**Supporting Information**

**Sustainable Production of Alternative Aviation Fuel via Thermolytic Conversion of Polyethylene Waste: Techno-economic Analysis and Life Cycle Assessment**

Junyoung Park a, 1, Dongho Choi a, 1, Hyukwon Kwon b, c, Taewoo Lee d, Jaewon Lee e, \*, and Hyungtae Cho a, \*

*a Department of Chemical Engineering, College of Engineering, Kyung Hee University, Yongin 17104, Republic of Korea; b Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul 03722, Republic of Korea; c Green Materials and Processes R&D Group, Korea Institute of Industrial Technology, Ulsan 44413, Republic of Korea; d Department of Earth Resources & Environmental Engineering, Hanyang University, Seoul 04763, Republic of Korea; e Department of Materials Science and Chemical Engineering, Hanyang University, Ansan 15588, Republic of Korea*

1 These authors contributed equally to this study.

\* Corresponding authors: Jaewon Lee ([jwlee11@hanyang.ac.kr](mailto:jwlee11@hanyang.ac.kr)) and Hyungtae Cho (htcho@khu.ac.kr)

# **A. System description**

## **A.1. Pyrolysis process**

**도표, 평면도, 기술 도면, 개략도이(가) 표시된 사진

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**Figure S1.** Schematic of pyrolysis process

**Table S1.** Detailed distillation column conditions of aviation fuel production process

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **AFP-500** | | **AFP-600** | |
| **Parameter** | **Value** | **Parameter** | **Value** |
| COL-1 | Number of stages | 33 | Number of stages | 33 |
|  | Reflux ratio | 2.968 | Reflux ratio | 2.324 |
|  | Distillate to feed ratio | 0.460 | Distillate to feed ratio | 0.667 |
|  | Feed stream stage | 17 (On-stage) | Feed stream stage | 17 (On-stage) |
|  | Pressure | 1.013 | Pressure | 1.013 |
| COL-2 | Number of stages | 25 | Number of stages | 25 |
|  | Reflux ratio | 3 | Reflux ratio | 2.428 |
|  | Distillate to feed ratio | 0.083 | Distillate to feed ratio | 0.199 |
|  | Feed stream stage | 11 (On-stage) | Feed stream stage | 11 (On-stage) |
|  | Pressure | 1.013 | Pressure | 1.013 |

**Table S2.** Detailed stream conditions of pyrolysis process within AFP-500 and AFP-600

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Stream** | **AFP-500** | | | **AFP-600** | | |
| **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** | **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** |
| 101 | 35 | 1.013 | 5,000 | 35 | 1.013 | 5,000 |
| 102 | 35 | 1.013 | 33 | 35 | 1.013 | 33 |
| 103 | 500 | 1.013 | 5,033 | 600 | 1.013 | 5,033 |
| 104 | 228 | 1.013 | 5,033 | 307 | 1.013 | 5,033 |
| 105 | 113 | 1.013 | 5,033 | 107 | 1.013 | 5,033 |
| 106 | 44 | 1.013 | 5,033 | 42 | 1.013 | 5,033 |
| 107 | 20 | 1.013 | 5,033 | 20 | 1.013 | 5,033 |
| 108 | 20 | 1.013 | 4,225 | 20 | 1.013 | 2,501 |
| 109 | 360 | 1.013 | 4,225 | 360 | 1.013 | 2,501 |
| 110 | 35 | 3.000 | 630 | 35 | 1.013 | 1,050 |
| 111 | 35 | 3.000 | 630 | 35 | 1.013 | 1,050 |
| 112 | 135 | 1.013 | 630 | 135 | 1.013 | 1,050 |
| 113 | 35 | 1.013 | 14,225 | 35 | 1.013 | 44,057 |
| 114 | 90 | 1.013 | 14,225 | 52 | 1.013 | 44,057 |
| 115 | 20 | 1.013 | 808 | 20 | 1.013 | 2,532 |
| 116 | 741 | 1.013 | 1,503 | 716 | 1.013 | 46,590 |
| 117 | 161 | 1.013 | 1,262 | 134 | 1.013 | 1,193 |
| 118 | 81 | 1.013 | 60 | 83 | 1.013 | 153 |
| 119 | 186 | 1.013 | 1,202 | 170 | 1.013 | 1,039 |
| 120 | 359 | 1.013 | 2,963 | 354 | 1.013 | 1,308 |

