Cover sheet – Supporting Information

Editorial Office

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Manuscript title: *"Towards a computer-aided for synthesis and design of biorefinery networks – data collection and management using a generic modeling approach"*

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## SUPPORTING INFORMATION

This summary table of the simulation results verified and compared to seven NREL technical reports.

**Table S1.** The simulation results (1st case) verified by NREL technical report [18]

| | | Pretreatment step | | | | Primary conversion step | | | Gas cleaning/conditioning step | | | | Product synthesis step | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 2666.4 | 0 | 444.4 | 2222 | 0 | 1703.7 | 106 | 3818.54 | | 2019.56 | 550 | 3134.0 | 3269.1 | | 1292.17 | | | 426.91 | 4237.1 | 4.4 | 53 | 378.7 | 266.1 |
| H2O | 666.6 | | 444.4 | 222.2 | | 960 | | 988.43 | | | 550 | 1228.2 | 45 | | 0 | | | | 642 | | | | |
| H2 | 101.2 | | | 101.2 | | | | 122.8 | | 134 | | | 288 | | 81 | | | | 225 | 4.4 | | | |
| O2 | 812.6 | | | 812.6 | | 700 | | 0.1 | | | | | | | 0 | | | | 0 | | | | |
| N2 | 16 | | | 16 | | | | 17.7 | | | | 17.7 | | | 0 | | | | 0 | | | | |
| S | 4.4 | | | 4.4 | | | | 0.1 | | | | | | | 0 | | | | 0 | | | | |
| C | 945.6 | | | 945.6 | | | | 0.1 | | | | | | | 0 | | | | 0 | | | | |
| ASH | 120 | | | 120 | | | | 0.1 | | | | | | | 0 | | | | 0 | | | | |
| Steam | | | | | | | | | | | | | | | 0 | | | | 0 | | | | |
| CO | | | | | | | | 1457 | | 823 | | 26.1 | 1818 | | 500 | | | | 1391 | | | | |
| CO2 | | | | | | | | 1184 | | 175.7 | | 1854.7 | 190 | | 106 | | | | 296 | | | | |
| H2S | | | | | | | | 4.5 | | | | 4.5 | 0.03 | | 0 | | | | 0 | | | | |
| NH3 | | | | | | | | - | | | | | | | 0 | | | | 0 | | | | |
| TAR | | | | | | | | - | | | | | | | 0 | | | | 0 | | | | |
| COS | | | | | | | | - | | 1.12 | | 0.22 | 1.2 | | 0.68 | | | | 1.88 | | | | |
