Thermo-economic comparison of DME production plants using green electricity and different biomass sources

Supplementary material

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The supplementary material consists of 15 pages, 3 figures and 16 tables.

It is divided into 3 sections:

S1. Flowsheets and stream data

S2. Calculation of capital costs of DME production plants

S3. Calculation of operating costs of DME production plants

1. Flowsheets and stream data
   1. Wheat straw and 2-stage DME synthesis



Figure S.1. Detailed flowsheet of DME production plant using wheat straw and 2-stage synthesis

Table S.1. Thermodynamic data for the plant with wheat straw and 2-stage synthesis.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | T [°C] | P [bar] | [kg/s] |  | T [°C] | P [bar] | [kg/s] |  | T [°C] | P [bar] | [kg/s] |
| 1 | 660 | 1.47 | 4.09 | 25 | 90 | 8.00 | 3.23 | 49 | 80 | 1.08 | 0.90 |
| 2 | 500 | 1.46 | 4.09 | 26 | 25 | 8.00 | 0.25 | 50 | 20 | 1.01 | 3.46 |
| 3 | 500 | 1.45 | 4.09 | 27 | 19 | 2.10 | 0.25 | 51 | 20 | 1.64 | 3.46 |
| 4 | 600 | 1.44 | 4.09 | 28 | 19 | 2.10 | 0.32 | 52 | 116 | 1.64 | 3.46 |
| 5 | 1300 | 1.37 | 4.82 | 29 | 129 | 8.00 | 2.98 | 53 | 116 | 1.63 | 3.46 |
| 6 | 1009 | 1.30 | 5.22 | 30 | 129 | 10.10 | 2.98 | 54 | 131 | 1.63 | 3.59 |
| 7 | 953 | 1.29 | 5.22 | 31 | 260 | 10.00 | 2.98 | 55 | 800 | 1.62 | 3.59 |
| 8 | 210 | 1.28 | 5.22 | 32 | 374 | 9.30 | 3.78 | 56 | 800 | 1.62 | 1.07 |
| 9 | 50 | 1.27 | 3.32 | 33 | 159 | 9.20 | 3.78 | 57 | 250 | 1.61 | 1.07 |
| 10 | 51 | 1.27 | 1.92 | 34 | 138 | 9.10 | 3.78 | 58 | 250 | 1.61 | 0.13 |
| 11 | 158 | 85.10 | 3.30 | 35 | 100 | 9.00 | 3.78 | 59 | 252 | 1.63 | 0.13 |
| 12 | 76 | 85.10 | 9.66 | 36 | 94 | 6.80 | 3.78 | 60 | 250 | 1.61 | 0.94 |
| 13 | 210 | 85.00 | 9.66 | 37 | 30 | 6.80 | 2.08 | 61 | 72 | 1.61 | 0.94 |
| 14 | 245 | 84.33 | 9.66 | 38 | 135 | 6.80 | 1.69 | 62 | 30 | 1.60 | 0.39 |
| 15 | 132 | 84.23 | 9.66 | 39 | 99 | 2.10 | 1.69 | 63 | 600 | 1.59 | 0.39 |
| 16 | 50 | 84.13 | 9.66 | 40 | 122 | 2.10 | 0.90 | 64 | 800 | 1.62 | 2.52 |
| 17 | 25 | 84.03 | 9.66 | 41 | 30 | 1.60 | 0.55 | 65 | 800 | 1.62 | 1.86 |
| 18 | 25 | 84.03 | 6.42 | 42 | 83 | 2.10 | 0.80 | 66 | 800 | 1.45 | 1.86 |
| 19 | 25 | 84.03 | 6.36 | 43 | 83 | 10.10 | 0.80 | 67 | 800 | 1.45 | 0.73 |
| 20 | 26 | 85.10 | 6.36 | 44 | 260 | 10.00 | 0.80 | 68 | 800 | 1.45 | 1.13 |
| 21 | 25 | 84.03 | 0.06 | 45 | 15 | 1.01 | 0.58 | 69 | 800 | 1.62 | 0.66 |
| 22 | 20 | 2.10 | 0.06 | 46 | 94 | 2.00 | 0.58 | S1 | 15 | 1.62 | 3.79 |
| 23 | 25 | 84.03 | 3.23 | 47 | 328 | 1.10 | 0.90 | S2 | 660 | 1.62 | 0.35 |
| 24 | 27 | 8.10 | 3.23 | 48 | 210 | 1.09 | 0.90 |  |  |  |  |

Table S.1. Heat and electricity streams for the plant with wheat straw and 2-stage synthesis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Heat [MW] |  | Heat [MW] |  | Power [MW] |
| 301 | 1.3 | 318 | 2.0 | 101 | 5.2 |
| 302 | 0.8 | 319 | 0.3 | 102 | 0.0 |
| 303 | 0.8 | 320 | 1.7 | 103 | 0.0 |
| 304 | 9.8 | 321 | 2.9 | 104 | 0.0 |
| 305 | 6.5 | 322 | 3.1 | 105 | 0.4 |
| 306 | 4.0 | 323 | 0.3 | 106 | 0.0 |
| 307 | 3.1 | 324 | 1.1 | 107 | 0.0 |
| 308 | 8.2 | 325 | 0.3 | 108 | 39.1 |
| 309 | 3.1 | 326 | 0.1 | 109 | 0.0 |
| 310 | 4.1 | 327 | 0.1 |  |  |
| 311 | 0.7 | 328 | 1.6 | NET | 43.9 |
| 312 | 0.7 | 329 | 8.1 |  |  |
| 313 | 0.5 | 330 | 5.5 |  |  |
| 314 | 0.1 | 331 | 3.8 |  |  |
| 315 | 2.4 | 332 | 1.0 |  |  |
| 316 | 1.7 | 333 | 1.6 |  |  |
| 317 | 0.7 | 334 | 2.7 |  |  |

Table S.2. Stream composition of the DME production plant with wheat straw and 2-stage synthesis; top: weight distribution between liquid and gas constituents; bottom: molar composition of the gas phase.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Stream number | 1-4 | 5 | 6-8 | 9 | 10 | 11 | 12-13 | 14-17 | 18-22 | 23-25 | 26-27 | 28 | 29-31 | 32-36 | 37 | 38-39 | 40 | 41 | 42-44 | 45-46 | 47-49 | 50-53 | 54-55 | 56-61 | 63-64 | 65-70 |
| Liquids (wt. %) | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Bio-oil | 7.6 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| Aq. Organics | 2.3 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| Water | - | - | - | - | 100.0 | - | - | - | - | - | - | - | - | - | - | - | 100.0 | 100.0 | - | - | - | 100.0 | - | - | - | - |
| Gas (wt. %) | 90.0 | 100.0 | 100.0 | 100.0 | - | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | 100.0 | - | - | 100.0 | 100.0 | 100.0 | - | 100.0 | 100.0 | 100.0 | 100.0 |
| Gas Composition (mole-%) | | |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| H2O | 50.9 | 34.3 | 27.4 | 0.9 | - | 0.4 | 0.1 | 0.8 | 0.0 | 4.4 | 0.0 | 0.0 | 4.7 | 41.5 | - | 66.7 | - | - | 0.2 | - | 11.3 | - | 90.2 | 18.0 | 2.7 | - |
| H2 | 7.3 | 23.3 | 47.7 | 65.1 | - | 65.4 | 62.0 | 49.1 | 59.8 | 0.2 | 3.7 | 27.9 | - | - | - | - | - | - | - | - | - | - | 9.8 | 82.0 | 97.3 | - |
| N2 | 0.0 | 0.4 | 0.2 | 0.3 | - | 0.3 | 10.0 | 13.3 | 16.1 | 0.1 | 1.9 | 8.1 | - | - | - | - | - | - | - | 79.0 | 57.9 | - | - | - | - | - |
| CO | 25.7 | 27.7 | 22.4 | 30.5 | - | 30.7 | 21.0 | 12.3 | 14.9 | 0.1 | 1.8 | 7.5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| CO2 | 10.4 | 14.3 | 2.4 | 3.2 | - | 3.2 | 6.7 | 8.2 | 8.8 | 5.4 | 90.3 | 55.1 | 0.0 | 0.0 | 0.0 | - | - | - | - | - | 23.5 | - | - | - | - | - |
| CH4 | 3.8 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| ETHENE | 0.9 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| PROPENE | 0.4 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| BENZENE | 0.0 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| ETHANE | 0.4 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| PENTENE | 0.3 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| MEOH | - | - | - | - | - | - | 0.2 | 16.3 | 0.3 | 89.7 | 2.3 | 1.4 | 95.3 | 20.7 | 0.0 | 33.3 | 0.0 | - | 99.6 | - | - | - | - | - | - | - |
| DME | - | - | - | - | - | - | - | - | - | - | - | - | - | 37.8 | 100.0 | 0.1 | - | - | 0.3 | - | - | - | - | - | - | - |
| O2 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 21.0 | 7.3 | - | - | - | - | 100.0 |