## **A.2. Catalytic cracking process**

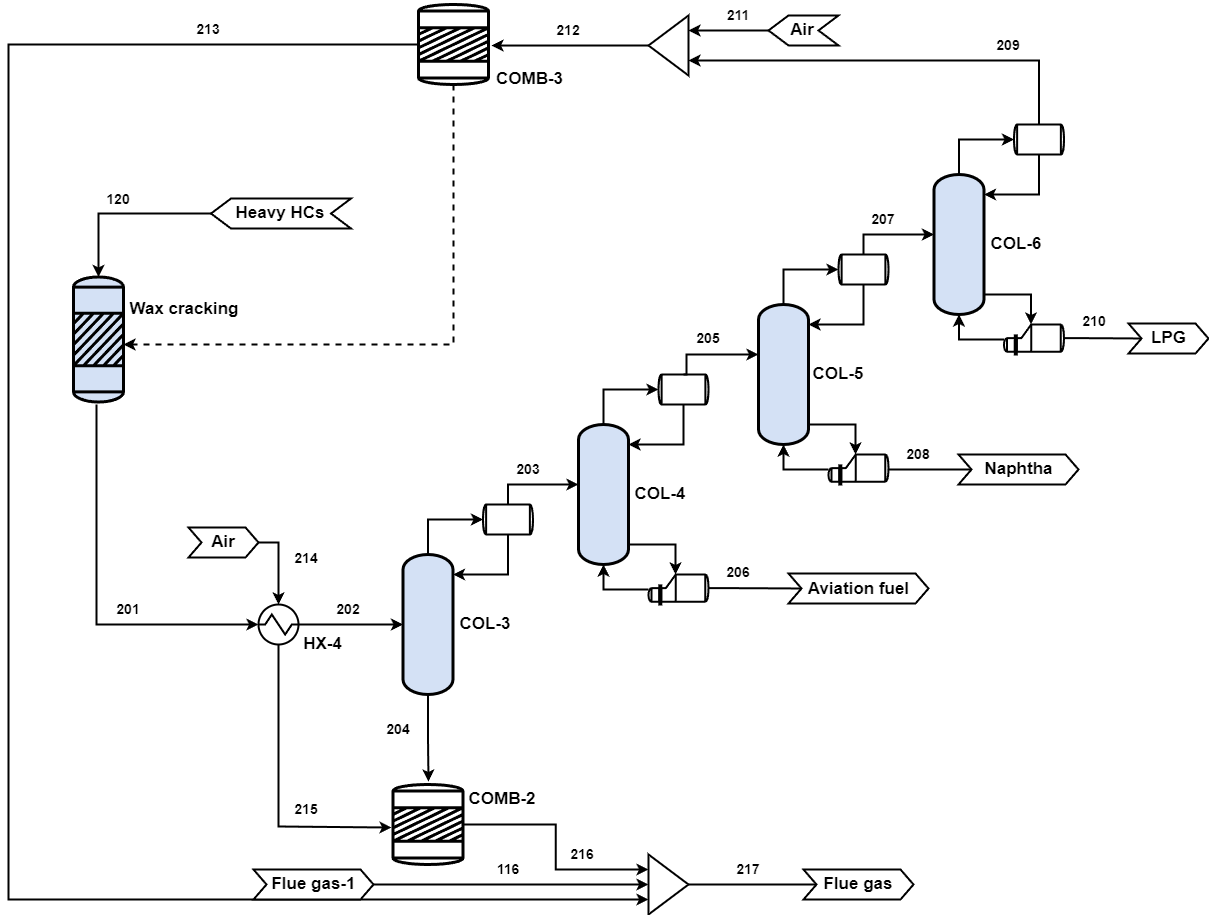
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**Figure S2.** Product yields in the catalytic cracking of HDPE waxes under conditions of 560°C and a C/O ratio of 7 g/g

**Table S3.** Comparison of HDPE wax compositions from pyrolysis at 500 and 600℃ with literature data

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Wax composition, [wt.%]** | | **Pyrolysis at 500 ℃** | **Pyrolysis at 600 ℃** | **Literature [1]** |
| Naphtha / LCO | C5-20 | 19 | 22 | 18 |
| HCO | C20+ | 81 | 78 | 82 |
| Total | | 100 | 100 | 100 |

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**Figure S3.** Schematic of wax cracking process