| AR | | | | | | 43.7 | | 43.7 | | 502.9 | | 2.6 | 544 | | 305 | | | | 850 | | | | |
| CH4 | | | | | | | | | | 63.4 | | | 63.4 | | 38.6 | | | | 107 | | 14.9 | | |
| SLAG | | | | | | | 100 | | | | | | | | 0 | | | | 0 | | | | |
| SOOT | | | | | | | 6 | | | | | | | | 0 | | | | 0 | | | | |
| C2H6 | | | | | | | | | | | | | | | 65 | | | | 180 | | | | |
| C2H4 | | | | | | | | | | | | | | | 86 | | | | 0 | | | | |
| C6H6 | | | | | | | | | | | | | | | 101.9 | | | | 0 | | | | |
| CHAR | | | | | | | | | | | | | | | 1.39 | | | | 0 | | | | |
| C3 | | | | | | | | | | 141.56 | | | 141.56 | | 1.5 | | | | 239 | | 37.8 | | |
| C4 | | | | | | | | | | 167.55 | | | 167.55 | | 0.7 | | | | 283 | | | | |
| C5 | | | | | | | | | | 2.29 | | | 2.29 | | 0.72 | | | 15.49 | 3.87 | | | | |
| C6 | | | | | | | | | | 2.46 | | | 2.46 | | 0.72 | | | 16.65 | 4.16 | | | | |
| C7 | | | | | | | | | | 1.15 | | | 1.15 | | 0.72 | | | 17.54 | 1.95 | | | | |
| C8 | | | | | | | | | | 1.18 | | | 1.18 | | 0.71 | | | 17.99 | 2 | | 112.6 | | |
| C9 | | | | | | | | | | 1.11 | | | 1.11 | | 0.33 | | | 18.1 | 2.01 | | | | |
| C10 | | | | | | | | | | 1.16 | | | 1.16 | | 0.32 | | | 18.12 | 2.01 | | | | |
| C11 | | | | | | | | | | 0.83 | | | 0.83 | | 0.31 | | | 17.62 | 1.96 | | | | |
| C12 | | | | | | | | | | 0.13 | | | 0.13 | | 0.29 | | | 17.25 | 0.91 | | | | |
| C13 | | | | | | | | | | 0.02 | | | 0.02 | | 0.28 | | | 16.7 | 0.88 | | | | |
| C14 | | | | | | | | | | | | | | | | | | 16.16 | 0.85 | | | | |
| C15 | | | | | | | | | | | | | | | | | | 15.57 | 0.82 | | | | |
| C16 | | | | | | | | | | | | | | | | | | 14.93 | 0.79 | | | 266.1 | |
| C17 | | | | | | | | | | | | | | | | | | 14.75 | | | | | |
| C18 | | | | | | | | | | | | | | | | | | 14.05 | | | | | |
| C19 | | | | | | | | | | | | | | | | | | 13.35 | | | | | |
| C20 | | | | | | | | | | | | | | | | | | 12.64 | | | | | |
| Waxes | | | | | | | | | | | | | | | | | | 170 | | | | | |

