

Journal Name

ARTICLE

Bio-electrochemical Conversion of Industrial Wastewater combined with downstream Methanol Synthesis – Economic- and Life Cycle Assessment

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Electronic Supplementary Information

S1 Variable List

Descriptor	Full Name	Unit
A_E	Electrode Surface Area, MEC system	m^2
B_n	Revenues in year n	€
CD	Current Density	mA/cm^2 , A/m^2
CH_3OH_{mol}	Molar CH_3OH Flow	mol/s
CH_4-LN	Methane Input (Standard Litres)	L_N
CH_4-LHV	Methane Lower Heating Value	kWh/Nm^3
C_n	Operational costs in year n	€
COD	Chemical Oxygen Demand	g

$COD_{Acetate}$ in Biomass	Bacterial biomass expressed as acetate COD	g
COD_{ox}	COD oxidized to CO_2	g
COD_r	COD removal rate	%
COD_{mol}	COD molar flow in wastewater	mol/s
ΔCOD_{mol}	COD molar flow in wastewater that is oxidized in MEC	mol/s
$CO_{2,mol}$	Molar CO_2 Flow	mol/s
$CO_{2,Biomass\ spec}$	Carbon dioxide emissions per gram biomass	g
$CO_{2, Wastewater\ COD}$	Carbon dioxide emissions from wastewater COD oxidation	g
$CO_{2, Sludge}$	Carbon dioxide emissions from sludge digestion	g
DM	Dry Matter	kg
E_n	Savings of wastewater treatment fees	€
ES	Excess Sludge	kg
e^-	Electron	
\dot{e}	Actual electron flow from substrate	$electrons/s$
\dot{e}_{pot}	potential electron flow from substrate	$electrons/s$
$\dot{H}_{2,mol}$	H_2 molar flow	mol/s
I_{MEC}	MEC Current	A, kA
I_0	Investment costs in year 0	€
M_n	Methanol production in year n	tonnes
MPC	Methanol Production Costs	€/t _{CH₃OH}
$M_{Biomass}$	Molar weight of biomass	g/mol

M_{CO_2}	Molar weight of carbon dioxide	g/mol
M_{O_2}	Molar weight of oxygen	g/mol
N_A	Avogadro's Number	mol^{-1}
NPV	Net Present Value	€
oDM	Organic Dry Matter	kg
r	Discount rate	
q_e	Elementary Charge	Coulomb [C]
U_{Cell}	MEC Cell Voltage	mV
V_s	MEC System Volume	m^3
V_{Cell}	MEC Cell Volume	m^3
W_{el}	Electric Production	kWh
Y_{CH_4}	Methane Yield	Nm^3
$\Delta COD_{Acetate}$	Removed wastewater COD	g

$\Delta\text{COD}_{\text{mol}}$	Removed wastewater COD (molar)	mol
ΔoDM	Fraction of oDM digested during anaerobic process	kg
$\Delta\text{m}_{\text{Biomass}}$	Bacterial biomass metabolized in anaerobic digester	g
η_{CE}	Coulomb Efficiency	
η_{CCE}	Cathodic Conversion Efficiency	
$\eta_{\text{electrical}}$	Electrical Efficiency of CHP	

S2 Estimation of linearized MEC Polarization Curve

For the calculation of the MEC electricity demand a linearized polarization curve has been constructed based on anodic and cathodic half-cell polarization curves from literature.

In case of the anode, a polarization curve recorded with *Geobacter sulfurreducens* (using carbon electrodes) and an acetate-based medium has been considered.¹ The experimental curve has been linearized and extrapolated to a maximum current density (CD) of 2 mA/cm². Furthermore, to account for a possibly reduced performance of a mixed consortium it has been shifted towards more positive values by 50 mV. Regarding the cathode, published polarization data of MoS₂-based hydrogen evolution cathodes