* 1. Wheat straw and 1-stage DME synthesis



Figure S.2. Detailed flowsheet of DME production plant using wheat straw and 1-stage synthesis

* 1. Bamboo and 2-stage DME synthesis



Figure S.3. Detailed flowsheet of DME production plant using bamboo and 2-stage synthesis

* 1. Bamboo and 1-stage DME synthesis



Figure S.4. Detailed flowsheet of DME production plant using bamboo and 1-stage synthesis

1. Composite curves and utility estimations

In the following subsections, the composite curves and the utility composite curves of the investigated plants are shown (Figure S.5 - Figure S.12) . The utility composite curve shows the grand composite curve plus the utility integration. The plots were generated using the software Aspen Energy Analyzer V11.

The considered utilities were:

1. Steam at 200 °C (15.55 bar) for process heat provision
2. Water heated from 40 °C to 75 °C for district heating provision
3. Water heated from 15 °C to 20 °C used as cooling water
4. Evaporating refrigerant at -55 °C in the plants with 1-stage synthesis for low-temperature cooling

The results for the required utility capacities based on the results of the pinch analysis are shown in Table S. 3.

Table S. 3. Utility estimations

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Process heat**  **[MW]** | **District heating**  **[MW]** | **Cooling water**  **[MW]** | **Refrigeration**  **[MW]** |
| **Wheat, 2-stage** | 9.5 | 11.3 | 2.7 | - |
| **Wheat, 1-stage** | 19.5 | 6.8 | 2.7 | 3.1 |
| **Bamboo, 2-stage** | 1.6 | 11.6 | 2.7 | - |
| **Bamboo, 1-stage** | 10.7 | 3.9 | 2.1 | 2.3 |

* 1. Wheat straw and 2-stage DME synthesis

A computer screen shot of a computer screen

Description automatically generated

Figure S.5. Composite curves of the plant using wheat straw and 2-stage synthesis

A person holding a flag

Description automatically generated

Figure S.6. Utility composite curve of the plant using wheat straw and 2-stage synthesis

* 1. Wheat straw and 1-stage DME synthesis

A screenshot of a computer

Description automatically generated

Figure S.7. Composite curves of the plant using wheat straw and 1-stage synthesis

A white background with black and red lines

Description automatically generated

Figure S.8. Utility composite curve of the plant using wheat straw and 1-stage synthesis

* 1. Bamboo and 2-stage DME synthesis

A white screen with black text

Description automatically generated

Figure S.9. Composite curves of the plant using bamboo and 2-stage synthesis A flag of the united states of america

Description automatically generated

Figure S.10. Utility composite curve of the plant using bamboo and 2-stage synthesis

* 1. Bamboo and 1-stage DME synthesis

A screen shot of a graph

Description automatically generated

Figure S.11. Composite curves of the plant using bamboo and 1-stage synthesis

A white background with black and red lines

Description automatically generated

Figure S.12. Utility composite curve of the plant using bamboo and 1-stage synthesis

1. Calculation of capital costs of DME production plants

The cost of the DME production plants presented in this work were calculated as grassroot costs , as presented by Turton et al. [1]. The grassroot costs describe the cost of a completely new facility on essentially undeveloped land. The grassroot costs can be calculated from the total module cost and the bare module costs of the equipment at base conditions with eq. (1)

|  |  |
| --- | --- |
|  | (1) |

The total module cost describes the cost of all the equipment of the plant including all direct and indirect costs connected to the different equipment in the plant as well as the contingency and fee costs. The total module costs are calculated using eq. (2), assuming values of 15 % and 3% of the bare module cost for contingency costs and fees, respectively. These are appropriate for systems that are well understood [1].

|  |  |
| --- | --- |
|  | (2) |

Eqs. (1) and (2) can be summarized to eqs. (3) and (4), where denotes the contribution of equipment to the grassroot cost of the overall plant. Eqs. (3) and (4) were used in this work for calculating the grassroots costs of the plants.

|  |  |
| --- | --- |
|  | (3) |
|  | (4) |

Different methods were used for estimating the bare module costs and of the equipment in the plants. The different methods are explained in detail in the following subsections.

For all the used methods, the bare module costs and hence the grassroot costs were calculated for a specific reference year . The cost was updated to the year 2022 taking inflation into account by using the Chemical Engineering Plant Cost Index (CEPCI) as shown in eq. (5). The values for the CEPCI of the last 20 years can be found in

Lastly, the grassroot costs were converted to €, using the exchange rate from € to $ . This value corresponds to the average exchange rate of the year 2022 (01/01/2022-31/12/2022), as found on the webpage of The European Central Bank [2].

Note: In this part of the work, the capital cost of the solid oxide electrolysis was not considered as the size and cost estimation of the electrolyser was part of the last step of this work, explained in chapter S5.

.

|  |  |
| --- | --- |
|  | (5) |

Lastly, the grassroot costs were converted to €, using the exchange rate from € to $ . This value corresponds to the average exchange rate of the year 2022 (01/01/2022-31/12/2022), as found on the webpage of The European Central Bank [2].

Note: In this part of the work, the capital cost of the solid oxide electrolysis was not considered as the size and cost estimation of the electrolyser was part of the last step of this work, explained in chapter S5.

* 1. Bare module costs of standard equipment from Turton et al.

For most of the equipment included in the investigated plants, the module costing technique presented by Turton et al. [1] was used for estimating the bare module cost. The bare module cost , which includes all direct and indirect costs associated with the equipment, is calculated with eq. (6), where denotes the purchased equipment cost for base conditions and denotes the bare module factor.

|  |  |
| --- | --- |
|  | (6) |

The purchased equipment cost at ambient operating pressure and using carbon steel construction was calculated with eq. (7).

|  |  |
| --- | --- |
|  | (7) |

Where denotes the capacity or size parameter and , and the parameters for each specific equipment. The parameters for the used equipment in this work are listed in Table S.12.

The bare module costs of the equipment at base conditions is calculated in analogy with eq. (6) with eq. (8).

|  |  |
| --- | --- |
|  | (8) |

Where denotes the bare module factor at base conditions.

The calculation of the bare module factor is depending on the used equipment. In the following subsections, the data for the calculation of the purchased equipment cost, the equation and data used for the bare module factor and the method for sizing is explained in detail for the investigated equipment.