**Table S2.** The simulation results (2nd case) validated by NREL technical report [18]

| | | Pretreatment step | | | | Primary conversion step | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 2666.4 | 0 | 444.4 | 2222 | 0 | 913 | 216.6 | 2917.2 | | 2069.14 | 1000 | 2284.0 | 3705.2 | | 559.46 | 4260.1 | 1132 | 330.3 | 2796.5 | 3.4 | 41 | 87 | 205 |
| H2O | 666.6 | | 444.4 | 222.2 | | 352 | | 413.4 | | 0 | 1000 | 409.0 | 850 | | | 672 | 1132 | | | | | | |
| H2 | 101.2 | | | 101.2 | | | | 47.75 | | 120 | | | 222 | | 32.6 | 271 | | | 163 | 3.4 | | | |
| O2 | 812.6 | | | 812.6 | | 528 | | | | | | | | | | | | | | | | | |
| N2 | 16 | | | 16 | | | | | | | | | | | | | | | | | | | |
| S | 4.4 | | | 4.4 | | | | | | | | | | | | | | | | | | | |
| C | 945.6 | | | 945.6 | | | | | | | | | | | | | | | | | | | |
| ASH | 120 | | | 120 | | | 120 | | | | | | | | | | | | | | | | |
| Steam | | | | | | | | | | | | | | | | | | | | | | | |
| CO | | | | | | | | 797 | | 795 | | 15.3 | 1854 | | 215 | 1791 | | | 1074 | | | | |
| CO2 | | | | | | | | 1418 | | 559 | | 1809.0 | 167.8 | | 151 | 755 | | | 755 | | | | |
| H2S | | | | | | | | 4.6 | | | | 4.4 | 0.13 | | | | | | | | | | |
| NH3 | | | | | | | | 19 | | 0.28 | | 17.36 | 1.5 | | 0.08 | 0.38 | | | 0.38 | | | | |
| TAR | | | | | | | | 10.5 | | | | 10.57 | 0 | | | | | | | | | | |
| COS | | | | | | | | | | | | | | | | | | | | | | | |
| AR | | | | | | 33 | | 33 | | 380 | | | 411 | | 103 | 514 | | | 514 | | | | |
| CH4 | | | | | | | | 103 | | 52 | | 4.56 | 52 | | 14 | 66 | | | 70.3 | | 11.5 | | |
| SLAG | | | | | | | | | | | | | | | | | | | | | | | |
| SOOT | | | | | | | | | | | | | | | | | | | | | | | |
| C2H6 | | | | | | | | 21.8 | | 13.55 | | 5.75 | 7.7 | | 3.6 | 11.4 | | | 18 | | | | |
| C2H4 | | | | | | | | 45 | | 0.36 | | 8.11 | 0.39 | | | 0.5 | | | 0.5 | | | | |
| C6H6 | | | | | | | | 4.1 | | 36.54 | | | 39.5 | | 9.8 | 49 | | | 49.4 | | | | |
| CHAR | | | | | | | 96.6 | | | | | | 0 | | | | | | | | | | |
| C3 | | | | | | | | | | 58.6 | | | 54.2 | | 15.8 | 70 | | | 79.2 | | 29.2 | | |
| C4 | | | | | | | | | | 41.7 | | | 34.3 | | 11.3 | 46 | | | 56.4 | | | | |
| C5 | | | | | | | | | | 2.21 | | | 2.21 | | 0.6 | 2.8 | | 11.9 | 2.98 | | | | |
| C6 | | | | | | | | | | 2.37 | | | 2.37 | | 0.64 | 3 | | 12.8 | 3.2 | | | | |
| C7 | | | | | | | | | | 1.11 | | | 1.11 | | 0.3 | 1.4 | | 13.5 | 1.5 | | | | |
| C8 | | | | | | | | | | 1.14 | | | 1.14 | | 0.31 | 1.45 | | 13.9 | 1.54 | | | 87 | |
| C9 | | | | | | | | | | 1.15 | | | 1.15 | | 0.31 | 1.39 | | 14.0 | 1.55 | | | | |
| C10 | | | | | | | | | | 1.15 | | | 1.15 | | 0.31 | 1.44 | | 14.0 | 1.55 | | | | |
| C11 | | | | | | | | | | 0.54 | | | 0.54 | | 0.15 | 0.65 | | 13.9 | 0.73 | | | | |
| C12 | | | | | | | | | | 0.53 | | | 0.44 | | 0.14 | 0.59 | | 13.5 | 0.71 | | | | |
| C13 | | | | | | | | | | 0.51 | | | 0.34 | | 0.14 | 0.47 | | 13.1 | 0.69 | | | | |
| C14 | | | | | | | | | | 0.49 | | | 0.2 | | 0.13 | 0.34 | | 12.6 | 0.66 | | | | |
| C15 | | | | | | | | | | 0.46 | | | | | 0.13 | 0.13 | | 11.9 | 0.63 | | | | |
| C16 | | | | | | | | | | 0.45 | | | | | 0.12 | 0.16 | | 11.5 | 0.6 | | | | 205 |
| C17 | | | | | | | | | | | | | | | | | | 11.4 | | | | | |
| C18 | | | | | | | | | | | | | | | | | | 10.9 | | | | | |
| C19 | | | | | | | | | | | | | | | | | | 10.3 | | | | | |
| C20 | | | | | | | | | | | | | | | | | | 9.8 | | | | | |
| Waxes | | | | | | | | | | | | | | | | | | 131.5 | | | | | |