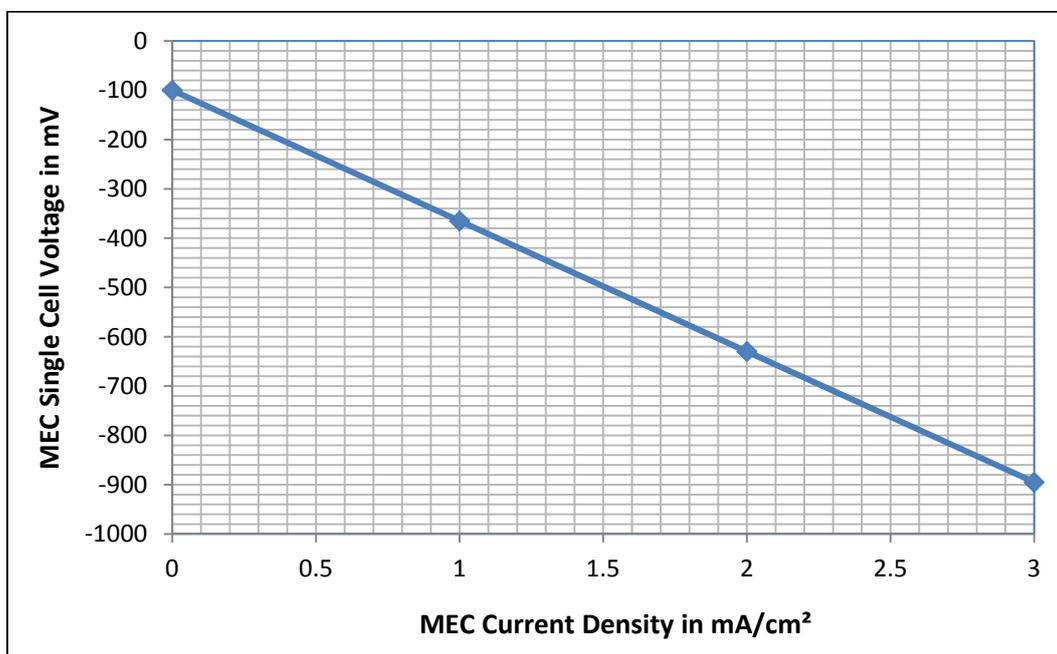
operated in acidic waste water (originating from chemical production processes) have been considered.²

For linearization, the onset overpotential (approx. open circuit potential; -120 mV vs. RHE) and the approximate overpotential at a current density of 2 mA/cm² (~ -350 mV vs. RHE) available from linear sweep experiments were taken into account. This approximation can be regarded as conservative estimate, since in long-term experiments at constant current density the MoS₂-cathodes exhibited a noticeable improved performance, as reported in the cited paper. Constructed from the individual half-cell curves the linearized overall MEC polarization curve follows the relation as depicted in the following equation (Eq. S1).

$$U_{\text{cell}} = -265 \frac{\text{mV}}{\text{mA}/\text{cm}^2} * \text{CD} - 100 \text{ mV} \quad \text{Eq. S1}$$

With U_{cell} = MEC cell voltage, CD = MEC current density

Figure S1: Linearized polarization curve for the wastewater MEC of the BioMethanol System.



S3 Process Data for Methanol Synthesis from CHEMCAD

Table S1: Additional parameters of the CHEMCAD simulation of methanol synthesis plant.

Parameter	Value
Feed Reactor 1 [Nm ³ /h]	164.4
Feed Reactor 2 [Nm ³ /h]	109.7
CO ₂ +CO Conversion Efficiency per pass, Reactor 1 / Reactor 2	22% / 13%
Recycling Rate, mass (Recycle/Feed)	2.1

S4 Excess Sludge Formation in MEC and WWTP

Table S2: Input values for the calculation of sewage sludge formation in microbial electrolysis and activated sludge process according to Teichgräber *et al.*^{3 a} info of industrial operator, ^b value was chosen, so that sludge age does not affect sludge formation, ^c for 60% COD degradation in microbial electrolysis, ^d maximum value of source

Item	AS	MEC
Biomass yield [gCOD _{Biomass} /gCOD _{degraded}]	0.67 ³	0.05 ⁴
Decay coefficient [d ⁻¹]	0.17 ³	0.17 ³
Temperature [°C]	12 ⁵	30 ^a
Sludge age [d]	9 ⁵	1 ^b
Influent COD [mg/L]	3,900	-
Degradable COD	-	2,340 ^c
Dry matter content of excess sludge [%]	1 ^{6,d}	

The sludge formation in the wastewater treatment plant and the microbial electrolysis cell system has been estimated via a method described by Teichgräber *et al.*³ We did not have access to the report so that the methodology, as cited by Hiegemann *et al.*⁵ is shown. In the project industrial wastewater flow no particulate COD was present, so that in turn the calculations only considered soluble COD. Calculations according to **Error! Reference source not found.** to Eq. S8. For the calculations of MEC sludge formation, the metabolised COD has been inserted as degradable COD ($C_{COD,deg,ZB}$). Furthermore, the inert soluble COD in the influent ($S_{COD,inert,ZB}$) has not been considered. Otherwise the method was conducted as described using the values in **Error! Reference source not found.**:

- Inert particulate COD in the influent $X_{COD,inert,ZB}$ [mg/L]: $C_{COD,ZB}$ = COD influent concentration

$$X_{COD,inert,ZB} = 0.3 * (C_{COD,ZB} - S_{COD,ZB}) \quad \text{Eq. S2}$$

- Inert soluble COD in the influent of activated sludge process $S_{COD,inert,ZB}$ [mg/L]:

$$S_{COD,inert,ZB} = 0.05 * C_{COD,ZB} \quad \text{Eq. S3}$$

- Degradable COD, $C_{COD,deg,ZB}$ [mg/L]: $X_{COD,inert,ZB}$ =

$$C_{COD,deg,ZB} = C_{COD,ZB} - S_{COD,inert,ZB} - X_{COD,inert,ZB} \quad \text{Eq. S4}$$

