | 156125 | 136982 | 124667 | 12682 | 220 | 2909 | 9056 |
| | lb mole/hr | 65.38 | 280.95 | 57.47 | 403.79 | | 403.79 | 354.28 | 322.43 | 32.80 | 0.57 | 7.52 | 23.42 |
| | lb/hr | 1716.0 | 6473.5 | 116.1 | 8308.5 | | 8308.6 | 8342.3 | 7440.0 | 755.7 | 17.8 | 278.5 | 824.7 |

**RUN NO:** AF-R10.5 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 4/3/94 | 2:00 |
| End Date | 4/3/94 | 14:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 146.92 |
| End | 158.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 573 |
| Pressure (psig) | 1735 |
| Space Velocity (sL/kg-hr) | 8281 |
| Vg (inlet) | 0.44 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 40.9 |
| Slurry Level (%) | 91 |
| Gas Holdup (vol %) | 41.8 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 15.7 |
| H2 Conversion (%) | 47.9 |
| H2 Conversion (%) | 47.9 |
| Syngas Conversion (%) | 25.7 |
| MeOH Production (g/kg-oxide-hr) | 718.8 |
| IBOH Production (g/kg oxide-hr) | 23.2 |
| C2-C6 OH Production (g/kg oxide-hr) | 95.9 |

**Atom Balance Closure (% of inlet)**

| | |
|---|---|
| C | -0.64 |
| H | 1.76 |
| H | 1.76 |
| O | -1.03 |
| N | 0.14 |

**Liquid Product Analysis (wt%)**

| | Sample# 6:30 A | Sample# 6:30 B | Sample# 12:45 A | Sample# 12:45 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 82.469 | 82.474 | 83.866 | 83.906 | | |
| Ethanol | 3.188 | 3.176 | 2.990 | 2.928 | | |
| 1-Propanol | 3.459 | 3.461 | 3.196 | 3.222 | | |
| iso-Propanol | 0.041 | 0.040 | 0.036 | 0.038 | | |
| 1-Butanol | 0.755 | 0.756 | 0.695 | 0.703 | | |
| 2-Butanol | 0.243 | 0.244 | 0.223 | 0.226 | | |
| iso-Butanol | 2.352 | 2.349 | 2.006 | 2.024 | | |
| 2-Methyl-1-Butanol | 0.684 | 0.685 | 0.597 | 0.602 | | |
| 1-Pentanol | 0.403 | 0.405 | 0.367 | 0.374 | | |
| 2-Methyl-1-Pentanol | 0.368 | 0.358 | 0.298 | 0.308 | | |
| 1-Hexanol | 0.159 | 0.166 | 0.143 | 0.147 | | |
| 2-Methyl-1-Isobutyrate | 0.203 | 0.200 | 0.165 | 0.167 | | |
| Methyl Acetate | 0.948 | 0.946 | 0.954 | 0.944 | | |
| Ethyl Acetate | 0.000 | 0.018 | 0.000 | 0.000 | | |
| Methyl Formate | 0.952 | 0.952 | 1.113 | 1.098 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.181 | 0.183 | 0.144 | 0.146 | | |
| Oil + Others (*) | 0.426 | 0.426 | 0.432 | 0.432 | | |
| Total | 96.831 | 96.839 | 97.225 | 97.265 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.5 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS : SV=8200