**Table S3.** The simulation results (3rd case) validated by NREL technical report [12]

| | | Pretreatment step | | | | Primary conversion step | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 3999.9 | | | 2105.0 | | 5478.8 | 18.4 | 2534.0 | 5034.1 | 2303.3 | 3123.2 | 1088.6 | 3063.4 | 3940.4 | 43.8 | | | 3103.9 | | | | 763.3 | 2340.6 |
| H2O | 2000.0 | | | 105.0 | | 887.0 | | 901.3 | 279.4 | 68.8 | 60.9 | 514.7 | 9.2 | 604.0 | | | | 14.5 | | | 10.9 | 3.5 | 0.1 |
| H2 | 120.8 | | | 120.8 | | | | 37.7 | | | | | 168.7 | | | | | 72.7 | | | | 0.2 | 72.5 |
| O2 | 838.0 | | | 838.0 | | 1063.1 | | | 177.2 | 43.1 | 708.6 | | | 86.4 | | | | | | | | | |
| N2 | 3.4 | | | 3.4 | | 3469.6 | | | 3469.8 | | 2312.7 | | 45.4 | 2314.9 | | | | 45.4 | | | | 0.2 | 45.3 |
| S | 1.8 | | | 1.8 | | | | | | | | | | | | | | | | | | | |
| C | 1017.6 | | | 1017.6 | | | | | | | | | | | | | | | | | | | |
| ASH | 18.4 | | | 18.4 | | | 18.4 | | | | | | | | | | | | | | | | |
| Steam | | | | | | | | | | | | | | | | | | | | | | | |
| CO | | | | | | | | 874.3 | | 903.6 | | | 2345.7 | | | | | 951.8 | | | | 4.5 | 947.4 |
| CO2 | | | | | | | | 408.1 | 1048.5 | 1153.8 | 1.5 | 572.7 | 405.3 | 895.6 | | | | 1212.6 | | | | 62.2 | 1150.4 |
| H2S | | | | | | | | 1.8 | | 0.3 | | 1.3 | 0.3 | | | | | 0.3 | | | | 0.1 | 0.2 |
| NH3 | | | | | | | | 3.9 | | 0.3 | | | 0.3 | | | | | 0.3 | | | | 0.2 | 0.2 |
| TAR | | | | | | | | 19.8 | | | | | | | | | | 0.0 | | | | | |
| COS | | | | | | | | | | | | | | | | | | 0.0 | | | | | |
| AR | | | | | | 59.2 | | | 59.2 | | 39.4 | | 43.0 | 39.4 | | | | | | | | | |
| CH4 | | | | | | | | 180.5 | | 84.9 | | | | | | | | 89.4 | | | | 1.0 | 88.4 |
| SLAG | | | | | | | | | | | | | | | | | | | | | | | |
| SOOT | | | | | | | | | | | | | | | | | | | | | | | |
| C2H6 | | | | | | | | 5.2 | | 3.5 | | | 0.1 | | | | | 3.7 | | | | 0.2 | 3.5 |
| C2H4 | | | | | | | | 86.8 | | 6.6 | | | 6.9 | | | | | 6.9 | | | | 0.4 | 6.6 |
| C2H2 | | | | | | | | 8.2 | | 0.6 | | | 0.7 | | | | | 0.7 | | | | 0.0 | 0.6 |
| C6H6 | | | | | | | | 6.6 | | | | | | | | | | | | | | | |
| CHAR | | | | | | | | | | | | | | | | | | | | | | | |
| C3 | | | | | | | | | | 17.4 | | | 17.4 | | 2.1 | | | 20.1 | | | | 8.6 | 11.5 |
| C4 | | | | | | | | | | 3.2 | | | 3.2 | | 2.3 | | | 5.6 | | | | 4.0 | 1.5 |
| C5 | | | | | | | | | | 0.6 | | | 0.6 | | 1.7 | | | 2.3 | | | | 2.1 | 0.2 |
| C1-ol | | | | | | | | | | 4.3 | | | 4.3 | | 32.6 | | | 39.6 | | | | 38.2 | 1.4 |
| C2-ol | | | | | | | | | | 11.6 | | | 11.6 | | 5.1 | | | 549.6 | | | | 539.5 | 10.1 |
| C3-ol | | | | | | | | | | 0.7 | | | 0.7 | | | | | 77.5 | | | | 76.8 | 0.7 |
| C4-ol | | | | | | | | | | | | | | | | | | 9.6 | | | | 9.5 | |
| C5-ol | | | | | | | | | | | | | | | | | | 1.3 | | | | 1.3 | |