Table S.4. Chemical Engineering Plant Cost Index (CEPCI) for the past years. At the bottom of the list, the CEPCI used for the cost functions of Turton et al. [1] is reported.

|  |  |
| --- | --- |
| **Year** | **CEPCI** |
| 2022 | 816 |
| 2021 | 708.8 |
| 2020 | 596.2 |
| 2019 | 607.5 |
| 2018 | 603.1 |
| 2017 | 567.5 |
| 2016 | 541.7 |
| 2015 | 556.8 |
| 2014 | 576.1 |
| 2013 | 567.3 |
| 2012 | 584.6 |
| 2011 | 585.7 |
| 2010 | 550.8 |
| 2009 | 521.9 |
| 2008 | 575.4 |
| 2007 | 525.4 |
| 2006 | 499.6 |
| 2005 | 468.2 |
| 2004 | 444.2 |
| 2003 | 402.0 |
| 2002 | 395.6 |
| 2001 | 394.3 |
| 2001Turton | 397.0 |

* + 1. Reactors

There were five different reactors included in the investigated plants, which can be clustered into two types of reactors:

**Adiabatic reactors**: POX reactor, rWGS reactor, adiabatic methanol dehydration reactor

**Boiling water reactors**: methanol reactor, one-stage DME reactor

* + - 1. Adiabatic reactors:

For the adiabatic reactors, the cost functions for horizontal pressure vessels were used. The sizing factor for horizontal process vessels in eq. (7) is the reactor volume . For the POX reactor and the rWGS reactor, the volume of the reactor was calculated with eq. (9). The residence times were assumed to be 3 s and 10 s for POX and rWGS reactor, respectively. The outlet volume flow rate from the reactors was used for the calculations.

|  |  |
| --- | --- |
|  | (9) |

For the adiabatic DME reactor in the two-stage plants used for methanol dehydration, the size of the reactor was derived using the a kinetic reactor model in order to find the length of the reactor achieving the same outlet methanol mole flow as in an equilibrium reactor model with a temperature approach of . The reactor diameter was fixed to .

The bare module factor for process vessels is calculated using eq. (10)

|  |  |
| --- | --- |
|  | (10) |

Where denotes the material factor and denotes the pressure factor.

The pressure factor for process vessels is calculated with eq. (11)

|  |  |
| --- | --- |
|  | (11) |

Where P is the pressure in bar and D the diameter in meters. Note that the equation was changed from [1] in order to be based on the pressure in bar instead of barg. If is less than 1, then is used. For all reactors a diameter of was used for the calculations.

The material factor depends on the used material. For the POX and rWGS reactor, stainless steel (SS) was used due to potential corrosion connected to the tars in the POX and the high temperature hydrogen in the rWGS reactor. For the adiabatic DME reactor, carbon steel (CS) was used. In Table S.5, the material factor for horizontal and vertical process vessels for different materials are listed. The values were read from Figure A.18 in [1].

Table S.5. Material factors for horizontal and vertical process vessels for different materials.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Material** | **CS** | **SS clad** | **SS** | **Ni alloy clad** | **Ni alloy** | **Ti clad** | **Ti** |
| Material factor | 1 | 1.75 | 3.1 | 3.6 | 7.1 | 4.65 | 9.4 |

The bare module factor at base conditions is calculated with eq. (12).

|  |  |
| --- | --- |
|  | (12) |

The constants and used in eqs. (10) and (12) are shown in Table S.13.

* + - 1. Boiling water reactors:

For the boiling water reactors, the purchased equipment costs were calculated in analogy to a shell and tube heat exchanger. The sizing factor for shell and tube heat exchangers in in eq. (7) is the heat transfer area , which corresponds to the outside area of the tubes in the reactor/heat exchanger. The heat transfer area was calculated with eq. (13).

|  |  |
| --- | --- |
|  | (13) |

The tube diameter was fixed to for all reactors. The reactor length was for the methanol reactor in the two-stage synthesis plants and for the DME reactor in the one-stage plants. The number of tubes was determined as described in the article, by ensuring a sufficient residence time in the reactor for approaching equilibrium at the outlet as much as possible, while ensuring that the maximum temperature within the reactor was kept below for avoiding damages on the catalyst.

As shown in Table S.12, the application of the cost function for shell-and-tube heat exchangers is limited to a maximum heat transfer area of . While boiling water reactors can be larger than this, the use of eq. (7) at higher values was avoided in order to avoid extrapolation error. Instead, the use of parallel reactors was assumed in case of . The number of parallel units was calculated with eq. (14).

|  |  |
| --- | --- |
|  | (14) |

The area per unit, used in eq. (7) was then calculated as, and the calculated value was then multiplied by the number of units .

|  |  |
| --- | --- |
|  | (15) |

The bare module factor and the bare module factor at base conditions were calculated with eqs. (10) and (12), respectively. The constants and used are shown in Table S.13.

The pressure factor for heat exchangers is calculated with eq. (16)

|  |  |
| --- | --- |
|  | (16) |

The units of are barg unless stated otherwise. The values of the parameters , and are listed in Table S.14.

The material factor depends on the used material. For the methanol reactor in the two-stage synthesis plants and for the DME reactor in the one-stage plants, stainless steel construction (SS/SS) was used. In Table S.6, the material factor for shell-and-tube heat exchangers for different materials are listed. The values were read from Figure A.18 in [1].

Table S.6. Material factors for shell-and-tube heat exchangers for different materials.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Material** | **CS/CS** | **CS/Cu** | **Cu/Cu** | **CS/SS** | **SS/SS** | **CS/Ni alloy** | **Ni alloy/Ni alloy** | **CS/Ti** | **Ti/Ti** |
| Material factor | 1 | 1.4 | 1.7 | 1.8 | 2.8 | 2.7 | 3.7 | 4.6 | 11.4 |

* + 1. Pumps

For the pumps in the system, the cost function for centrifugal pumps was used. The sizing factor for centrifugal pumps in in eq. (7) is the shaft power, which was extracted directly from the simulation results in aspen Plus. The bare module factor and the bare module factor at base conditions were calculated with eqs. (10) and (12), respectively. The constants and used are shown in Table S.13. The pressure factor for centrifugal pumps is calculated with eq. (16). The values of the parameters , and are listed in Table S.14.

The material factor depends on the used material. For the pump in delivering water to the electrolyser, carbon steel (CS) was used. For the methanol pumps in the synthesis blocks, recycling and pumping methanol and methanol-DME-water mixtures, stainless steel (SS) was used. In Table S.7the material factor for centrifugal pumps for different materials are listed. The values were read from Figure A.18 in [1].

Table S.7. Material factors for centrifugal pumps for different materials.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Material** | **Cast iron** | **CS** | **SS** | **Ni alloy** |
| Material factor | 1 | 1.75 | 2.45 | 4.35 |

* + 1. Compressors

For the compressors in the system, the cost function for centrifugal compressors was used. The sizing factor for centrifugal compressors in in eq. (7) is the fluid power. From the simulation results in Aspen Plus, the electrical power was then calculated with eq. (17), using an isentropic efficiency and a mechanical efficiency .

|  |  |
| --- | --- |
|  | (17) |

The bare module factor and the bare module factor at base conditions for compressors depend solely on the material used. For all compressors in the plants carbon steel (CS) was used as material. For the determination of the lowers bare module factor was used, namely the one for carbon steel. In Table S.8, the bare module factors for centrifugal compressors for different materials are listed. The values were read from Figure A.19 in [1].

Table S.8. Bare module factors for centrifugal compressors for different materials.

|  |  |  |  |
| --- | --- | --- | --- |
| **Material** | **CS** | **SS** | **Ni alloy** |
| Material factor | 2.75 | 5.8 | 11.4 |

* + 1. Fans

For the fans and blowers in the system, the cost function for centrifugal radial fans was used. The sizing factor for centrifugal radial fans in in eq. (7) is the gas flow rate. The inlet gas flow rate to the fans was used in this work. For fans, the bare module costs are calculated using eq. (18).

|  |  |
| --- | --- |
|  | (18) |

The pressure factor for centrifugal radial fans is calculated with eq. (16). The values of the parameters , and are listed in Table S.14. For the pressure the pressure difference across the fan in kPa is used.