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 293.8 | 123.2 | 85.9 | 388.7 | | 371.7 | 546.8 | 86.8 | 74.5 | 68.9 | 125.2 | 80.0 |
| P | psig | 783.9 | 831.9 | 830.8 | 1748.0 | | 1748.0 | 1734.8 | 695.7 | 661.6 | 31.9 | 163.3 | 1.0 |
| Comp | H2 | 7.21 | 17.00 | 100.00 | 29.44 | | 29.44 | 18.28 | 16.56 | 17.00 | 5.62 | 2.46 | 0.00 |
| | CO | 91.94 | 75.87 | 0.00 | 65.66 | | 65.66 | 65.90 | 74.61 | 75.87 | 53.94 | 31.78 | 0.00 |
| | N2 | 0.76 | 2.98 | 0.00 | 2.12 | | 2.12 | 2.52 | 2.86 | 2.98 | 1.51 | 0.81 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.09 | 4.15 | 0.00 | 2.78 | | 2.78 | 5.52 | 5.98 | 4.15 | 30.09 | 61.52 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.46 | 0.53 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.45 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.45 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.60 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 7.23 | 0.00 | 0.00 | 8.37 | 2.90 | 91.13 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.32 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.20 | 0.00 | 0.00 | 0.00 | 0.00 | 2.34 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.16 | 0.00 | 0.00 | 0.00 | 0.00 | 1.95 |
| | Iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 1.03 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.34 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.11 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.26 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.15 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.11 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.07 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.06 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.68 | 0.00 | 0.00 | 0.00 | 0.00 | 0.05 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.65 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 26.152 | 24.254 | 2.020 | 20.804 | | 20.804 | 24.893 | 24.664 | 24.254 | 31.783 | 37.426 | 34.983 |
| Flow | SCFH | 24676 | 105916 | 26556 | 157148 | | 157148 | 131945 | 116252 | 5213 | 257 | 3898 | 11948 |
| | lb mole/hr | 63.82 | 273.94 | 68.68 | 406.44 | | 406.44 | 341.26 | 300.67 | 13.48 | 0.67 | 10.08 | 30.90 |
| | lb/hr | 1669.0 | 6644.2 | 138.7 | 8455.7 | | 8455.7 | 8494.7 | 7415.7 | 327.0 | 21.1 | 377.4 | 1081.1 |

**RUN NO:** AF-R10.6 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 4/4/94 | 0:00 |
| End Date | 4/4/94 | 12:00 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 168.92 |
| End | 180.92 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 572 |
| Pressure (psig) | 1735 |
| Space Velocity (sL/kg-hr) | 3026 |
| Vg (inlet) | 0.16 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 35.5 |
| Slurry Level (%) | 91 |
| Gas Holdup (vol %) | 27.9 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 20.9 |
| H2 Conversion (%) | 48.3 |
| H2 Conversion (%) | 48.3 |
| Syngas Conversion (%) | 29.3 |
| MeOH Production (g/kg-oxide-hr) | 214.2 |
| IBOH Production (g/kg oxide-hr) | 23.8 |
| C2-C6 OH Production (g/kg oxide-hr) | 60.6 |