- Temperature factor for endogenous respiration, F_t :

$$F_t = 1.072^{(T-15)} \quad \text{Eq. S5}$$

- Produced biomass, $X_{COD,BM}$ [mg/L]: Y = growth yield, b = decay rate, t_{TSS} = sludge age [d]

$$X_{COD,BM} = C_{COD,deg,ZB} * Y * ((1/(1 + b * t_{TSS} * F_t))) \quad \text{Eq. S6}$$

- Inert COD of Biomass, $X_{COD,inert,BM}$ [mg/L]

$$X_{COD,inert,BM} = 0.2 * X_{COD,BM} * t_{TSS} * b * F_t \quad \text{Eq. S7}$$

- Daily excess sludge production, ES_{d,C} [kg TSS/d]

$$ES_{d,C} = Q_d * \left(\frac{X_{COD, inert, ZB}}{1.33} + \frac{X_{COD, BM} + X_{COD, inert, BM}}{0.92 * 1.42} + X_{inorg, TSS, ZB} \right) / 1000 \quad \text{Eq. S8}$$

S5 Anaerobic Digestion of Sewage Sludge

Table S3: Input values for the calculation of biogas formation in anaerobic sludge digestions. ^a Cornel *et al.* (2006) as cited in indicated source, ^b German Association for Water, Wastewater and Waste as cited in listed source, Y_{CH_4} = methane yield, $COD_{degraded}$ =chemical oxygen demand which is degraded in anaerobic digestion, $COD_{Biomass}$ = specific COD of one unit of biomass, oDM = organic dry matter, DM = dry matter, $oDM_{degraded}$ = oDM degraded in anaerobic digestion

Parameter	Value	Unit
CH ₄ per $COD_{degraded}$ (Y_{CH_4}/COD)	350 ^{7,8, a}	Nm ³ / t COD
COD in biomass (COD/oDM)	1.42 ³	kg COD/ kg oDM
oDM per DM (oDM/DM)	70 ^{8,9,b}	%
oDM _{degraded} (ΔoDM)	50 ⁸	%
Sludge concentration in	1.5	%
Sludge concentration out	3	%

For the anaerobic digestion of sewage sludge, the process parameters and outputs have been calculated using the values in S4 Excess Sludge Formation in MEC and WWTP

Table S2: Input values for the calculation of sewage sludge formation in microbial electrolysis and activated sludge process according to Teichgräber *et al.*^{3 a} info of industrial operator, ^b value was chosen, so that sludge age does not affect sludge formation, ^c for 60% COD degradation in microbial electrolysis, ^d maximum value of source

Item	AS	MEC
Biomass yield [gCODBiomass/gCODdegraded]	0.673	0.054
Decay coefficient [d-1]	0.173	0.173
Temperature [°C]	125	30a
Sludge age [d]	95	1b
Influent COD [mg/L]	3,900	-
Degradable COD	-	2,340c
Dry matter content of excess sludge [%]	16,d	

The sludge mass after anaerobic digestion was calculated via Eq. S9:

$$DM_{out} = \text{Sludge } DM_{in} - (DM_{in} \times oDM/DM \times \Delta oDM) \quad \text{Eq. S9}$$

With DM = dry matter, oDM = organic dry matter

S6 Wastewater Treatment Plant Reference System: Allocation of Aeration Electricity

In the activated sludge process of wastewater treatment, aeration is required for the oxidation of both, COD and TN, resulting in an electricity demand for an air pump (0.2 kWh/kg $COD_{removed}$).¹⁰ The mentioned electricity demand is for the oxidation of both, COD and TN. In contrast, during microbial electrolysis, primarily COD is removed. In the LCA of the *BioMethanol* System, the MEC receives a credit from the substitution of COD treatment in the activated

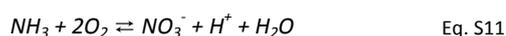
sludge process of conventional wastewater treatment. In order to determine the electricity demand for isolated COD- and TN-treatment in the activated sludge process, allocation is required. This has been performed via partitioning allocation based on the oxygen consumption of COD and TN during treatment. For the COD, the calculation is straight forward, as it directly represents oxygen demand (Eq. S10). However, attention needs to be paid to one detail: the bacterial sludge grows on wastewater carbon which constitutes a certain amount of COD per carbon atom. In the process of bacterial growth, the oxidation state of wastewater

carbon is altered by incorporation into bacterial biomass (and thereby also the COD per carbon atom). Therefore the COD of the bacterial biomass is unequal the COD that has been removed from wastewater for bacterial biomass build-up and cannot be directly subtracted in Eq. S10. In turn, to figure out the COD removed by bacterial growth, a factor is applied to convert the COD of bacterial biomass to acetate COD (acetate is considered to constitute wastewater COD). The factor is based on the COD per carbon atom relation in acetate and bacterial biomass ($(\text{CH}_{1.8}\text{O}_{0.5}\text{N}_{0.2})_n$; $M = 24.6 \text{ g/mol}$; ¹¹). For the COD of biomass an average value from Teichgräber et al. ³ has been assumed ($1.42 \text{ g(COD)/g(biomass)}^3$).