The bare module factor and the bare module factor at base conditions for fans depend solely on the material used. For all fans in the plants carbon steel (CS) was used as material, except of the fan used for recycling the volatiles to the pyrolysis reactor in the bamboo plants. Here, stainless steel (SS) was used due to potential corrosion connected to the tars. For the determination of the lowest bare module factor was used, namely the one for carbon steel and a pressure factor of was used. In Table S.9, the bare module factors for centrifugal radial fans for different materials are listed. The values were read from Figure A.19 in [1].

Table S.9. Bare module factors for centrifugal radial fans for different materials.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Material** | **CS** | **Fiberglass** | **SS** | **Ni alloy** |
| Material factor | 2.75 | 5 | 5.8 | 11.4 |

* + 1. Distillation columns

For the distillation columns, the cost functions for vertical process vessels and sieve trays were used. Below, the followed approach for the two equipment types are explained:

* + - 1. Vertical process vessels

The sizing factor for vertical process vessels in eq. (7) is the volume . The volume was calculated from the column diameter and the height with eq.

|  |  |
| --- | --- |
|  | (19) |

The diameter and height were taken from the build-in column internals in Aspen Plus. The height is determined based on the number of stages and required height for each stage. The diameter is determined to ensure a proper hydraulic behaviour. For all distillation columns, the number of stages was fixed . It should be mentioned that for some distillation columns, a lower number of stages would be sufficient to fulfil the distillation requirements, but an optimization of the number of stages was deemed unnecessary for the purpose of this work.

The bare module factor and the bare module factor at base conditions were calculated with eqs. (10) and (12), respectively. The constants and used are shown in Table S.13. The pressure factor for process vessels is calculated with eq. (11). The material factor depends on the used material. Carbon steel (CS) was used as material for all investigated distillation columns. In Table S.5, the material factor for horizontal and vertical process vessels for different materials are listed. The values were read from Figure A.18 in [1].

* + - 1. Sieve trays

The sizing factor for sieve trays in eq. (7) is the area . The calculated purchased equipment cost is the cost of one tray. The area was calculated from the column diameter with eq. (20).

|  |  |
| --- | --- |
|  | (20) |

The diameter was taken from the build-in column internals in Aspen Plus. The diameter is determined to ensure a proper hydraulic behaviour. For all distillation columns, the number of stages was fixed to . It should be mentioned that for some distillation columns, a lower number of stages would be sufficient to fulfil the distillation requirements, but an optimization of the number of stages was deemed unnecessary for the purpose of this work.

The bare module cost for sieve trays is calculated with eq. (21)

|  |  |
| --- | --- |
|  | (21) |

Where is the number of trays and is a quantity factor for trays given by eq.

|  |  |
| --- | --- |
|  | (22) |

The bare module factor and the bare module factor at base conditions for trays depend solely on the material used. For all trays in the plants carbon steel (CS) was used as material. For the determination of the lowest bare module factor was used, namely the one for carbon steel. In Table S.10, the bare module factors for centrifugal sieve trays for different materials are listed. The values were read from Figure A.19 in [1].

Table S.10. Bare module factors for sieve trays for different materials.

|  |  |  |  |
| --- | --- | --- | --- |
| **Material** | **CS** | **SS** | **Ni alloy** |
| Material factor | 1 | 2 | 5.6 |

* + 1. Gas engines

For the gas engines in the system, the cost function for internal combustion engines was used. The sizing factor for internal combustion engines in in eq. (7) is the shaft power. The shaft power was taken from the simulation results in Aspen Plus.

The bare module factor of internal combustion engines is independent of material and pressure and is constant at

* + 1. Refrigeration plants

The capital cost of the refrigeration plant was calculated as the cost of the compressor and the condenser. The cost for the throttling valve was neglected, while the cost of the evaporator(s) was not considered here, as it was already included in the heat exchanger network.

* + - 1. Compressor

For the compressor, the same procedure as presented in section S3.1.3 was conducted. The electrical power was calculated from the refrigeration capacity of the plants, determined as shown in chapter S2. The electrical power was then calculated with eq. (23), using a

|  |  |
| --- | --- |
|  | (23) |

* + - 1. Condenser

For the condenser, the cost function for flat plate heat exchangers was used. The sizing factor for flat plate heat exchanger in in eq. (7) is the heat transfer area. The heat transfer area was estimated using eq.

|  |  |
| --- | --- |
|  | (24) |

The heat transferred in the condenser was calculated based on the energy balance of the refrigeration plant:

|  |  |
| --- | --- |
|  | (25) |

The overall heat transfer coefficient was calculated with:

|  |  |
| --- | --- |
|  | (26) |

Where denotes the convective heat transfer coefficient of the condensing refrigerant and the convective heat transfer coefficient of the cooling water.

The logarithmic mean temperature difference was calculated with eq. (27).

|  |  |
| --- | --- |
|  | (27) |

Where is the condensation temperature of the refrigerant and and are the cooling water inlet and outlet temperature.

The bare module factor and the bare module factor at base conditions were calculated with eqs. (10) and (12), respectively. The constants and used are shown in Table S.13.

The pressure factor for flat plate heat exchangers is for pressures of , while there are no data available for higher pressures. However, for typical refrigerants it is realistic to have pressures below 20 bar at a condensation temperature of 25 °C.

The material factor depends on the used material. Carbon steel (CS) was used as material. In Table S.11, the material factor for flat plate heat exchangers for different materials are listed. The values were read from Figure A.18 in [1].

Table S.11. Material factors for flat plate heat exchangers for different materials.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Material** | **CS** | **Cu** | **SS** | **Ni alloy** | **Ti** |
| Material factor | 1 | 1.35 | 2.4 | 2.7 | 4.6 |

* + 1. Heat exchanger network

Table S.12. Parameters for calculation of purchased equipment costs with eq. (7)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Equipment type** | **Equipment Description** |  |  |  | **Capacity, Units** | **Min size** | **Max Size** |
| Process vessels | Horizontal | 3.5565 | 0.3776 | 0.0905 | Volume, m3 | 0.1 | 628 |
| Heat exchangers | Floating head (=shell-and-tube) | 4.8306 | -0.8509 | 0.3187 | Area, m2 | 10 | 1000 |
| Pumps | Centrifugal | 3.3892 | 0.0536 | 0.1538 | Shaft power, kW | 1 | 300 |
| Compressors | Centrifugal | 2.2897 | 1.3604 | -0.1027 | Fluid power | 450 | 3000 |
| Fans | Centrifugal radial | 3.5391 | -0.3533 | 0.4477 | Gas flowrate, m3/s | 1 | 100 |
| Process vessels | Vertical | 3.4974 | 0.4485 | 0.1074 | Volume, m3 | 0.3 | 520 |
| Trays | Sieve | 2.9949 | 0.4465 | 0.3961 | Area, m2 | 0.07 | 12.3 |
| Drives | Int. Comb. Engine | 2.7635 | 0.8574 | -0.0098 | Shaft power, kW | 10 | 10000 |
| Heat exchangers | Flat plate | 4.6656 | -0.1557 | 0.1547 | Area, m2 | 10 | 1000 |

Table S.13. Constants for calculation of bare module factor with eqs. (10) and (12)

|  |  |  |  |
| --- | --- | --- | --- |
| **Equipment type** | **Equipment Description** |  |  |
| Process vessels | Horizontal | 1.49 | 1.52 |
| Heat exchangers | Floating head (=shell-and-tube) | 1.63 | 1.66 |
| Pumps | Centrifugal | 1.89 | 1.35 |
| Process vessels | Vertical | 2.25 | 1.82 |
| Heat exchangers | Flat plate | 0.96 | 1.21 |

Table S.14. Parameter for calculation of pressure factor with eq. (16)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Equipment type** | **Equipment Description** |  |  |  | **Pressure Range (barg)** |
| Heat exchangers | Floating head (=shell-and-tube) | 0 | 0 | 0 | P<5 |
| 0.03881 | -0.11272 | 0.08183 | 5<P<140 |
| Pumps | Centrifugal | 0 | 0 | 0 | P<10 |
| -0.3935 | 0.3957 | -0.00226 | 10<P<100 |
| Fans | Centrifugal radial | 0 | 0 | 0 | ΔP<1 kPa |
| 0 | 0.20899 | -0.0328 | 1<ΔP<16 |

* 1. Bare module costs of gasifiers and other components

The cost functions presented by Turton et al. [1] do not include data that can be used for estimating the grassroot cost of the used biomass gasification units and some equipment for biomass handling and gas conditioning. In the following subsections, the method and references used for estimating the capital cost of this equipment is described.

