**Supplementary information**

**Assessing the economic viability of the plastic biorefinery and its contribution to a more circular plastic sector**

**Megan Roux and Cristiano Varrone**

*Table S1: Major cost inputs to the model*

|  |  |  |
| --- | --- | --- |
| **Component** | **Cost (USD/kg)** | **Reference** |
| **Raw materials** |
| LCC enzyme | 25.0 | [1] |
| NaOH | 0.32 | [2] |
| H2SO4 | 0.07 | [2] |
| THF | 1.53 | [3] |
| O2 | 0.04 | [3] |
| Cellulose | 0.45 | [3] |
| Crude glycerol | 0.14 | [4] |
| *C. butirycum* culture | 213 | [5] |
| PDO pre-culture medium | 0.007 | [2] |
| PDO fermentation broth | 0.004 | [2] |
| Methanol | 0.24 | [2] |
| Water | 1.33 | [6] |
| **Catalysts\*** |
| Pt/C | 194 | [3] |
| RuSn4/C | 539 | [3] |
| TBT | 150 | [7] |
| **Utilities** |
| Cooling water | 0.00005 | [2] |
| Chilled water | 0.0004 | [2] |
| Steam | 0.012 | [2] |
| High pressure steam | 0.02 | [2] |
| Electricity\*\* | 0.1 | [2] |
| **Revenues** |
| Na2SO4 | 1.00 | [2] |
| Activated carbon | 1.20 | [3] |
| PEF | 2.70 | Assumed |
| PTT | 2.70 | Assumed |

\*Catalyst life span is assumed 6 months, with 10 % replacement at 20 % of the cost [3].

\*\*In USD/kW-h

*Table S2: Inputs to the DCCF analysis*

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | **Reference** |
| Cost of PET pre-treatment (USD/kg PET) | 277 | [8] |
| Cost of labour (USD/h) | 34.5 | [9] |
| Construction period (years) | 3 | [10] |
| 1st year expenditures (%) | 8.0 | [10] |
| 2nd year expenditures (%) | 60 | [10] |
| 3rd year expenditures (%) | 32 | [10] |
| Tax rate (%) | 22 | [11] |
| Depreciation (years)\* | 5.0 | [12] |
| Working capital (% of fixed capital) | 15 | [12] |
| Start-up time (years) | 0.5 | [10] |
| Revenue during start-up (% of normal) | 50 | [10] |
| Operating costs during start-up (% of normal) | 75 | [10] |
| Discount rate (%) | 10 | [10] |

\*Straight-line depreciation over 5 years

*Table S3: Summary of capital and operating costs, and revenues.*

|  |  |
| --- | --- |
| Fixed capital (USD) | 498 379 707 |
| Working capital (USD) | 74 810 956 |
| Total capital investment (USD) | 573 550 663 |
| Revenues (USD/year) | 391 411 846 |
| Operating costs (USD/year) | 367 323 069 |

*Table S4: DCCF of Scenario 1 in USD*

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|   | 2022 | 2023 | 2024 | 2025 | 2026 | 2027 | 2028 | 2029 | 2030 | 2031 | 2032 | 2033 | 2034 | 2035 |
| Revenue |   |   |   |  195,705,923  |  391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  | 391,411,846  |
| Operating Costs |   |   |   |  275,492,302  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |  367,323,069  |
| Gross Profit |   |   |   |  -79,786,379 |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |  24,088,777  |
| Depreciation |   |   |   |  99,747,941  |  99,747,941  |  99,747,941  |  99,747,941  |  99,747,941  |   |   |   |   |   |   |
| Net Profit |   |   |   |  -140,036,770 |  -59,014,149 | -59,014,149 | -59,014,149 | -59,014,149 |  18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| Cash Flow |  -39,899,177 |  -299,243,824 |  -234,407,662 |  -40,288,829 |  40,733,793  | 40,733,793  | 40,733,793  | 40,733,793  |  18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  | 18,789,246  |
| CCF |  -39,899,177 |  -339,143,001 |  -573,550,663 |  -80,188,005 |  -298,409,208 |  -257,675,415 |  -216,941,622 |  -176,207,830 |  -157,418,584 |  -138,629,338 |  -119,840,093 |  -101,050,847 |  -82,261,601 |  -63,472,356 |
| DCF |  -36,271,979 |  -247,308,946 |  -176,113,946 |  -27,517,812 |  25,292,481  |  22,993,164  |  20,902,876  |  19,002,615  |  7,968,474  |  7,244,068  |  6,585,516  |  5,986,833  |  5,442,575  |  4,947,796  |
| DCCF |  -36,271,979 |  -283,580,924 |  -459,694,871 |  -487,212,683 |  -258,288,444 |  -235,295,280 |  -214,392,403 |  -195,389,788 |  -187,421,314 |  -180,177,246 |  -173,591,730 |  -167,604,898 |  -162,162,323 |  -157,214,527 |