$$O_2 = \text{COD}_{\text{Carbon}} = \text{COD}_{\text{Acetate in}} \times \text{COD}_r - \text{COD}_{\text{Acetate_Biomass}} \quad \text{Eq. S10}$$

With O_2 = oxygen demand, $\text{COD}_{\text{Carbon}}$ = chemical oxygen demand from carbon atoms, $\text{COD}_{\text{Acetate in}}$ = acetate COD influent, COD_r = COD removal rate, $\text{COD}_{\text{Acetate_Biomass}}$ = acetate COD that is taken up by biomass growth

The oxygen required for biological TN oxidation is consumed to convert ammonia (assumed to constitute all nitrogen in wastewater) to nitrate (Eq. S11-Eq. S13). For the calculations the nitrogen content of biomass was assumed to be 7%. ³



$$O_2 = \text{TN}_{\text{metabolized}} / M_N \times 2 \times M_{\text{O}_2} \quad \text{Eq. S12}$$

$$\text{TN}_{\text{metabolized}} = \text{TN}_{\text{in}} - \text{TN}_r - \text{TN}_{\text{Biomass}} \quad \text{Eq. S13}$$

With $\text{TN}_{\text{metabolized}}$ = the TN that is oxidized to NO_3^- , 2 = 2 moles of O_2 per mole of NH_3 , M_N = molar mass of nitrogen, M_{O_2} = molar mass of molecular oxygen, TN_{in} = TN influent, TN_r = TN removal rate, $\text{TN}_{\text{Biomass}}$ = TN taken up by bacterial growth

S7 Calculation of hardware requirements

MEC Electrodes

The electrode material demand has been calculated according to the experimental design of Kokko *et al.* ² and the electrode surface of the *BioMethanol* System MEC (cf. main paper). For molybdenum, the required mass has been calculated according to the weight percentage in molybdenum sulfide.

MEC Membrane

The membrane material demand for different membrane options has been estimated by Eq. S14 using values from Table S4.

$$m_{\text{material}} = \rho_{\text{material}} * d_{\text{membrane}} * A_{\text{membrane}} \quad \text{Eq. S14}$$

With m_{material} = membrane material mass, ρ_{membrane} = membrane material density, d_{membrane} = membrane thickness, A_{membrane} = MEA surface

MEC Housing & Current Collectors

The material needs for MEC housing were estimated based on a lab scale MEC in flat-plate design. Per cell, two endplates made from 2.5 mm thick polypropylene sheets with a total weight of $5 \text{ kg/m}^2_{\text{MEA}}$ have been considered. Furthermore, each cell is equipped with two current collector meshes (80% open area) made

either from 650 μm stainless steel (V2A) or 550 μm copper, corresponding to 2 kg of current collector material per m^2_{MEA} .

MEC Power Electronics

The weight of the power electronics is 500 kg/10kA, as stated in the product datasheets. ¹² In the LCA, the power electronics have been modelled with the Ecoinvent processes “market for inverter, 2.5 kW [GLO]” and “market for transformer [GLO]”. The inverter process gives an output according to power [kW], while the transformer process gives an output in mass [kg]. To depict the hardware needs of the MEC power electronics, the product mass of the inverter process “market for inverter, 2.5 kW [GLO]” to cater for 45 kW electrolysis (plus little extra) have been calculated. The rectifier mass has been subtracted from the expected total mass. The remainder was modelled as the material demand for the process “market for transformer [GLO]”.

Gas Cleaning

The requirements for gas cleaning have been modelled in orientation to supplier data for activated carbon filters for biogas plants. ¹³ According to the supplier, the consumption of activated carbon shows a linear dependency on volumetric flow and the respective H_2S -impurities. The base data was: 50 kg/month at a volumetric flow of 120 m^3/h and 200 ppm. Accordingly, the activated carbon consumption has been calculated for the volumetric flow of the MEC output gases. Furthermore, the electricity consumption of a ventilator was estimated (15-21 kWh/a).

Biogas Plant & Sludge Press

The material needs for the construction of the biogas plant & sludge press have been calculated from the inventory of Foley *et al.* ¹⁴ with applications of different capacity. The material demand from the reference was scaled:

- 1) For the biogas plant according to necessary surface area. Therefore the required plant volume for the *BioMethanol* System was calculated by multiplying excess sludge output per day with sludge retention of 25 days. The surface area was then calculated assuming a cylindrical body of 10 m height.
- 2) The sludge press was scaled according to the sludge output per day (using the average value in reference).