* + 1. LT-CFB gasifer

The low-temperature circulating fluidized bed (LT-CFB) gasifier was used for wheat straw gasification. The LT-CFB gasifier consists of four components (see figure XX):

1. Fluidized bed pyrolysis reactor, where the wheat straw is pyrolyzed. The pyrolysis char is exiting at the top of the reactor together with the pyrolysis gas, gasifier gas and bio-ash.
2. Char cyclone, where the pyrolysis char is separated from the gas and bio-ash and led to the char gasifier
3. Fluidized bed char reactor, where the pyrolysis char is gasified using pure oxygen. The produced gas and the remaining bio-ash are returned to the pyrolysis reactor, where they are then exiting the LT-CFB gasifier at the top together with the pyrolysis gas.
4. Ash cyclone, where the bio-ash is separated from the produced gas.

For estimating the capital cost of the components, the method and data presented by Larson et al. [3] were used. The purchased equipment cost was calculated using eq. (28)

|  |  |
| --- | --- |
|  | (28) |

Where denotes the purchased equipment cost at reference size, denotes the reference size, denotes the equipment size in the plant and denotes the scaling factor. The data for the investigated equipment are shown in Table S.15. For completeness, the maximum size of the equipment is also shown, needed for determining the number of units needed. In this work, the fluidized bed reactors and the cyclones were all below the maximum size, and hence no parallel equipment was required.

Table S.15. Parameters for calculation of purchased equipment costs with eq. (28)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Equipment** |  |  |  |  | **Scaling factor** |  |
| Fluidized bed gasifier | 41.7 | 120 |  | 6.41 | 0.7 | 30 |
| Cyclone | 68.7 | 180 |  | 0.91 | 0.7 | - |

For the pyrolysis reactor and the char reactor, the data for a fluidized bed gasifier were used. In Table S.15, a reference pressure is shown, as the reference cost and size denote to the corresponding operation pressure. As described by Larson et al. in footnote (c) of Table 7 in [3], the size of a fluidized bed gasifier processing the same amount of biomass decreases with increasing operating pressures. Larson et al. derived eq. (29) for the dependency of the maximum gasifier size .

|  |  |
| --- | --- |
|  | (29) |

The pressure dependency of the reference size is proportional to the dependency of the maximum size. Therefore, eq. (30) was used for calculating the reference size at the operating pressure of the LT-CFB gasifier.

|  |  |
| --- | --- |
|  | (30) |

For calculating the total module cost, Larson et al. used a different than the one presented by Turton et al. First, the direct costs (DC) associated with the equipment are calculated by adding the balance of plant (BOP) costs to the purchased equipment cost. Larson et al. derived an estimate for the BOP cost as percentage of the purchased equipment cost as a function of the biomass input to the system (HHV).

|  |  |
| --- | --- |
|  | (31) |

For the investigated plants, the resulting values are between 30 % and 40 %. For simplification, a value of 35 % was used for all plants. The direct cost () was then calculated with:

|  |  |
| --- | --- |
|  | (32) |

Secondly, the indirect cost ( ) was calculated as a percentage of the direct cost. Larson et al. suggest that the indirect cost for gasifier and gas clean up equipment can be calculated as % of the direct cost, including contingency and fees. The total module cost is the calculated with eq. (33)

|  |  |
| --- | --- |
|  | (33) |

For the calculation of the grassroot cost in eq. (1), the bare module cost at base conditions of the equipment are required. In analogy to eq. (2), of the fluidized bed reactors and the cyclones was estimated with eq. (34).

|  |  |
| --- | --- |
|  | (34) |

* + 1. Entrained flow gasifier

The entrained flow gasifier (EFG) was used for bamboo gasification. The entrained flow gasifier consists of four components:

1. Steam dryer, where the moisture content of the biomass is reduced from 25 % to 2 %.
2. Updraft pyrolysis reactor, where bamboo is pyrolyzed as pretreatment step for the entrained flow gasifier
3. Grinder, where the pyrolysis char pulverized to the necessary particle size of the gasifier
4. Entrained flow gasifier, where the pyrolysis char is fed through lock hoppers using downstream CO2. The pyrolysis char and the volatiles from the pyrolysis are gasified using pure oxygen. The product gas leaves the gasifier at the top.

For the steam dryer and the updraft pyrolysis reactor, the method and data from Butera et al. [4] were used. From the data, the bare module cost of the equipment was calculated using eq. (35).

|  |  |
| --- | --- |
|  | (35) |

Where denotes the bare module cost at reference size, denotes the reference size, denotes the equipment size in the plant and denotes the scaling factor. The data for the investigated equipment are shown in Table S. 16.

The total module cost was then calculated using eq. (2). For the calculation of the grassroot cost in eq. (1), the bare module cost was used instead of the bare module cost at base conditions .

Table S. 16. Parameters for calculation of bare module costs with eq. (35)(28)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Equipment** |  |  |  | **Scaling factor** |
| Steam Dryer | 71 |  | 18.07 | 0.6 |
| Updraft pyrolysis reactor | 7 |  | 1.6 | 0.6 |

For the entrained flow gasifier and the grinder, the method from Hamelinck et al [5] were used. The purchased equipment cost was calculated using eq. (28). The data for the investigated equipment are shown in Table S. 17. Data for the entrained flow gasifier were taken from Pandey et al. [6], but they follow the same method as presented by Hamelinck et al. [5].

Table S. 17. Parameters for calculation of purchased equipment cost with eq. (28) and total module cost with eq. (36)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Equipment** |  |  |  | **Reference year** | **Scaling factor** | **Installation factor** | **Reference** |
| Entrained flow gasifier | 17.5 |  | 23.2 | 2007 | 0.7 | 2.48 | [6] |
| Grinder | 33.5 |  | 0.48 | 2002 | 0.6 | 2 | [5] |
| Particle filter | 12.1 |  | 1.9 | 2002 | 0.65 | 2 | [5] |
| Sulphur removal | 8 |  | 0.024 | 2002 | 1 | 3 | [5] |
| Selexol Co2 removal | 9909 |  | 63 | 2002 | 0.7 | 1 | [5] |
| Biomass conveyers | 33.5 |  | 0.41 | 2002 | 0.8 | 2 | [5] |
| Biomass storage | 33.5 |  | 1.16 | 2002 | 0.65 | 2 | [5] |

The total module cost was calculated using eq. (36). As explained by Hamelinck et al. in Table 6 of [5], the installation factor includes all the direct and indirect cost, including contingency and fees.

|  |  |
| --- | --- |
|  | (36) |

For the calculation of the grassroot cost in eq. (1), the bare module cost at base conditions of the equipment are required. In analogy to eq. (2), of the fluidized bed reactors and the cyclones was estimated with eq. (34).

* + 1. Other equipment for biomass handling and gas conditioning

For the biomass storage and conveyer, as well as the particle filter, sulphur removal and CO2 removal equipment in the plants, the data and method of Hamelinck et al [5]. were used as explained above. The data for the investigated equipment are shown in Table S. 17.

* 1. Capital cost estimates for the investigated DME plants

In the following tables, the capacities and the estimated cost of the investigated plants and the corresponding equipment are shown.