**Atom Balance Closure (% of inlet)**

| | |
|---|---|
| C | 1.55 |
| H | 0.75 |
| H | 0.75 |
| O | -0.27 |
| N | 0.09 |

**Liquid Product Analysis (wt%)**

| | Sample# 4:50 A | Sample# 4:50 B | Sample# 10:45 A | Sample# 10:45 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 68.455 | 68.637 | 68.662 | 68.799 | | |
| Ethanol | 2.824 | 2.833 | 2.815 | 2.832 | | |
| 1-Propanol | 5.003 | 4.995 | 5.017 | 5.033 | | |
| iso-Propanol | 0.041 | 0.042 | 0.045 | 0.041 | | |
| 1-Butanol | 1.002 | 0.998 | 1.001 | 1.001 | | |
| 2-Butanol | 0.265 | 0.262 | 0.263 | 0.259 | | |
| Iso-Butanol | 7.178 | 7.147 | 7.155 | 7.176 | | |
| 2-Methyl-1-Butanol | 1.646 | 1.615 | 1.618 | 1.621 | | |
| 1-Pentanol | 0.581 | 0.575 | 0.578 | 0.576 | | |
| 2-Methyl-1-Pentanol | 0.845 | 0.832 | 0.835 | 0.836 | | |
| 1-Hexanol | 0.218 | 0.211 | 0.210 | 0.213 | | |
| 2-Methyl-1-Isobutyrate | 0.987 | 0.991 | 0.981 | 0.980 | | |
| Methyl Acetate | 1.295 | 1.313 | 1.285 | 1.277 | | |
| Ethyl Acetate | 0.032 | 0.030 | 0.029 | 0.039 | | |
| Methyl Formate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 1.641 | 1.676 | 1.635 | 1.619 | | |
| Oil + Others (*) | 1.156 | 1.156 | 1.687 | 1.687 | | |
| Total | 93.169 | 93.313 | 93.816 | 93.989 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.6 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 266.9 | 131.6 | 70.0 | 340.9 | | 318.6 | 547.3 | 75.7 | 68.6 | 64.8 | 133.1 | 80.0 |
| P | psig | 720.0 | 819.9 | 846.8 | 1730.9 | | 1730.9 | 1735.0 | 733.0 | 720.0 | 30.3 | 158.5 | 1.0 |
| Comp | H2 | 42.85 | 16.53 | 100.00 | 29.44 | | 29.44 | 18.47 | 17.42 | 16.53 | 4.52 | 1.93 | 0.00 |
| | CO | 56.46 | 76.66 | 0.00 | 66.74 | | 66.74 | 64.04 | 72.09 | 76.66 | 46.52 | 24.35 | 0.00 |
| | N2 | 0.61 | 2.04 | 0.00 | 1.34 | | 1.34 | 1.63 | 1.86 | 2.04 | 0.96 | 0.43 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.07 | 4.78 | 0.00 | 2.48 | | 2.48 | 7.94 | 8.61 | 4.78 | 42.63 | 68.98 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.74 | 1.20 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.67 |
| | [illegible] | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.67 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 6.01 | 0.00 | 0.00 | 4.62 | 3.12 | 81.68 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 3.47 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.18 | 0.00 | 0.00 | 0.00 | 0.00 | 2.34 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.23 | 0.00 | 0.00 | 0.00 | 0.00 | 3.18 |
| | Iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.29 | 0.00 | 0.00 | 0.00 | 0.00 | 3.68 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.03 | 0.00 | 0.00 | 0.00 | 0.00 | 0.51 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.13 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.04 | 0.00 | 0.00 | 0.00 | 0.00 | 0.70 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.25 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.31 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 2.48 |
| | 2-Methyl 1-isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.37 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 1.09 | 0.00 | 0.00 | 0.00 | 0.00 | 0.18 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 16.884 | 24.479 | 2.020 | 20.756 | | 20.757 | 25.563 | 24.860 | 24.479 | 33.972 | 38.886 | 37.720 |
| Flow | SCFH | 27204 | 30223 | 0 | 57427 | | 57427 | 47330 | 41302 | 7520 | 236 | 2575 | 4002 |
| | lb mole/hr | 70.36 | 78.17 | 0.00 | 148.53 | | 148.53 | 122.41 | 106.82 | 19.45 | 0.61 | 6.66 | 10.35 |
| | lb/hr | 1187.9 | 1913.5 | 0.0 | 3082.9 | | 3082.9 | 3129.3 | 2655.5 | 476.1 | 20.8 | 259.0 | 390.4 |

**RUN NO:** AF-R10.7 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS**

| | | |
|---|---|---|
| **Balance Period:** | | |
| Start Date | 4/4/94 | 17:00 |
| End Date | 4/5/94 | 8:00 |

| | |
|---|---|
| **Time From Start of Run (hr)** | |
| Start | 185.92 |
| End | 200.92 |

| | |
|---|---|
| **Reaction Conditions** | |
| Temperature (°F) | 572 |
| Pressure (psig) | 1300 |
| Space Velocity (sL/kg-hr) | 5070 |
| Vg (Inlet) | 0.36 |

| | |
|---|---|
| **Slurry Data** | |
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 38.9 |
| Slurry Level (%) | 91 |
| Gas Holdup (vol %) | 37.5 |

| | |
|---|---|
| **Performance Results** | |
| CO Conversion (%) | 14.2 |
| H2 Conversion (%) | 39.4 |
| H2 Conversion (%) | 39.4 |
| Syngas Conversion (%) | 22.1 |
| MeOH Production (g/kg-oxide-hr) | 329.8 |
| IBOH Production (g/kg oxide-hr) | 19.2 |
| C2-C6 OH Production (g/kg oxide-hr) | 64.2 |

| | |
|---|---|
| **Atom Balance Closure (% of inlet)** | |
| C | 0.56 |
| H | -0.94 |
| H | -0.94 |
| O | -0.13 |
| N | -0.82 |