**Table S4.** The simulation results (4th case) validated by NREL technical report [6]

| | | Pretreatment step | | | | Primary conversion step | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 3999.9 | | | 2105.2 | | 881.3 | 113.4 | 1704.3 | 1169.8 | 2717.9 | 822.0 | 2320.1 | 2925.4 | | 49.8 | | | 611.8 | 2365.7 | | | 556.7 | 54.9 |
| H2O | 2000.0 | | | 105.3 | | 421.1 | | 270.0 | 185.3 | 0.4 | 822.0 | 1022.2 | 10.3 | | 15.4 | | | 18.3 | 0.2 | | | 2.8 | 15.5 |
| H2 | 120.8 | | | 120.8 | | | | 24.5 | 16.8 | 81.5 | | | 167.0 | | | | | 0.1 | 88.5 | | | | 0.1 |
| O2 | 838.0 | | | 838.0 | | 435.2 | | | | | | | | | | | | | | | | | 0.0 |
| N2 | 3.4 | | | 3.4 | | 0.8 | | 0.5 | 0.3 | 24.2 | | | 26.3 | | | | | 0.1 | 26.3 | | | | 0.1 |
| S | 1.8 | | | 1.8 | | | | | | | | | | | | | | | | | | | 0.0 |
| C | 1017.6 | | | 1017.6 | | | | | | | | | | | | | | | | | | | 0.0 |
| ASH | 18.4 | | | 18.4 | | | 18.4 | | | | | | | | | | | | | | | | 0.0 |
| Steam | | | | | | | | | | | | | | | | | | | | | | | |
| CO | | | | | | | | 276.6 | 189.9 | 725.6 | | | 1935.7 | | | | | 2.6 | 786.8 | | | 0.1 | 2.5 |
| CO2 | | | | | | | | 869.5 | 596.8 | 1475.0 | | 1296.5 | 397.2 | | 0.2 | | | 39.5 | 1026.2 | | | 8.3 | 31.2 |
| H2S | | | | | | | | 1.0 | 0.7 | 0.3 | | 1.0 | 0.3 | | 0.0 | | | 0.1 | 0.2 | | | | |
| NH3 | | | | | | | | 2.4 | 1.6 | 0.2 | | 0.4 | 0.2 | | 0.1 | | | 0.1 | 0.1 | | | 0.1 | |
| TAR | | | | | | | | 28.1 | 19.3 | | | | | | | | | | | | | | |
| COS | | | | | | | | | | | | | | | | | | 1.4 | 179.6 | | | 0.1 | 1.3 |
| AR | | | | | | 24.2 | | 14.4 | 9.9 | | | | | | | | | 1.9 | 234.9 | | | 0.1 | 1.8 |
| CH4 | | | | | | | | 151.6 | 104.0 | 166.4 | | | 180.8 | | | | | 0.1 | 3.0 | | | | 0.1 |
| SLAG | | | | | | | | | | | | | | | | | | | | | | | |
| SOOT | | | | | | | | | | | | | | | | | | | | | | | |
| C2H6 | | | | | | | | 13.5 | 9.2 | 217.8 | | | 198.7 | | | | | | | | | | |
| C2H4 | | | | | | | | 52.4 | 36.0 | 2.9 | | | 0.2 | | | | | | | | | | |
| C2H2 | | | | | | | | | | | | | | | | | | 0.5 | | | | 0.5 | |
| C6H6 | | | | | | | | | | | | | | | | | | | | | | | |
| CHAR | | | | | | | 95 | | | | | | | | | | | | | | | | |
| C3 | | | | | | | | | | 7.1 | | | 0.5 | | 1.1 | | | 3.1 | 5.6 | | | 2.4 | 0.6 |
| C4 | | | | | | | | | | 1.1 | | | | | 0.9 | | | 1.4 | 0.7 | | | 1.3 | 0.1 |
| C5 | | | | | | | | | | 0.2 | | | 7.1 | | 0.6 | | | 0.6 | 0.1 | | | 0.6 | |
| C1-ol | | | | | | | | | | 2.9 | | | 1.1 | | 27.3 | | | 30.9 | 1.5 | | | 30.7 | 0.2 |
| C2-ol | | | | | | | | | | 11.7 | | | 0.2 | | 4.2 | | | 439.4 | 11.1 | | | 438.1 | 1.3 |
| C3-ol | | | | | | | | | | 0.7 | | | | | | | | 62.9 | 0.7 | | | 62.9 | 0.1 |
| C4-ol | | | | | | | | | | | | | | | | | | 7.8 | 0.0 | | | 7.8 | |
| C5-ol | | | | | | | | | | | | | | | | | | 1.0 | 0.0 | | | 1.0 | |