Methanol Plant: Reactor, Heat Exchanger, Distillation, Catalyst

The required catalyst mass for methanol synthesis was calculated via catalyst volume. Volume was calculated by Eq. S15. The feed gas volume was obtained from CHEMCAD simulation (Table S1). A standard GHSV of 10,000^{-d} and catalyst density of 1.2 kg/L were

applied.¹⁵ Furthermore, the catalyst volume was assumed to be 80% of reactor volume. Catalyst composition was assumed to be 68 wt% CuO, 23 wt% ZnO and 9 wt% Al₂O₃ in orientation to Ref.¹⁵

$$GHSV = \frac{V_{cat}}{V_{gas}} \quad \text{Eq. S15}$$

With GHSV= gas hourly space velocity, V_{cat}=volume of the catalyst, V_{gas}=volume flow of the feed-gas in Nm³

The heat exchanger surface necessary for heat integration of synthesis and distillation was estimated from CHEMCAD data and resulted in 7.3 m² surface area. The material requirements of the reactors and distillation have not been specified. For the economic assessment the costs were taken into account via supplier data and cost functions (cf. S8). For LCA, the dataset "market for methanol factory [GLO]" from Ecoinvent v. 3.4 has been considered.

Sludge & Wastewater Pumps

Table S4: Input values for the calculation of material needs for the microbial electrolysis cell membrane. ^aassumption based on membrane used by project partners fumasep® FAA-3-PK-130

Material	Density [g/cm ³]	Weight[g/cm ²]	Thickness [μm]
Nafion/PTFE ¹⁷	-	43	22
Polysulfone ¹⁸	1.24	-	130 ^a

Table S5: Parameters for the calculation of required wastewater- & sludge pump capacity for the microbial electrolysis cell system. ^aaverage of source

Parameter	Foley et al., 2010 ¹⁴	BioMethanol
Wastewater stream [m ³ /d]	2,200	950
COD conc. [mg/L]	4,000	3,900
Wastewater pump [kW]	11	4.75
Sludge after press [t/d]	6.65 ^a	0.144
Sludge pump [kW]	15	0.3

S8 Details on Prices, Costs & Revenues

The currency exchange rates that have been used can be found in Table S6.

Table S6: Currency exchange rate from Euro to Dollar for the years 2005-2016¹⁹

Year	Euro [€] in Dollar [\$]
2005	1.244
2006	1.256
2007	1.371
2008	1.471
2009	1.395
2010	1.326

For the calculation of the capacity of wastewater- & sludge pumps for the microbial electrolysis cell, the equations Eq. S16 & Eq. S17 and values in

Table S5 have been used. For both pumps the calculated pump capacity has been increased to an available pump size of a 5.5 kW.¹⁶ The operation time of the sludge pump has been assumed to be 1h per week or 52 hours per year in orientation to Foley et al.¹⁴.

$$P_{WWPump} = \frac{P_{WWPump_Foley}}{V_{Foley}} * V_{BioMethanol} \quad \text{Eq. S16}$$

$$P_{SludgePump} = \frac{P_{SludgePump_Foley}}{\dot{m}_{Sludge_Foley}} * \dot{m}_{sludge_BioMethanol} \quad \text{Eq. S17}$$

With P_{X-Pump}= pump capacity of pump X, P_{X-Pump-Foley}= pump capacity in Foley et al.¹⁴ for pump X, V_{Foley}= wastewater volume flow in Foley et al.¹⁴, V_{BioMethanol}= wastewater volume flow in BioMethanol system, \dot{m}_{sludge_Foley} = sludge mass flow in in Foley et al.¹⁴, $\dot{m}_{sludge_BioMethanol}$ = sludge mass flow in BioMethanol system

2011	1.392
2012	1.285
2013	1.328
2014	1.329
2015	1.11
2016	1.107

Investment Cost Factors

For the microbial electrolysis cell system and methanol synthesis + distillation the cost factors described in Table S7 have been applied. The abbreviations listed in the table are used in the following cost formulae. A contingency factor of 10% has been applied to total investment.

Table S7: Cost factors topped up on system costs. MEC=microbial electrolysis cell, ^a internal information from course on cost estimation by German DECHEMA ^c assumed safety factor

Other factors	Price	Note
Piping + measurement & control (<i>pmc</i>)	1.75 ²⁰	Factored on reactor costs (MEC), and total material costs (methanol synthesis)
Installation (<i>i</i>)	1.15 ²⁰	Factored on total investment
Planning (<i>p</i>)	1.08 ^a	Factored on total investment
Contingency (<i>c</i>)	1.1 ^c	Safety factor, factored on total investment

Investment Costs for Microbial Electrolysis Cell System

The cost details for the calculation of microbial electrolysis investment costs can be found in Table S8. On top of the reactor costs the factors for piping and measurement and control as specified in Table S7 have been applied.