*Table S5(a): Stream table showing most important process streams relating to Fig.2 in the main report. Flows are in kg/h.*

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| PET | 6437.83 | 649.56 |  |  |  |  |  |  |  |  |  |  |  |
| LCC | 12.86 | 12.86 |  |  |  |  |  |  |  |  |  |  |  |
| NaOH | 1576.34 |  |  |  |  |  |  |  |  |  |  |  |  |
| H2SO4 |  |  |  | 23506.30 |  |  |  | 577.34 | 48.30 |  |  |  |  |
| Water | 25082.45 |  | 25082.45 |  | 43889.76 |  | 4.38 | 1109.00 | 26.38 |  |  |  |  |
| EG |  |  | 2654.25 |  | 2654.25 | 11.61 | 2609.40 |  |  |  |  |  |  |
| Na2TP |  |  | 4710.37 |  | 0.01 | 0.01 |  |  |  |  |  |  |  |
| PTA |  |  |  |  | 5550.30 |  |  |  |  |  |  |  |  |
| Na2SO4 |  |  |  |  | 3859.02 | 3859.02 |  |  |  |  |  |  |  |
| Cellulose |  |  |  |  |  |  |  | 16654.05 |  |  |  |  |  |
| THF |  |  |  |  |  |  |  | 242.32 | 242.32 |  |  |  |  |
| CaOH |  |  |  |  |  |  |  | 399.70 |  |  |  |  |  |
| HMF |  |  |  |  |  |  |  |  |  | 5462.53 |  |  |  |
| CaSO4 |  |  |  |  |  |  |  |  | 928.74 |  |  |  |  |
| Humins |  |  |  |  |  |  |  |  |  | 10064.04 |  |  |  |
| Oxygen |  |  |  |  |  |  |  |  |  |  | 1664.53 |  |  |
| AC |  |  |  |  |  |  |  |  |  |  |  | 6061.48 |  |
| FDCA |  |  |  |  |  |  |  |  |  |  |  |  | 6328.71 |
| GVL |  |  |  |  |  |  |  |  |  |  |  |  | 1.13 |

LCC= leaf compost cutinase, Na2TP=sodium terephthalate, THF=tetrahydrofuran, AC=activated carbon, GVL=gamma-valerolactone

*Table S5(b): Stream table showing most important process streams relating to Fig.2 in the main report. Flows are in kg/h.*

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 |
| Water |  | 9.93 |  |  |  | 978.03 | 3007 | 3311.64 | 33.27 |  |  |  |  |
| PTA |  |  |  |  |  |  |  |  |  |  | 902.87 | 40.63 | 40.63 |
| DMFD |  | 47.33 | 6148.94 |  |  |  |  |  |  |  |  |  |  |
| Methanol | 527 | 6.31 |  |  |  |  |  |  |  | 383.00 | 5.56 |  |  |
| PEF |  |  |  | 7420.96 | 5550.30 |  |  |  |  |  |  |  |  |
| *C. butirycum* cells |  |  |  |  |  | 5.51 | 2772.40 | 2772.40 |  |  |  |  |  |
| Fermentation media |  |  |  |  |  | 2037.90 |  |  |  |  |  |  |  |
| Glycerol |  |  |  |  |  | 6601.70 |  |  |  |  |  |  |  |
| FFA |  |  |  |  |  | 81.50 | 81.50 | 81.50 |  |  |  |  |  |
| KCl |  |  |  |  |  | 489.02 | 489.02 |  | 9.75 |  |  |  |  |
| PDO |  |  |  |  |  |  | 3630.94 | 21.17 | 3609.77 |  |  |  |  |
| DMT |  |  |  |  |  |  |  |  |  |  | 36.4 | 5347.97 |  |
| PTT |  |  |  |  |  |  |  |  |  |  |  |  | 6667.27 |

FFA=free fatty acids



***Figure S1(a):*** *Process flow diagram of Area 1 (PET depolymerisation). Stream 1-1: PET, stream 1-15: PTA, stream 1-19: Na2SO4, stream 1-23: EG.*

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***Figure S1(b):*** *Process flow diagram of Area 2 (FDCA production). Stream 2-1: cellulose, stream 2-29: FDCA, stream 2-20b: GVL recycle to stream 20 (not implemented due to limit in number of unit operations, but modelled in stream 2-20)*

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***Figure S1(c):*** *Process flow diagram of Area 3 (PEF synthesis). Stream 2-29: FDCA, stream 3-1: methanol make-up, stream 1-23: EG, stream 3-31: PEF.*



***Figure S1(d):*** *Process flow diagram of Area 4 (PDO production). Stream 4-1: starter culture, stream 4-3: fermentation media, stream 4-5: crude glycerol, stream 4-36: PDO.*



***Figure S1(e):*** *Process flow diagram of Area 5 (PTT synthesis). Stream 1-15: PTA, stream 5-1: methanol make-up, stream 4-36: PDO, stream 5-30: PTT.*

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