**Table S5.** The simulation results (5th case) validated by NREL technical report [5]

| | | Pretreatment step | | | | Primary conversion step | | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 2857.1 | | | 2222.2 | | 5301.3 | 795.0 | 18.4 | 2674.6 | 5625.4 | 2632.2 | 2761.6 | 1277.6 | 2850.8 | 3939.4 | 8213.6 | | | 1762.5 | 9305.4 | | 73.6 | 1328.9 | 360.8 |
| H2O | 857.1 | | | 222.2 | | 102.5 | 795.0 | | 1018.2 | 346.1 | 12.7 | 53.9 | 695.2 | 4.5 | 417.0 | | | | 78.5 | | | 71.6 | 6.7 | 0.2 |
| H2 | 120.8 | | | 120.8 | | | | | 33.5 | | 58.2 | | | 194.4 | | 406.0 | | | 1.4 | 462.7 | | | | 1.4 |
| O2 | 838.0 | | | 838.0 | | 1179.7 | | | | 196.6 | | 626.6 | | | 83.6 | | | | | | | | | |
| N2 | 3.4 | | | 3.4 | | 3850.3 | | | | 3850.5 | 11.0 | 2044.9 | | 11.0 | 2047.7 | 66.6 | | | 0.4 | 77.2 | | | | 0.3 |
| S | 1.8 | | | 1.8 | | | | | | | | | | | | | | | | | | | | |
| C | 1017.6 | | | 1017.6 | | | | | | | | | | | | | | | | | | | | |
| ASH | 18.4 | | | 18.4 | | | | 18.4 | | | | | | | | | | | | | | | | |
| Steam | | | | | | | | | | | | | | | | | | | | | | | | |
| CO | | | | | | | | | 825.2 | | 574.5 | | | 2165.9 | | 3387.1 | | | 25.0 | 3927.4 | | | 0.1 | 24.9 |
| CO2 | | | | | | 3.3 | | | 394.3 | 1166.6 | 1754.2 | 1.4 | 581.8 | 405.3 | 1356.2 | 3075.8 | | | 348.7 | 3889.6 | | | 38.0 | 310.7 |
| H2S | | | | | | | | | 0.6 | | 0.3 | | 0.6 | 0.3 | | 0.2 | | | 0.5 | | | | 0.2 | 0.3 |
| NH3 | | | | | | | | | 3.9 | | 0.1 | | | 0.4 | | 0.1 | | | 0.2 | | | | 0.1 | |
| TAR | | | | | | | | | 20.9 | | | | | | | | | | | | | | | |
| COS | | | | | | | | | | | | | | | | | | | | | | | | |
| AR | | | | | | 65.7 | | | | 65.7 | | 34.9 | | | 34.9 | | | | | | | | | |
| CH4 | | | | | | | | | 172.2 | | 168.3 | | | 57.2 | | 765.4 | | | 12.1 | 909.9 | | | 0.2 | 12.0 |
| SLAG | | | | | | | | | | | | | | | | | | | | | | | | |
| SOOT | | | | | | | | | | | | | | | | | | | | | | | | |
| C2H6 | | | | | | | | | 6.2 | | 7.5 | | | 0.1 | | 11.9 | | | 0.9 | 15.1 | | | 0.1 | 0.9 |
| C2H4 | | | | | | | | | 85.3 | | 8.6 | | | 8.7 | | 17.2 | | | 1.7 | 21.5 | | | 0.1 | 1.6 |
| C2H2 | | | | | | | | | 7.4 | | 0.7 | | | 0.7 | | | | | 0.1 | | | | 0.0 | 0.1 |
| C6H6 | | | | | | | | | 7.0 | | | | | 0.1 | | | | | 0.1 | | | | 0.1 | |
| CHAR | | | | | | | | | | | | | | | | | | | | | | | | |
| C3 | | | | | | 0.3 | | | 0.3 | | 4.0 | | | 2.1 | | 2.0 | | | 3.0 | 2.0 | | 1.9 | | 1.1 |
| C4 | | | | | | | | | | | | | | | | | | | | | | | | |
| C5 | | | | | | | | | | | | | | | | | | | | | | | | |
| C1-ol | | | | | | 98.7 | | | 98.7 | | 24.8 | | | | | 477.2 | | | 669.6 | | | | 664.9 | 5.3 |
| C2-ol | | | | | | 0.8 | | | 0.8 | | 7.1 | | | | | 4.0 | | | 562.4 | | | | 560.6 | 2.0 |
| C3-ol | | | | | | | | | | | 0.3 | | | | | | | | 57.9 | | | | 57.8 | 0.1 |
| C4-ol | | | | | | | | | | | | | | | | | | | 0.1 | | | | 0.1 | |
| C5-ol | | | | | | | | | | | | | | | | | | | | | | | | |