Table S8: Cost details for the components of the microbial electrolysis cell system, as considered in the *BioMethanol* System. MEA=Membrane electrode assembly; MEC=microbial electrolysis cell

MEA	Price [€/m ²]	Note
MEA price moderate ²¹	100	Estimate for production of >30.000 m ²
MEA price optimistic ²²	7	In orientation to cost goal of source
MEA costs = MEA price x MEC electrode surface		(Eq. S18)
MEC Reactor Component	Price/Factor	Note
Polypropylene Endplates (<i>E</i>)	5.5 €/m ² _{MEA}	5 kg _{Polypropylene} /m ² _{MEA} ²³
Current collector steel (<i>CC</i>)	3.5 €/m ² _{MEA}	2 kg _{Steel} /m ² _{MEA} (cf. A6) with a cost of 1.75 €/kg _{Steel} in orientation to manufactured V2A steel products ²⁴

Current collector copper (CC)	10 €/m ² _{MEA}	2 kg _{Copper} /m ² _{MEA} (cf. A6) with a cost of 5 €/kg _{Steel} in orientation to copper raw material price ²⁵
Factor for manufacturing ²⁶ (f1)	1.25x	manufacturing and profit for endplates and current collectors
MEC reactor costs = (E + CC) x MEC electrode surface x f1		(Eq. S19)
MEC Assembly Component	Price/Factor	Note
Wastewater pump ¹⁶ (P1)	4,300 €	Per pump 5,5 kW
Sludge pump ¹⁶ (P2)		
Rectifier & transformer ¹² (R1)	287,000 €	For 130 kA capacity
MEC reactor & assembly costs = [(MEC reactor costs x pmc) + P1 + P2 + R1] x i x p		(Eq. S20)

Investment Costs for Gas Cleaning

Table S9: Cost details for the components of gas cleaning considered in the *BioMethanol* System.

Gas Cleaning	Price	Note
Activated Carbon ¹³	3€/kg	50 kg/month @ 120 m ³ /h, 200 ppm H ₂ S
Activated Carbon Container ¹³	11,000€	500 kg capacity for consumption of 50 kg/month; scaled by six-tenth power rule according to monthly consumption
Activated Carbon Costs = 3€/kg * [(50 kg*month ⁻¹ / 120m ³ /h x 200 ppm H ₂ S)* (Volumetric Flow*H ₂ S content)]*(8,500h/8760h)		
Activated Carbon Container = 11,000€ * (Activated Carbon Consumption/50 kg*month ⁻¹)^(2/3)		

Investment Costs for Compressors

The costs for compression are based on vendor requests at a different capacity and listed in Table S10.

Table S10: Cost details of the components of compression and methanol synthesis considered in the *BioMethanol* system.

Compressor	Request	Final price	Note
H ₂	45,000 ²⁷ € (2 stages, 2.5 kW)	53,800 € (4 stages, 8.7 kW)	Scaling by six tenth power rule, 25% top up from two to four stage compressor assumed
CO ₂	18,000 ²⁷ € (2 stages, 9,2 kW)	38,300 € (4 stages, 2.9 kW)	
CO ₂	18.000 ²⁷ € (2 stages, 9,2 kW)	34,800 € (2 stages, 3.5 kW)	Scaling by six tenth power rule
Recirculation	25,000 ²⁷ € (2.7 kW)	7,600 € (0.45 kW)	
New price = Old price x (new capacity/old capacity) ^(2/3) x 25% top up for stage difference			(Eq. S21)

Investment Costs for Methanol Synthesis & Distillation

Table S11: Cost details of components of methanol synthesis & distillation considered in the *BioMethanol* System.

Component	Request	Final price	Note
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Reactor ²⁸	5,000 € (64.7 L)	1,500 € & 2,000 €	Scaling by six tenth power rule, new reactor sizes 11 & 16.4 L
Heat exchanger ^{29,30}	-	6,500 €	Scaling by six tenth power rule, CEPCI & currency exchange applied; from the publications the following values have been used 32.800 \$/80m ² // 30.000\$/112.5m ²
New price reactor = Old price x (new volume/ old volume) ^(2/3)			(Eq. S22)
New price heat exchanger = [price from source x (surface / surface in source) ^(2/3)] /CEPCI ₁₀ * CEPCI ₁₁			(Eq. S23)
Component			
Price		Note	
Methanol reactor fittings (<i>fc</i>)	5,000 €	Assumption	
Methanol synthesis catalyst	100 €/kg	In source 2.5 kg 150€/kg ³¹ ; assumption: price drops for more purchase	
Distillation column	13,700 €	1.6 x reactor costs ³²	
Catalyst costs = catalyst mass x catalyst price			(Eq. S24)
Distillation column costs = 1.6 x (methanol synthesis reactor costs + <i>fc</i>)			(Eq. S25)

Operational Expenses

The operational expenses have been calculated according to the values in Table S12. Electricity prices varied with each market scenario as specified in the main paper.

Table S12: Cost details for operational costs of the BioMethanol system.