**Table S4.** Detailed distillation column conditions of catalytic cracking of HDPE waxes within AFP-500 and AFP-600

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **AFP-500** | | **AFP-600 ℃** | |
| **Parameter** | **Value** | **Parameter** | **Value** |
| COL-3 | Number of stages | 3 | Number of stages | 3 |
| Distillate to feed ratio | 0.967 | Distillate to feed ratio | 0.95 |
| Feed stream stage | 3 (On-stage) | Feed stream stage | 3 (On-stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |
| COL-4 | Number of stages | 30 | Number of stages | 30 |
| Reflux ratio | 1.366 | Reflux ratio | 2.223 |
| Distillate to feed ratio | 0.813 | Distillate to feed ratio | 0.833 |
| Feed stream stage | 15 (Above-stage) | Feed stream stage | 15 (Above-stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |
| COL-5 | Number of stages | 10 | Number of stages | 10 |
| Reflux ratio | 1.998 | Reflux ratio | 2.003 |
| Distillate to feed ratio | 0.542 | Distillate to feed ratio | 0.560 |
| Feed stream stage | 5 (Above-stage) | Feed stream stage | 5 (Above-stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |
| COL-6 | Number of stages | 10 | Number of stages | 10 |
| Reflux ratio | 2.033 | Reflux ratio | 2.033 |
| Distillate to feed ratio | 0.461 | Distillate to feed ratio | 0.330 |
| Feed stream stage | 4 (Above-stage) | Feed stream stage | 7 (Above-stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |

**Table S5.** Detailed stream conditions of catalytic cracking processes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Stream** | **AFP-500** | | | **AFP-600 ℃** | | |
| **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** | **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** |
| 201 | 560 | 1.013 | 2,744 | 560 | 1.013 | 1,213 |
| 202 | 370 | 1.013 | 2,744 | 370 | 1.013 | 1,213 |
| 203 | 129 | 1.013 | 1,712 | 71 | 1.013 | 720 |
| 204 | 313 | 1.013 | 1,032 | 198 | 1.013 | 493 |
| 205 | 36 | 1.013 | 1,391 | 32 | 1.013 | 600 |
| 206 | 142 | 1.013 | 321 | 131 | 1.013 | 120 |
| 207 | -37 | 1.013 | 754 | -37 | 1.013 | 336 |
| 208 | 47 | 1.013 | 637 | 47 | 1.013 | 264 |
| 209 | -75 | 1.013 | 347 | -93 | 1.013 | 111 |
| 210 | -35 | 1.013 | 407 | -42 | 1.013 | 225 |
| 211 | 35 | 1.013 | 6,508 | 35 | 1.013 | 2,116 |
| 212 | 26 | 1.013 | 6,856 | 25 | 1.013 | 2,227 |
| 213 | 1,351 | 1.013 | 6,856 | 1,138 | 1.013 | 2,227 |
| 214 | 35 | 1.013 | 18,979 | 35 | 1.013 | 8,009 |
| 215 | 127 | 1.013 | 18,979 | 131 | 1.013 | 8,009 |
| 216 | 806 | 1.013 | 20,011 | 687 | 1.013 | 8,502 |
| 217 | 783 | 1.013 | 41,900 | 729 | 1.013 | 57,319 |

## **A.3. CO2 capture process**

도표, 평면도, 기술 도면, 텍스트이(가) 표시된 사진

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**Figure S4.** Schematic of CO2 capture process

**Table S6.** Detailed equipment conditions ofCO2 capture processes within AFP-500 and AFP-600

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameter** | **AFP-500** | | **AFP-600** | |
| **Parameter** | **Value** | **Parameter** | **Value** |
| Absorber | Number of stages | 12 | Number of stages | 12 |
| LEAN IN stream stage | 1 | LEAN IN stream stage | 1 |
| Feed stream stage | 12 (On-stage) | Feed stream stage | 12 (On-stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |
| Stripper | Number of stages | 10 | Number of stages | 10 |
| Reflux ratio | 1 | Reflux ratio | 1 |
| Reboiler duty, [kW] | 11,400 | Reboiler duty, [kW] | 18,400 |
| Feed stream stage | 2 (Above-stage) | Feed stream stage | 2 (Above stage) |
| Pressure, [bar] | 1.013 | Pressure, [bar] | 1.013 |