**Liquid Product Analysis (wt%)**

| | Sample# 0:35 A | Sample# 0:35 B | Sample# 5:30 A | Sample# 5:30 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 76.516 | 76.569 | 78.674 | 78.542 | | |
| Ethanol | 3.212 | 3.242 | 3.297 | 3.291 | | |
| 1-Propanol | 4.444 | 4.474 | 4.292 | 4.318 | | |
| iso-Propanol | 0.040 | 0.041 | 0.040 | 0.040 | | |
| 1-Butanol | 0.893 | 0.900 | 0.858 | 0.863 | | |
| 2-Butanol | 0.885 | 0.886 | 0.741 | 0.745 | | |
| iso-Butanol | 4.415 | 4.446 | 3.763 | 3.792 | | |
| 2-Methyl-1-Butanol | 1.085 | 1.109 | 0.958 | 0.971 | | |
| 1-Pentanol | 0.490 | 0.496 | 0.466 | 0.465 | | |
| 2-Methyl-1-Pentanol | 0.599 | 0.603 | 0.514 | 0.523 | | |
| 1-Hexanol | 0.193 | 0.190 | 0.177 | 0.179 | | |
| 2-Methyl-1-Isobutyrate | 0.452 | 0.453 | 0.321 | 0.322 | | |
| Methyl Acetate | 0.940 | 0.934 | 0.849 | 0.833 | | |
| Ethyl Acetate | 0.024 | 0.026 | 0.000 | 0.000 | | |
| Methyl Formate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.906 | 0.890 | 0.823 | 0.795 | | |
| Oil + Others (*) | 1.020 | 1.020 | 0.700 | 0.700 | | |
| Total | 96.114 | 96.279 | 96.473 | 96.379 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.

RUN NO: AF-R10.7 TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS

| | | FRESH MAKE-UP | RECYCLE | HP H2 MAKEUP | DRY FEED | ALCOHOL INJECT. | REACT FEED | REACT EFFL | 22.10 VAPOR | PURGE 1 PIC-201 | PURGE 2 22.11 | PURGE 3 07.20 | LIQUID PROD |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T | F | 274.2 | 141.9 | 76.6 | 365.8 | | 345.8 | 554.1 | 84.1 | 74.0 | 72.0 | 133.3 | 80.0 |
| P | psig | 756.2 | 882.4 | 835.7 | 1309.9 | | 1309.9 | 1300.1 | 718.8 | 700.5 | 30.3 | 150.0 | 1.0 |
| Comp | H2 | 51.50 | 21.04 | 100.00 | 29.96 | | 29.96 | 21.02 | 21.79 | 21.04 | 6.93 | 3.01 | 0.00 |
| | CO | 47.84 | 72.45 | 0.00 | 65.29 | | 65.29 | 64.82 | 69.90 | 72.45 | 51.78 | 29.74 | 0.00 |
| | N2 | 0.60 | 2.77 | 0.00 | 2.10 | | 2.10 | 2.43 | 2.65 | 2.77 | 1.36 | 0.73 | 0.00 |
| | CH4 | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | CO2 | 0.06 | 3.75 | 0.00 | 2.65 | | 2.65 | 5.29 | 5.65 | 3.75 | 32.27 | 63.25 | 0.00 |
| | DME | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.28 | 0.62 | 0.00 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.43 |
| | MeAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.43 |
| | EtAc | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| | MeFm | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| | MeOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 5.27 | 0.00 | 0.00 | 7.36 | 2.64 | 87.40 |
| | H2O | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 1.71 |
| | Etoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.16 | 0.00 | 0.00 | 0.00 | 0.00 | 2.55 |
| | 1-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.15 | 0.00 | 0.00 | 0.00 | 0.00 | 2.63 |
| | iso-Proh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.02 |
| | IBOH | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.13 | 0.00 | 0.00 | 0.00 | 0.00 | 2.00 |
| | 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.43 |
| | 2-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.40 |
| | 2-Methyl 1-Buoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 | 0.00 | 0.42 |
| | 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.20 |
| | 2-Methyl 1-Peoh | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.20 |
| | 1-hexanol | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.37 |
| | 2-Methyl 1-Isobutyrate | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.14 |
| | others | 0.00 | 0.00 | 0.00 | 0.00 | | 0.00 | 0.66 | 0.00 | 0.00 | 0.00 | 0.00 | 0.10 |
| | TOTAL | 100.00 | 100.00 | 100.00 | 100.00 | | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |
| Mole Wt | lb/lb mole | 14.634 | 23.140 | 2.020 | 20.649 | | 20.649 | 24.074 | 23.248 | 23.140 | 31.718 | 37.568 | 35.858 |
| Flow | SCFH | 28789 | 67430 | 0 | 96219 | | 96219 | 83168 | 76637 | 5537 | 221 | 2591 | 5457 |
| | lb mole/hr | 74.46 | 174.40 | 0.00 | 248.86 | | 248.86 | 215.10 | 198.21 | 14.32 | 0.57 | 6.70 | 14.11 |
| | lb/hr | 1089.6 | 4035.6 | 0.0 | 5138.5 | | 5138.5 | 5178.4 | 4608.1 | 331.4 | 18.1 | 251.8 | 506.1 |