Table S. 18. Capital cost estimates for plant using wheat straw and 2-stage DME synthesis

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Capacities** | | | | **Grass root costs [M€]** | |
| **Subgroups** | **Unit** | **Required Capacity** | **Number of Units** | **Capacity per unit** | **Unit of Capacity** | **Per unit** | **Per subgroup** |
| Biomass Handling | Conveyors | 3.8 | 1 | 3.8 | t\_wet\_biomass/h | 1.1 | 4.7 |
| Biomass storage | 3.8 | 1 | 3.8 | t\_wet\_biomass/h | 3.6 |
| LT-CFB gasifier | Pyrolysis reactor | 10.9 | 1 | 10.9 | t\_dry\_biomass/h | 33.8 | 48.2 |
| Char reactor | 2.4 | 1 | 2.4 | t\_dry\_biomass/h | 11.8 |
| Char Cyclone | 11.3 | 1 | 11.3 | m^3/s | 1.3 |
| Ash Cyclone | 11.3 | 1 | 11.3 | m^3/s | 1.3 |
| Gas Cleaning | Particle filter | 8.0 | 1 | 8.0 | m^3/s | 8.1 | 10.9 |
| POX reactor | 66.4 | 1 | 66.4 | m^3 | 0.6 |
| RWGS reactor | 322.7 | 1 | 322.7 | m^3 | 2.0 |
| Sulfur removal | 7.1 | 1 | 7.1 | Nm^3/s | 0.2 |
| Turbomachinery | SYN-COM1 | 1159.0 | 1 | 1159.0 | kW | 2.3 | 10.9 |
| SYN-COM2 | 1017.0 | 1 | 1017.0 | kW | 2.1 |
| SYN-COM3 | 997.0 | 1 | 997.0 | kW | 2.0 |
| SYN-COM4 | 987.0 | 1 | 987.0 | kW | 2.0 |
| SYN-COM5 | 1101.0 | 1 | 1101.0 | kW | 2.2 |
| REC-COMP | 0.1 | 1 | 0.1 | m^3/s | 0.2 |
| MEOH-PUMP | 1.5 | 1 | 1.5 | kW | 0.0 |
| MEOH-PUMP2 | 1.5 | 1 | 1.5 | kW | 0.0 |
| ELEC-PUMP | 0.0 | 1 | 0.0 | kW | 0.0 |
| H2-REC | 0.7 | 1 | 0.7 | m^3/s | 0.0 |
| Synthesis reactors | MeOH reactor | 681.7 | 1 | 681.7 | m^2 | 2.0 | 2.1 |
| DME reactor | 2.3 | 1 | 2.3 | m^3 | 0.1 |
| Distillation colums | TOP-COL | 2.7 | 1 | 2.7 | m^3 | 0.1 | 0.5 |
| DME-COL | 6.2 | 1 | 6.2 | m^3 | 0.2 |
| MEOH-COL | 10.1 | 1 | 10.1 | m^3 | 0.2 |
| Gas Engine | Gas engine | 418.0 | 1 | 418.0 | kW | 0.6 | 0.6 |
| Heat exchanger Network | Heat exchanger | 4609.0 | 49 | 94.1 | m^2 | 13.0 | 13.0 |
| **Total Grassroot costs** |  |  |  |  |  | **90.9** | **90.9** |

Table S. 19. Capital cost estimates for plant using wheat straw and 1-stage DME synthesis

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Capacities** | | | | **Grass root costs [M€]** | |
| **Subgroups** | **Unit** | **Required Capacity** | **Number of Units** | **Capacity per unit** | **Unit of Capacity** | **Per unit** | **Per subgroup** |
| Biomass Handling | Conveyors | 5.3 | 1 | 5.3 | t\_wet\_biomass/h | 1.5 | 5.9 |
| Biomass storage | 5.3 | 1 | 5.3 | t\_wet\_biomass/h | 4.5 |
| LT-CFB gasifier | Pyrolysis reactor | 15.2 | 1 | 15.2 | t\_dry\_biomass/h | 42.8 | 60.4 |
| Char reactor | 3.4 | 1 | 3.4 | t\_dry\_biomass/h | 15.0 |
| Char Cyclone | 12.2 | 1 | 12.2 | m^3/s | 1.3 |
| Ash Cyclone | 12.2 | 1 | 12.2 | m^3/s | 1.3 |
| Gas Cleaning | Particle filter | 11.3 | 1 | 11.3 | m^3/s | 10.1 | 13.7 |
| POX reactor | 93.5 | 1 | 93.5 | m^3 | 0.8 |
| RWGS reactor | 437.2 | 1 | 437.2 | m^3 | 2.6 |
| Sulfur removal | 8.0 | 1 | 8.0 | Nm^3/s | 0.2 |
| Turbomachinery | SYN-COM1 | 1237.0 | 1 | 1237.0 | kW | 2.4 | 10.3 |
| SYN-COM2 | 960.0 | 1 | 960.0 | kW | 2.0 |
| SYN-COM3 | 936.0 | 1 | 936.0 | kW | 1.9 |
| SYN-COM4 | 926.0 | 1 | 926.0 | kW | 1.9 |
| SYN-COM5 | 923.0 | 1 | 923.0 | kW | 1.9 |
| REC-COMP | 0.9 | 1 | 0.9 | m^3/s | 0.1 |
| MEOH-PUMP | 4.2 | 1 | 4.2 | kW | 0.1 |
| ELEC-PUMP | 0.0 | 1 | 0.0 | kW | 0.0 |
| H2-REC | 0.0 | 1 | 0.0 | m^3/s | 0.0 |
| Synthesis reactors | DME reactor | 3430.6 | 4 | 857.7 | m^2 | 9.4 | 9.4 |
| Distillation colums | TOP-COL | 10.2 | 1 | 10.2 | m^3 | 0.2 | 0.5 |
| DME-COL | 4.5 | 1 | 4.5 | m^3 | 0.1 |
| MEOH-COL | 5.2 | 1 | 5.2 | m^3 | 0.2 |
| Gas Engine | Gas engine | 1519.0 | 1 | 1519.0 | kW | 1.6 | 1.6 |
| Refrigeration Plant | Refrigeration plant | 3107.0 | 1 | 3107.0 | kW\_Cooling | 6.1 | 6.1 |
| Heat exchanger Network | Heat exchanger | 7359.0 | 55 | 133.8 | m^2 | 17.1 | 17.1 |
| **Total Grassroot costs** | |  |  |  |  | **125.2** | **125.2** |

Table S. 20. Capital cost estimates for plant using bamboo and 2-stage DME synthesis