**Table S7.** Detailed stream conditions of CO2 capture processes within AFP-500 and AFP-600

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Stream** | **AFP-500** | | | **AFP-600** | | |
| **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** | **Temperature, [˚C]** | **Pressure, [bar]** | **Flow rate, [kg h-1]** |
| 301 | 51 | 1.013 | 41,900 | 50 | 1.013 | 57,319 |
| 302 | 40 | 1.013 | 41,900 | 40 | 1.013 | 57,319 |
| 303 | 45 | 1.013 | 79,915 | 48 | 1.013 | 134,735 |
| 304 | 45 | 1.500 | 79,915 | 48 | 1.500 | 134,735 |
| 305 | 70 | 1.500 | 79,915 | 70 | 1.500 | 134,735 |
| 306 | 105 | 1.013 | 70,439 | 105 | 1.013 | 116,814 |
| 307 | 25 | 1.013 | 31 | 25 | 1.013 | 56 |
| 308 | 40 | 1.013 | 8,969 | 40 | 1.013 | 10,313 |
| 309 | 38 | 1.013 | 79,439 | 40 | 1.013 | 127,183 |
| 310 | 40 | 1.08 | 79,439 | 39 | 1.08 | 127,183 |
| 311 | 35 | 1.013 | 13,250 | 35 | 1.013 | 17,000 |
| 312 | 35 | 3.000 | 13,250 | 35 | 3.000 | 17,000 |
| 313 | 135 | 3.000 | 13,250 | 135 | 3.000 | 17,000 |
| 314 | 135 | 3.000 | 1,383 | - | - | **-** |
| 315 | - | - | - | 35 | 1.013 | 12,260 |
| 316 | - | - | - | 135 | 3.000 | 12,260 |
| 317 | - | - | - | 135 | 3.000 | 5,926 |
| 318 | 135 | 3.000 | 15,263 | 135 | 3.000 | 24,384 |
| 319 | 25 | 1.013 | 31,000 | 25 | 1.013 | 45,400 |
| 320 | 48 | 1.013 | 31,000 | 47 | 1.013 | 45,400 |
| 321 | 69 | 1.013 | 42,217 | 71 | 1.013 | 57,866 |
| 322 | 75 | 1.013 | 9,476 | 83 | 1.013 | 17,942 |
| 323 | 25 | 1.013 | 51,900 | 25 | 1.013 | 86,000 |
| 324 | 100 | 1.013 | 51,900 | 100 | 1.013 | 86,000 |

# **B. Economic evalution model**

## **B.1. Annualized capital cost (CAPEX)**

The annualized capital cost (CAPEX) is calculated by dividing the Total Capital Investment (TCI) by the Annuity Factor (AF), as shown in Eq. (S1):

|  |  |
| --- | --- |
|  | (S1) |

The TCI refers to the total cost required to initiate and operate the process, encompassing the Fixed Capital Cost (FCI), Start-Up Cost (SUC), and Working Capital Investment (WCI), as expressed in Eq. (S2). :

|  |  |
| --- | --- |
|  | (S2) |

The FCI represents the initial costs needed to establish the physical infrastructure, including plant equipment, facilities, buildings, and construction expenses. It was calculated as 3.33 times the equipment cost, as described in Eq. (S3). :

|  |  |
| --- | --- |
|  | (S3) |

The equipment costs (*Cequipment*) in 2024 for pyrolysis reactor, wax cracking reactor, distillation columns, combustors, pumps, separators, and heat exchangers were estimated using Six-tenth rule. [2]-[5] To this end, chemical engineering plant cost index (*CEPCI*) and reference cost (*Cref*) were used. The corresponding equation is provided in Eq. (S4).

|  |  |
| --- | --- |
|  | (S4) |

Where and denote the CEPCI in 2024 and in the reference year, respectively; *PC* and denote the proposed and reference equipment capacities; and *n* refers to the cost exponent, assumed to be 0.6 when not explicitly stated in the literature.

The Start-Up Cost (SUC) represents the initial expenses incurred before the process becomes operational, including costs associated with initial testing, adjustments, training, and process commissioning. The SUC was calculated as 10% of the Fixed Capital Cost (FCI), as expressed in Eq. (S5). :

|  |  |
| --- | --- |
|  | (S5) |

The Working Capital Investment (WCI) refers to the operational costs required after the process begins, encompassing expenses such as raw material procurement, wages, and production operations. The WCI was also calculated as 10% of the FCI, as outlined in Eq. (S6). :

|  |  |
| --- | --- |
|  | (S6) |

The Annuity Factor (AF) is used to calculate the present value of a series of future annuities, and its formulation is provided in Eq. (S7). :

|  |  |
| --- | --- |
|  | (S7) |

In this equation, RP represents the periodic interest rate, and NP denotes the number of periods. In this study, RP was set at 5%, and NP was defined as 30 years.