**Table S6.** The simulation results (6th case) validated by NREL technical report [23]

| | | Pretreatment step | | | | Primary conversion step | | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 666.7 | | | 2147.3 | | 3399.8 | | 311.0 | 1305.8 | 3930.5 | | | | | | | 2924.5 | 514.3 | 321.2 | 3282.1 | | | | |
| H2O | 101.2 | | | 147.5 | | 181.5 | | | 256.6 | 147.8 | | | | | | | 482.1 | 252.0 | | 243.3 | | | | |
| H2 | 812.6 | | | 101.2 | | | | | | 0.1 | | | | | | | | | | | | | | |
| O2 | 16.0 | | | 812.6 | | | | | | | | | | | | | 568.9 | | | 94.8 | | | | |
| N2 | 4.4 | | | 16.0 | | 1811.6 | | | | 1820.2 | | | | | | | 1873.5 | | | 1873.6 | | | | |
| S | 945.6 | | | 4.4 | | | | | | | | | | | | | | | | | | | | |
| C | 120.0 | | | 945.6 | | | | | | | | | | | | | | | | | | | | |
| ASH | | | | 120.0 | | | | 1.1 | 0.2 | | | | | | | | | | | | | | | |
| CO | | | | | | 7.9 | | | | 118.9 | | | | | | | | | | | | | | |
| CO2 | | | | | | 1377.4 | | | 1.1 | 1622.5 | | | | | | | | 204.0 | | 1050.0 | | | | |
| H2S | | | | | | | | | | | | | | | | | | | | | | | | |
| NH3 | | | | | | | | | | | | | | | | | | | | | | | | |
| TAR | | | | | | | | | | | | | | | | | | | | | | | | |
| AR | | | | | | | | | | | | | | | | | | | | | | | | |
| CH4 | | | | | | 1.3 | | | | 19.3 | | | | | | | | 25.7 | | | | | | |
| C2H6 | | | | | | | | | | | | | | | | | | | | | | | | |
| C2H4 | | | | | | | | | | 0.5 | | | | | | | | | | | | | | |
| C2H2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C6H6 | | | | | | | | | | | | | | | | | | | | | | | | |
| CHAR | | | | | | 6.9 | | 309.9 | 53.0 | | | | | | | | | 32.6 | | 20.4 | | | | |
| C3 | | | | | | | | | | 0.5 | | | | | | | | | | | | | | |
| C2H4O2 | | | | | | 1.1 | | | 51.1 | 16.5 | | | | | | | | | | | | | | |
| C3H6O2 | | | | | | 1.9 | | | 300.6 | 28.7 | | | | | | | | | | | | | | |
| CH2O2 | | | | | | 8.7 | | | 177.8 | 131.3 | | | | | | | | | | | | | | |
| C7H8 | | | | | | 0.5 | | | 0.6 | 8.1 | | | | | | | | | | | | | | |
| C5H4O2 | | | | | | 1.0 | | | 58.0 | 14.8 | | | | | | | | | | | | | | |
| C10H12O2 | | | | | | | | | 327.7 | 1.1 | | | | | | | | | | | | | | |
| C7H8O2 | | | | | | | | | 10.4 | 0.0 | | | | | | | | | | | | | | |
| C8H10O | | | | | | | | | 67.9 | 0.2 | | | | | | | | | | | | | | |
| C6H6O | | | | | | | | | 0.8 | 0.0 | | | | | | | | | | | | | | |
| C8 | | | | | | | | | | | | | | | | | | | 160.6 | | | | | |
| C16 | | | | | | | | | | | | | | | | | | | 160.6 | | | | | |
| Pyrolysis | | | | | | | | | | | | | | | | | | | | | | | | |