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Capacities** | | | | **Grass root costs [M€]** | |
| **Subgroups** | **Unit** | **Required Capacity** | **Number of Units** | **Capacity per unit** | **Unit of Capacity** | **Per unit** | **Per subgroup** |
| Biomass Handling | Conveyors | 3.2 | 1 | 3.2 | t\_wet\_biomass/h | 1.0 | 4.2 |
| Biomass storage | 3.2 | 1 | 3.2 | t\_wet\_biomass/h | 3.2 |
| Entrained flow gasifier | Steam Dryer | 2.7 | 1 | 2.7 | t\_Steam/h | 5.5 | 44.3 |
| EF-gasifier | 2.2 | 1 | 2.2 | t\_dry\_biomass/h | 28.3 |
| Pyrolysis reactor | 41.4 | 1 | 41.4 | MW\_dry\_Biomass | 10.0 |
| Grinder | 2.2 | 1 | 2.2 | t\_dry\_biomass/h | 0.5 |
| Cyclone | 0.4 | 1 | 0.4 | m^3/s | 0.1 | 4.2 |
| Gas Cleaning | Particle filter | 0.4 | 1 | 0.4 | m^3/s | 1.2 |
| RWGS reactor | 8.9 | 1 | 8.9 | m^3 | 0.5 |
| Sulfur removal | 7.2 | 1 | 7.2 | Nm^3/s | 0.2 |
| AGR | 17.8 | 1 | 17.8 | kmol\_CO2/h | 2.1 |
| Turbomachinery | H2-COMP | 556.0 | 1 | 556.0 | kW | 1.3 | 4.8 |
| O-COMP | 119.0 | 1 | 119.0 | kW | 0.3 |
| SYN-COM | 832.0 | 1 | 832.0 | kW | 1.8 |
| ELEC-PUMP | 5.5 | 1 | 5.5 | kW | 0.0 |
| MEOH-PUMP | 1.2 | 1 | 1.2 | kW | 0.1 |
| MEOH-PUMP2 | 1.1 | 1 | 1.1 | kW | 0.0 |
| VOL-COMP | 0.2 | 1 | 0.2 | m^3/s | 0.2 |
| REC-COMP | 0.1 | 1 | 0.1 | m^3/s | 0.0 |
| STEAM-COMP | 30.6 | 1 | 30.6 | m^3/s | 0.2 |
| SYN-REC | 0.1 | 1 | 0.1 | m^3/s | 0.4 |
| H2-REC | 0.1 | 1 | 0.1 | m^3/s | 0.5 |
| Synthesis reactors | MeOH reactor | 395.8 | 1 | 395.8 | m^2 | 1.3 | 1.3 |
| DME reactor | 1.7 | 1 | 1.7 | m^3 | 0.1 |
| Distillation colums | TOP-COL | 1.8 | 1 | 1.8 | m^3 | 0.1 | 0.5 |
| DME-COL | 5.9 | 1 | 5.9 | m^3 | 0.2 |
| MEOH-COL | 8.7 | 1 | 8.7 | m^3 | 0.2 |
| Gas Engine | Gas engine | 470.0 | 1 | 470.0 | kW | 0.6 | 0.6 |
| Heat exchanger Network | Heat exchanger | 5774.0 | 52 | 111.0 | m^2 | 14.8 | 14.8 |
| **Total Grassroot costs** | |  |  |  |  | **74.7** | **74.7** |

Table S. 21. Capital cost estimates for plant using bamboo and 1-stage DME synthesis

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Capacities** | | | | **Grass root costs [M€]** | |
| **Subgroups** | **Unit** | **Required Capacity** | **Number of Units** | **Capacity per unit** | **Unit of Capacity** | **Per unit** | **Per subgroup** |
| Biomass Handling | Conveyors | 4.6 | 1 | 4.6 | t\_wet\_biomass/h | 1.3 | 5.4 |
| Biomass storage | 4.6 | 1 | 4.6 | t\_wet\_biomass/h | 4.1 |
| Entrained flow gasifier | Steam Dryer | 3.9 | 1 | 3.9 | t\_Steam/h | 6.8 | 56.4 |
| EF-gasifier | 3.1 | 1 | 3.1 | t\_dry\_biomass/h | 36.5 |
| Pyrolysis reactor | 59.5 | 1 | 59.5 | MW\_dry\_Biomass | 12.4 |
| Grinder | 3.1 | 1 | 3.1 | t\_dry\_biomass/h | 0.6 |
| Gas Cleaning | Cyclone | 0.6 | 1 | 0.6 | m^3/s | 0.2 | 6.9 |
| Particle filter | 0.6 | 1 | 0.6 | m^3/s | 1.5 |
| RWGS reactor | 10.8 | 1 | 10.8 | m^3 | 0.6 |
| Sulfur removal | 7.5 | 1 | 7.5 | Nm^3/s | 0.2 |
| AGR | 53.4 | 1 | 53.4 | kmol\_CO2/h | 4.5 |
| Turbomachinery | H2-COMP | 344.0 | 1 | 344.0 | kW | 0.8 | 2.6 |
|  | O-COMP | 179.0 | 1 | 179.0 | kW | 0.5 |
|  | SYN-COM | 149.0 | 1 | 149.0 | kW | 0.4 |
|  | ELEC-PUMP | 5.5 | 1 | 5.5 | kW | 0.0 |
|  | MEOH-PUMP | 1.3 | 1 | 1.3 | kW | 0.1 |
|  | VOL-COMP | 0.4 | 1 | 0.4 | m^3/s | 0.2 |
|  | REC-COMP | 0.2 | 1 | 0.2 | m^3/s | 0.1 |
|  | STEAM-COMP | 48.4 | 1 | 48.4 | m^3/s | 0.1 |
|  | SYN-REC | 0.2 | 1 | 0.2 | m^3/s | 0.2 |
|  | H2-REC | 0.0 | 1 | 0.0 | m^3/s | 0.1 |
| Synthesis reactors | DME reactor | 1595.9 | 2.0 | 798.0 | m^2 | 4.4 | 4.4 |
| Distillation colums | TOP-COL | 6.4 | 1 | 6.4 | m^3 | 0.2 | 0.4 |
| DME-COL | 4.3 | 1 | 4.3 | m^3 | 0.1 |
| MEOH-COL | 1.8 | 1 | 1.8 | m^3 | 0.1 |
| Gas Engine | Gas engine | 545 | 1 | 545.0 | kW | 0.7 | 0.7 |
| Refrigeration plant | Refrigeration plant | 2320 | 1 | 2320.0 | kW\_Cooling | 5.1 | 5.1 |
| Heat exchanger Network | Heat exchanger | 5463 | 50 | 109.3 | m^2 | 14.1 | 14.1 |
| **Total Grassroot costs** | |  |  |  |  | **96.0** | **96.0** |

1. Calculation of operating costs of DME production plants

The operating costs for the DME production plants were calculated following the method proposed by Turton et al. in Chapter 8 of [1]. Turton et al. use the term “Manufacturing Costs of a Chemical Product” for the operating costs of a plant. There are many factors influencing the operating costs of chemical plants. Table S. 22 lists the influencing factors and the formulas and values for their calculation as proposed by Turton et al [1].

Table S. 22. Factors influencing the operating costs, and typical ranges and average values for multiplying factors

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Cost item** | **Symbol** | **Formula a** | **Multiplying factor b** | | |
|  |  |  | **Lower range limit** | **Average** | **Higher range limit** |
| **1. Direct Manufacturing Costs** |  |  |  |  |  |
| a. Raw material |  |  |  |  |  |
| b. Waste treatment |  |  |  |  |  |
| c. Utilities |  |  |  |  |  |
| d. Operating labor |  |  |  |  |  |
| e. Direct supervisory and clerical labor |  |  | 0.1 | 0.18 | 0.25 |
| f. Maintenance and repairs |  |  | 0.02 | 0.06 | 0.1 |
| g. Operating supplies |  |  | 0.002 | 0.009 | 0.02 |
| h. Laboratory charges |  |  | 0.1 | 0.15 | 0.2 |
| i. Patents and royalties |  |  | 0 | 0.03 | 0.06 |
| **2. Fixed manufacturing Costs** |  |  |  |  |  |
| a. Depreciation c |  |  | 0.1 | 0.1 | 0.1 |
| b. Local taxes and insurance |  |  | 0.014 | 0.032 | 0.05 |
| c. Plant overhead costs |  |  | 0.55 / 0.01 | 0.708 / 0.036 | 0.875 / 0.07 |
| **3. General manufacturing Expenses** |  |  |  |  |  |
| a. Administration costs |  |  | 0.165 / 0.01 | 0.177 / 0.009 | 0.1875 / 0.07 |
| b. Distribution and selling costs |  |  | 0.02 | 0.11 | 0.2 |
| c. Research and development |  |  | 0.05 | 0.05 | 0.05 |

a In line 1f, 1g, 2a, 2b, 2c and 3a, Turton et al. use the fixed capital invest (FCI), which can be either the total module cost () or the grassroot cost (). In this work we used a conservative approach of using , leading to higher operating costs

b Some of the multiplying factors shown are not explicitly given in Table 8.2 of [1] and were derived from the given information for a clearer overview.

c In Table 8.2 of [1], an arbitrary multiplying factor of 0.1 was given for the depreciation. This value should be used carefully. In chapter 9 of [1], Turton et al. describe methods for calculating the depreciation costs in detail.