**Table S8.** Economic assessment results for the CAPEX

|  |  |  |  |
| --- | --- | --- | --- |
| **Classification** | **% of FCI** | **AFP-500,**  **[USD yr-1]** | **AFP-600,**  **[USD yr-1]** |
| *Direct cost* |  |  |  |
| *ISBL* |  |  |  |
| Equipment cost | 30 | 10,652,301 | 11,632,927 |
| Installation of equipment | 10 | 3,550,767 | 3,877,642 |
| Instrument and control | 5 | 1,775,384 | 1,938,821 |
| Piping | 10 | 3,550,767 | 3,877,642 |
| Electrical | 5 | 1,775,384 | 1,938,821 |
| *OSBL* |  |  |  |
| Building and building services | 8 | 2,840,614 | 3,102,114 |
| Yard improvements | 2 | 710,153 | 775,528 |
| Services facilities | 8 | 2,840,614 | 3,102,114 |
| Land | 2 | 710,153 | 775,528 |
| Total direct cost |  | 28,406,136 | 31,021,138 |
| *Indirect cost* |  |  |  |
| Engineering | 5 | 1,775,384 | 1,938,821 |
| Construction expenses | 5 | 1,775,384 | 1,938,821 |
| Contractor's fee | 5 | 1,775,384 | 1,938,821 |
| Contingency | 5 | 1,775,384 | 1,938,821 |
| Total indirect cost |  | 7,101,534 | 7,755,285 |
| Fixed capital investment (FCI) | 100 | 35,507,670 | 38,776,423 |
| Start up cost (SUC) | 10 | 7,101,534 | 7,755,285 |
| Working capital investment (WCI) | 10 | 7,101,534 | 7,755,285 |
| Total capital investment (TCI) |  | 49,710,739 | 54,286,992 |
| Annualized capital cost (CAPEX) |  | 3,233,755 | 3,531,447 |

## **B.2. Total product cost (OPEX)**

The Total Product Cost (OPEX) represents the annual operational cost incurred during the process, encompassing ongoing expenses such as raw material costs, energy costs, and labor costs. [6] The annual operating time for OPEX calculation was set at 8,500 hours, and OPEX is determined as the sum of Fixed Charges (FC), Direct Production Costs (DPC), Plant Overhead Costs (OVHD), and General Expenses (GE), as outlined in Eq. (S8). :

|  |  |
| --- | --- |
|  | (S8) |

Fixed Charges (FC) consist of local taxes and insurance costs, which were calculated as 10% of the Fixed Capital Cost (FCI), as expressed in Eq. (S9). :

|  |  |
| --- | --- |
|  | (S9) |

Direct Production Costs (DPC) include the combined costs of raw materials, water, electricity, maintenance, labor, supervision, operating supplies, and laboratory expenses, as detailed in Eq. (S10). :

|  |  |
| --- | --- |
|  | (S10) |

Plant Overhead Costs (OVHD) represent 60% of the sum of maintenance, labor, and supervision costs, and are calculated according to Eq. (S11). :

|  |  |
| --- | --- |
|  | (S11) |

Finally, General Expenses (GE) refer to costs associated with organizing and managing external activities, which form part of routine operations. These include administrative costs, marketing costs, and research and development costs, calculated as the sum of these components as shown in Eq. (S12). :