**RUN NO:** AF-R10.8 **TITLE: LPIBOH over Cs-Promoted BASF S3-86 CATALYST with SHELL SYNGAS**

**Balance Period:**

| | | |
|---|---|---|
| Start Date | 4/6/94 | 3:00 |
| End Date | 4/6/94 | 20:00 |

**Reaction Conditions**

| | |
|---|---|
| Temperature (°F) | 572 |
| Pressure (psig) | 1300 |
| Space Velocity (sL/kg-hr) | 5494 |
| Vg (inlet) | 0.39 |

**Performance Results**

| | |
|---|---|
| CO Conversion (%) | 6.8 |
| H2 Conversion (%) | 5.0 |
| H2 Conversion (%) | 5.0 |
| Syngas Conversion (%) | 6.2 |
| MeOH Production (g/kg-oxide-hr) | 634.1 |
| IBOH Production (g/kg oxide-hr) | 55.9 |
| C2-C6 OH Production (g/kg oxide-hr) | 190.8 |

**Time From Start of Run (hr)**

| | |
|---|---|
| Start | 219.92 |
| End | 236.92 |

**Slurry Data**

| | |
|---|---|
| Catalyst Weight (lb oxide) | 1100 |
| Slurry Concentration (wt %) | 40.1 |
| Slurry Level (%) | 91 |
| Gas Holdup (vol %) | 40.6 |

**Atom Balance Closure (% of Inlet)**

| | |
|---|---|
| C | -0.89 |
| H | -6.54 |
| H | -6.54 |
| O | -0.89 |
| N | 0.66 |

**Liquid Product Analysis (wt%)**

| | Sample# 07:45 A | Sample# 07:45 B | Sample# 12:30 A | Sample# 12:30 B | Sample# | Sample# |
|---|---|---|---|---|---|---|
| Methanol | 75.039 | 74.974 | 73.427 | 73.382 | | |
| Ethanol | 3.819 | 3.914 | 4.113 | 4.110 | | |
| 1-Propanol | 8.093 | 8.129 | 8.613 | 8.626 | | |
| iso-Propanol | 0.029 | 0.028 | 0.031 | 0.031 | | |
| 1-Butanol | 0.725 | 0.724 | 0.759 | 0.762 | | |
| 2-Butanol | 0.178 | 0.183 | 0.180 | 0.181 | | |
| iso-Butanol | 4.504 | 4.528 | 5.089 | 5.116 | | |
| 2-Methyl-1-Butanol | 0.602 | 0.612 | 0.519 | 0.519 | | |
| 1-Pentanol | 0.358 | 0.358 | 0.375 | 0.375 | | |
| 2-Methyl-1-Pentanol | 0.298 | 0.299 | 0.281 | 0.285 | | |
| 1-Hexanol | 0.137 | 0.140 | 0.146 | 0.144 | | |
| 2-Methyl-1-Isobutyrate | 0.313 | 0.310 | 0.359 | 0.358 | | |
| Methyl Acetate | 1.023 | 1.012 | 1.134 | 1.136 | | |
| Ethyl Acetate | 0.034 | 0.039 | 0.036 | 0.035 | | |
| Methyl Formate | 0.000 | 0.000 | 0.000 | 0.000 | | |
| DME | 0.000 | 0.000 | 0.000 | 0.000 | | |
| CO2 | 0.000 | 0.000 | 0.000 | 0.000 | | |
| Water | 0.622 | 0.613 | 0.624 | 0.625 | | |
| Oil + Others (*) | 0.499 | 0.499 | 0.443 | 0.443 | | |
| Total | 96.273 | 96.362 | 96.129 | 96.128 | | |

The balance of each sample comprises mainly higher alcohol isomers which are not individually analyzed. Assumed to average C6-OH.

(*) Standard oil analysis by evaporation yielded higher than typical results. Actual oil is probably 0.1-0.2 wt%. Balance is presumably other, less volatile higher alcohols.