In this work, the operating costs are divided into fixed and variable operating costs. The fixed operating costs are connected to the size of the plant, while the variable operating costs are connected to the amount of produced DME in the plants. In the following sections, the distinction is further explained, and the calculation of the costs is described.

**Note**: In this part of the work, the electricity consumption was not considered as the cost estimation for the electricity generation from renewables was part of the last step of this work, explained in chapter S5

* 1. Calculation of fixed operating costs

The fixed operating costs were defined as the yearly expenses which are not connected to the raw materials, waste treatment and utilities, namely the expenses 1d. – 1i., 2. and 3. from Table S. 22. Additionally, the cost for the catalyst in the methanol and DME reactors were added. Hence, the fixed operating costs can be calculated using eq. (37).

|  |  |
| --- | --- |
|  | (37) |

denotes the grassroot costs as described in chapter S3. The factor for the grassroot cost and the operating labour can be derived from the values given in Table S. 22. The values for using the values for the lower limit, average and higher limit of the range are shown in Table S. 23.

Table S. 23. Ranges of factors used in eq. (37).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | | |  | | |
| **Low** | **Average** | **High** | **Low** | **Average** | **High** |
| 0.06 | 0.18 | 0.45 | 2.06 | 2.73 | 3.64 |

denotes the cost of operating labour. was estimated using the method presented by Alkhayat and Gerrard [7] and reproduced in [1]. The cost of operating labour depends on the number of operators employed for the chemical plant. The number of operators per shift es estimated using eq. (38).

|  |  |
| --- | --- |
|  | (38) |

Where is the number of processing steps involving handling of particulate solids and denotes the number of nonparticulate processing steps, including compression, heating and cooling, mixing and reactions. Following the approach of Turton et al. [1], the number of P was assumed to be zero and is counted as

|  |  |
| --- | --- |
|  | (39) |

The number of operators needed in total in order to ensure continuous operation throughout the whole year is estimated under certain assumption [1] to be calculated with eq. (40)

|  |  |
| --- | --- |
|  | (40) |

The cost of operating labor was then calculated assuming an average salary of a chemical plant and system operator of $ 80 000 for the year 2022[8].

|  |  |
| --- | --- |
|  | (41) |

Lastly, the cost associated with the first filling of the methanol and DME reactors and exchange of used catalyst was calculated. The cost for the first filling was calculated using eq. (42).

|  |  |
| --- | --- |
|  | (42) |

Where denotes the reactor volume as calculated with eq. (43) and denotes the bulk density. Th bulk density was assumed to be equal for all used catalysts. The weight specific cost of the different catalysts are shown in Table S. 24. The prices was updated to the year 2022 using the CEPCI data shown in Table S.4.

|  |  |
| --- | --- |
|  | (43) |

Table S. 24. Catalyst price and expected lifetime for the catalysts used in the different DME production plants

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Reactor** | **Catalyst** |  | **Expected Catalyst lifetime**  **[years]** | **Reference** |
| Methanol synthesis | Cu-ZnO-Al2O3 | 9.69 |  | [9] |
| Methanol dehydration (indirect DME synthesis) | γ-Al2O3 | 10.30 |  | [9] |
| Direct DME synthesis | Cu-ZnO-Al2O3/γ-Al2O3 | 10.30 |  | -a |

a No comparable price and lifetime data were found for the bifunctional catalyst used for the direct DME synthesis. It was decided to use the same data as for the methanol dehydration catalyst, as it had the higher price than the methanol synthesis catalyst.

Based on the catalyst lifetime of four years and an assumed plant lifetime of 25 years, the catalyst needs to be exchanged six times over the plant lifetime after the first filling. Hence, a total number of seven fillings is required over the lifetime of the plant. Assuming that the catalyst price remains unchanged over the plant lifetime, the yearly cost for the catalyst was calculated with eq. (44)

|  |  |
| --- | --- |
|  | (44) |

* 1. Calculation of variable operating costs

The variable operating costs consist of the biomass cost , the cooling water cost and the revenue from selling bio-char .

|  |  |
| --- | --- |
|  | (45) |

The cost of biomass was calculated using eq. (46) with the biomass mass flow (S1) from the tables in chapter S1 and the biomass cost shown in Table S. 25.

|  |  |
| --- | --- |
|  | (46) |

Table S. 25. Biomass cost used in this work

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Wheat straw [€/GJ]**a[10] | | | **Bamboo [$/t]** | | |
| **Low cost** | **Base cost** | **High cost** | **Low cost** | **Base cost** | **High cost** |
| 5.0 | 6.4 | 9.1 | 100 | 150 | 200 |

a In order to the straw price in €/t, the above mentioned price was multiplied by the higher heating value of 14.5 GJ/t as used in the reference by Bang et al. [10]

The revenue from bio-char was calculated, assuming that the only revenue is achieved from CO2-certificate. Assuming an CO2 price of , the revenue was calculated with eq. (47).

|  |  |
| --- | --- |
|  | (47) |

For the plants using bamboo as feedstock, , as there is no bio-char production. For the plants using wheat straw as feedstock, is taken from the results in chapter S1 and the carbon content in the char is for both plants. The factor of denotes the weight ratio between carbon dioxide and pure carbon.

The cost for cooling water was calculated using eq. (48)

|  |  |
| --- | --- |
|  | (48) |

The cost of high-purity water for process use proposed by Turton et al [1] were used as specific cost for cooling water. The cooling water mass flow was calculated using eq. (49).

|  |  |
| --- | --- |
|  | (49) |

Where is the cooling water demand derived in chapter S2, is the heat released from the refrigeration plant as calculated with eq. (25), is the specific heat capacity and and are the inlet and outlet temperature of cooling water.

* 1. Operating cost estimates for the investigated DME plants

In the following tables, the results for the calculation of the fixed operating cost are shown. Based on the results shown in Table S. 26 it was decided to use the results obtained for the lower range of the factors in Table S. 23. The reason for this is that fixed operating costs corresponding to around 8 % to 10 % of the fixed capital investment, the result is much closer to the range of values used in other literature (e.g. [3,5,9], where usually values like 3% to 5 % of the fixed capital investment are assumed for operation and maintenance cost.

Table S. 26. Estimated fixed operating cost for the four plants, using the low, average and high values shown in Table S. 23. In addition to the absolute values, the relative value to the grassroot costs shown in Table S. 18-Table S. 21 are given for better comparison to other literature.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | |
|  | **Low** | | **Average** | | **High** | |
|  |  |  |  |  |  |  |
| **Wheat, 2-stage** | 9.2 | 9.6% | 21.8 | 22.8% | 49.2 | 51.4% |
| **Wheat, 1-stage** | 11.4 | 8.7% | 28.4 | 21.5% | 65.5 | 49.7% |
| **Bamboo, 2-stage** | 8.2 | 10.4% | 18.8 | 23.8% | 41.5 | 52.8% |
| **Bamboo, 1-stage** | 9.6 | 9.5% | 22.8 | 22.6% | 51.6 | 51.1% |

The results for the catalyst cost in Table S. 27, show that the importance of the catalyst price is very small compared to the overall fixed operating costs shown in Table S. 26

Table S. 27. Yearly cost associated with the filling an exchange of catalyst.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Methanol synthesis** | **Methanol dehydration** | **DME synthesis** | **Unit** |
| **Wheat, 2-stage** | 13513 | 4796 | - | $/year |
| **Wheat, 1-stage** | - | - | 72280 |
| **Bamboo, 2-stage** | 7846 | 3493 |  |
| **Bamboo, 1-stage** | - | - | 33625 |



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