**Table S7.** The simulation results (6th case) validated by NREL technical report [9]

| | | Pretreatment step | | | | Primary conversion step | | | | | Gas cleaning/conditioning step | | | | | Product synthesis step | | | | | Separation/purification step | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Biomass inlet | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | Recycle | R(i) | waste(i) | Fout1 | Fout2 | R(i) | waste(i) | Fout1 | Fout2 |
| Total (tpd) | 3999.8 | | | 2150.3 | | | 3810.0 | | 1650.4 | 4310.0 | | | | | | | 83.0 | 779.0 | | 397.5 | | | | |
| H2O | 2000.0 | | 1849.5 | 150.5 | | | | | 350.1 | 166.0 | | | | | | | | 779.0 | | 4.2 | | | | |
| H2 | 121.6 | | | 121.6 | | | | | | | | | | | | | 83.0 | | | 14.6 | | | | |
| O2 | 815.0 | | | 815.0 | | | 887.4 | | | 266.0 | | | | | | | | | | | | | | |
| N2 | 12.2 | | | 12.2 | | | 2922.7 | | | 2934.9 | | | | | | | | | | | | | | |
| S | 0.4 | | | 0.4 | | | | | | | | | | | | | | | | | | | | |
| C | 1012.0 | | | 1012.0 | | | | | | | | | | | | | | | | | | | | |
| ASH | 38.6 | | | 38.6 | | | | | | | | | | | | | | | | | | | | |
| CO | | | | | | | | | 0.1 | 5.6 | | | | | | | | | | | | | | |
| CO2 | | | | | | | | | 0.1 | 937.2 | | | | | | | | | | 190.3 | | | | |
| H2S | | | | | | | | | | | | | | | | | | | | | | | | |
| NH3 | | | | | | | | | | | | | | | | | | | | | | | | |
| TAR | | | | | | | | | | | | | | | | | | | | | | | | |
| AR | | | | | | | | | | | | | | | | | | | | | | | | |
| CH4 | | | | | | | | | | | | | | | | | | | | 72.8 | | | | |
| C2H6 | | | | | | | | | | | | | | | | | | | | 43.7 | | | | |
| C2H4 | | | | | | | | | | | | | | | | | | | | | | | | |
| C2H2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C6H6 | | | | | | | | | | | | | | | | | | | | | | | | |
| CHAR | | | | | | | | | | | | | | | | | | | | | | | | |
| C3 | | | | | | | | | 0.1 | | | | | | | | | | | 28.8 | | | | |
| C2H4O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C3H6O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| CH2O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C7H8 | | | | | | | | | | | | | | | | | | | | | | | | |
| C5H4O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C10H12O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C7H8O2 | | | | | | | | | | | | | | | | | | | | | | | | |
| C8H10O | | | | | | | | | | | | | | | | | | | | | | | | |
| C6H6O | | | | | | | | | | | | | | | | | | | | | | | | |
| C8 | | | | | | | | | | | | | | | | | | | 245.0 | | | | | |
| C16 | | | | | | | | | | | | | | | | | | | 313.0 | | | | | |
| Pyrolysis | | | | | | | | | 1300 | | | | | | | | | | | 43 | | | | |