|  |  |
| --- | --- |
|  | (S12) |

**Table S9.** Economic assessment results for the OPEX

|  |  |  |  |
| --- | --- | --- | --- |
| **Classification** |  | **AFP-500,**  **[USD yr-1]** | **AFP-600,**  **[USD yr-1]** |
| *Fixed charge (FC)* |  |  |  |
| Local taxes, Insurance | 1% of FCI | 355,077 | 387,764 |
| *Direct production cost (DPC)* |  |  |  |
| Raw materials |  | 1,714,323 | 1,888,957 |
| Electricity |  | 321,968 | 330,429 |
| Maintenance (M) | 8% of FC | 2,840,614 | 3,102,114 |
| Operating labor (OL) | 15% of OPEX | 2,234,428 | 2,438,801 |
| Supervision and support labor (S) | 30% of OL | 670,329 | 731,640 |
| Operating supplies | 15% of M | 426,092 | 465,317 |
| Laboratory charges | 15% of OL | 335,164 | 365,820 |
| Plant overhead cost (OVHD) | 60% of M+OL+S | 3,447,222 | 3,763,533 |
| *General expenses (GE)* |  |  |  |
| Admirative cost | 17.5% of OL | 391,025 | 426,790 |
| Distribution and marketing | 11% of OPEX | 1,638,581 | 1,788,454 |
| R&D cost | 3.5% of OPEX | 521,367 | 569,054 |
| Total product Cost (OPEX) |  | 14,896,189 | 16,258,673 |

**Table S10.** Parameters for the *LCOP* calculation

|  |  |  |
| --- | --- | --- |
| **Classification** | **Values** | |
| **For CAPEX calculation** | **For OPEX**  **calculation** |
| Number of periods, [year] | 30 | - |
| Annual operating time, [h year-1] | - | 8,500 |
| Rate per period, [%] | 5 | - |
| Electricity cost, [USD kWh-1] | - | 0.075 |
| Heating utility, [USD kJ-1] | - | 1.9 × 10-6 |
| Cooling utility, [USD kJ-1] | - | 2.13 × 10-7 |
| Deionized water cost, [USD m-3] | - | 1 |
| MEA cost, [USD kg MEA-1] | - | 2.09 |

## **B.3. Revenue**

In the process of producing sustainable aviation fuel, by-products such as LPG, naphtha, CO2, and coke are generated and sold, contributing to the overall revenue. [7]-[10] The total revenue is calculated using the following equation (Eq. (S13)) :

|  |  |
| --- | --- |
|  | (S13) |

represents the revenue from the sale of naphtha, denotes the revenue from LPG, corresponds to the revenue from CO2, and represents the revenue from the sale of low-pressure steam.

**Table S11.** The derived annual revenue of AFP-500 and AFP-600

|  |  |  |  |
| --- | --- | --- | --- |
| **Classification** | **Price** | **AFP-500, [USD]** | **AFP-600, [USD]** |
| Naphtha | 0.86 USD kg-1 | 5,099,025 | 3,048,270 |
| LPG | 0.47 USD L-1 | 2,632,189 | 1,454,036 |
| CO2 | 0.00595 USD kg-1 | 383,815 | 627,246 |
| LP Steam | 0.005 USD kg-1 | - | 260,785 |
| Total |  | 8,115,029 | 5,390,337 |

# **C. Life cycle analysis**

**Table S12.** Detailed LCA results of the aviation fuel production process involving pyrolysis at 500 ˚C (AFP-500)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Classification | GWP-100–fossil,  [kg CO2-eq] | GWP-100–biogenic,  [kg CO2-eq] | GWP-100–land transformation, [kg CO2-eq] | **Total**  [kg CO2-eq] |
| Aviation fuel | 0.490946 | - | - | 0.490946 |
| Monoethanolamine {GLO}| market for monoethanolamine | Cut-off, U | 0.0197404 | 2.254E-05 | 1.244E-05 | 0.0197754 |
| Water, deionised {RoW}| market for water, deionised | Cut-off, U | 0.001199 | 9.65E-05 | 1.76E-06 | 0.001298 |
| Polyethylene, high density, granulate, recycled {RoW}| polyethylene production, high density, granulate, recycled | Cut-off, U | 0.756911 | 0.072488 | 0.001273 | 0.830672 |
| Steam, in chemical industry {RoW}| market for steam, in chemical industry | Cut-off, U | 0.419137 | 7.12E-05 | 7.73E-05 | 0.419286 |
| Electricity, high voltage {GLO}| market group for electricity, high voltage | Cut-off, U | 0.063311 | 0.00012 | 0.000132 | 0.063564 |
| Metallurgical coke, at plant/RNA | -0.01426 | - | - | -0.01426 |
| Naphtha {RoW}| market for naphtha | Cut-off, U | -0.09839 | -3.9E-05 | -3.8E-05 | -0.09847 |
| Liquefied petroleum gas, at refinery/l/US | -0.03854 | - | - | -0.03854 |
| **Total** | - | - | - | 1.674277 |

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