Product	Price	Note
CO ₂ Purchase	100 €/t	Compromise of source values, CO ₂ ^{33–35}
CO ₂ Storage Tank Rent	10,000 €/a	Assumption based on request at Linde Gas AG. ³³ For reduced CO ₂ demand a linear price decrease assumed
CO ₂ purchase costs = CO ₂ demand x (100% - CO ₂ from MEC) * specific CO ₂ purchase price		(Eq. S26)
CO ₂ storage costs = 10,000 € * (100% - CO ₂ from MEC)		(Eq. S27)
Maintenance & Insurance ²⁰	4.5 %/a	Of system investment costs
Maintenance & insurance costs = total investment x 4.5%		(Eq. S28)
Staff	26,000 €/a	2 h/d á 50€/h, 5 days per week, 52 weeks/a ¹⁰
MEA cost degression ³⁶ (<i>d</i>)	4 %/a	Assumption: every 5 years MEA needs to be exchanged
MEA cost (year t) = MEA costs (year=0) x (1- <i>d</i>) ^t		(Eq. S29)
Sludge press ⁶	9.5 €/t sludge	Average value of source for mobile sludge press
Sludge transport ³⁷	21.4 €/m ³	-
Sludge treatment ³⁸	89.3 €/t	Costs at dry matter content of 27.5%
Sludge Disposal Costs = Sludge volume/mass x specific treatment costs (press, transport, treatment)		(Eq. 30)

Revenues

The prices and formula that were used for the calculation of the *BioMethanol* System revenues are illustrated in Table S13.

Table S13: Details on BioMethanol system revenues.

Item	Price	Note
WW savings ³⁹	0.35 €/m ³	COD removal of 60% and a nitrogen removal of 7% of organic excess sludge
Methanol	400/560/650 €/t	Assumed prices based on historic development ⁴⁰

H_2^{26}	3.82 €/kg	
WW savings = Operation time x wastewater volume per hours x 0.35 €/m ³		(Eq. S31)
Methanol revenue = methanol price x methanol yield		(Eq. S32)

S9 System Process Representation in Ecoinvent v.3.4

Table S14 lists the hardware requirements of the *BioMethanol* System and their representation with background processes from Ecoinvent v.3.4. Furthermore, the process representation is rated in a semi-quantitative manner and as described in table caption. Four reasons for the ratings are defined as following:

- Different process capacity: the Ecoinvent process represents the desired process but considers a different capacity. For that reason, scale effects are not taken into account.
- Average process: the Ecoinvent process Includes material and energy demand of a non-specified, average process
- Different material: the Ecoinvent was used as a proxy process as no process for the desired material was available
- Manufacturing not considered

Table S14: BioMethanol System process representation in Ecoinvent 3.4 database. Rating (R) as following: 1 = very good process representation, 2 = process representation ok, 3 = process representation a rough estimate, 4= poor process representation

Material/process	Ecoinvent 3.4 process representation	R	Rating Reason
Water & sludge pump	Market for pump 40W [GLO]	2	Different Capacity
Rectifier	Market for inverter, 2,5 kW [GLO]	2	Different Capacity
Transformer	Market for transformer [GLO]	3	Different capacity
Polypropylene	Market for polypropylene, granulate [GLO]	1	
Injection moulding, polypropylene	Injection moulding [RER]	2	Average process
Stainless steel	Market for steel, chromium steel 18/8 [GLO]	2	Different material
Current collector production	metal working, average for chromium steel product manufacturing [RER]	2	Average process
Carbon nanotubes	Market for graphite [GLO]	3	Different material
Molybdenum sulfide	Market for molybdenum [GLO]	3	Different material, No manufacturing
Nafion membrane	Market for tetrafluoroethylene film, on glass [GLO]	3	Different material, no manufacturing
Polysulfone membrane	Polysulfone production, for membrane filtration production [GLO]	3	Different material, no manufacturing
Mild steel	Market for steel, low-alloyed [GLO]	1	
Stainless steel	Market for steel, chromium steel 18/8 [GLO]	1	
Production of steel products	Metal working, average for steel product manufacturing	2	Average process

	[RER]		
Transport	Transport, lorry 16-32t,EURO4 [RER]	1	
Gas compressors	Market for air compressor, screw type compressor, 4kW [GLO]	3	Different process
CuO	Market for copper oxide [GLO]	2	No manufacturing
ZnO	Market for zinc oxide [GLO]	2	No manufacturing
AlO ₃	Market for aluminum oxide [GLO]	2	No manufacturing
Methanol factory	Market for methanol factory [GLO]	4	Different capacity
Average		2.2	

S10 Estimation of Input Data Quality

Table S15 lists the input data of the process analysis and estimates its quality.

Table S15: Data quality of input data for the process evaluation. Rating categories are as following: 1=good, 2=ok, 3=rough estimation, 4=poor data quality, ? = no data quality judgement possible, ** primary source not accessible

Item	Source	Rating	Reason
COD removal efficiency	Experimental data	1	
Coulomb efficiency	Literature Data	1	
Cathodic Conversion efficiency	Experimental data	1	
Current Density	Presupposition	?	
Cell Voltage	Based on experimental & literature data	2	
MEC Housing & Current collectors	Experimental data	1	
Membranes	Experimental data and other sources (see S7)	3	Estimation
Methanol yield	CHEMCAD simulation	2	
Carbon dioxide demand	CHEMCAD simulation	2	
Compressor electricity	CHEMCAD simulation	2	Isentropic compression
Excess heat	CHEMCAD simulation	2	
Heat exchanger surface	CHEMCAD simulation	3	Estimation
Sludge formation WWTP	³	2	Estimation
Sludge formation MEC	³	3	Estimation
Sludge pump electricity	Own calculations based on ref ¹⁴	2	Estimation
Wastewater pump electricity	Own calculations based on ref ¹⁴	2	Estimation
Sludge organic dry matter per dry matter	DWA,2003** as cited in ref ⁸	2	Average
COD per organic dry matter sludge	³	2	Average
oDM degradation in biogas digester	⁸	2	Average
Methane yield per COD in biogas digestion	Cornel,2006** in ref ⁸	2	Average
Methane lower heating value	⁴¹	1	
CHP electrical efficiency	based on ref ⁴²	2	Estimation
Activated Carbon Demand	Supplier Data ¹³		

Biogas digester steel demand	Own calculations based on ref ¹⁴	4	Weak data basis
Cooling pump electricity	Own calculation	3	Weak data basis
Sludge screw press electricity	⁶	2	Average
Sludge screw press steel demand	Own calculations based on ref ¹⁴	4	Weak data basis
Sludge incineration efficiency (el)	⁴²	2	Average
WWTP aeration electricity & COD/TN removal efficiency	WWTP Reference with project partner data	1	
WWTP electricity for other steps	⁴³	2	Average
Distance to sludge treat. after MEC	Google maps	1	
Transport to incineration plant	Assumption	4	Assumption
Rectifier & Transformer Efficiency	Supplier Data ¹²	3/A	
Grid hardware for renewable energy mix production	Ecoinvent v.3.3	3	Average assumption
CO ₂ formation	Stoichiometric calculation	2	
Sludge dry matter after MEC/AS	⁶	2	Average
Sludge dry matter after storage	Assumption	4	Assumption
Sludge dry matter after digestion	⁴⁴	3	Company data
Sludge dry matter after press	⁶	2	Average
Sludge dry matter after sludge drying	⁶	2	Average

S11 Influence of the Assumption of Wastewater Composition on Life Cycle Assessment Results

Table S16: LCA results for the consideration of a carbon source with oxidation state -4 (CH₄) in the wastewater stream of the WWTP Reference System. The values are rounded to the decimal at which a difference between the case for Acetate and CH₄ can be identified.

Unit	Ref	Base		Best		Worst	
		Ac-	CH ₄	Ac-	CH ₄	Ac-	CH ₄
GWP kg CO ₂ Eq/t t _{CH₃OH}	560	-815	-810	-1,010	-1,000	-622	-618
TAP kg SO ₂ Eq/t t _{CH₃OH}	1.6	2.62	2.65	1.81	1.86	3.39	3.41
POFP kg NMVOC Eq/t t _{CH₃OH}	1.8	1.21	1.23	0.43	0.47	1.8	1.81
FEP kg P-Eq/t t _{CH₃OH}	0.1	0.727	0.731	0.587	0.595	0.924	0.927
MDP kg Fe-Eq/t t _{CH₃OH}	30	234	236	172	175	332	334
CEDF GJ/t t _{CH₃OH}	33.8	7.59	7.65	4.57	4.7	10.9	10.95
CEDT GJ/t t _{CH₃OH}	34.2	20.6	21.1	14.6	15.7	24	24.5

Table S17: LCA results for the consideration of a carbon source with oxidation state +3 (CO) in the wastewater stream of the WWTP Reference System. The values are rounded to the decimal at which a difference between the case for Acetate and CO can be identified.

Unit	Ref	Base		Best		Worst	
		Ac-	CO	Ac-	CO	Ac-	CO
GWP kg CO ₂ Eq/t t _{CH₃OH}	560	-815	-816	-1,010	-1,012	-622	-624
TAP kg SO ₂ Eq/t t _{CH₃OH}	1.6	2.62	2.61	1.81	1.79	3.39	3.39
POFP kg NMVOC Eq/t t _{CH₃OH}	1.8	1.21	1.2	0.43	0.42	1.8	1.79
FEP kg P-Eq/t t _{CH₃OH}	0.1	0.727	0.726	0.587	0.585	0.924	0.923
MDP kg Fe-Eq/t t _{CH₃OH}	30	234.2	233.6	172	170	332.4	331.9
CEDF GJ/t t _{CH₃OH}	33.8	7.59	7.57	4.57	4.54	10.9	10.88
CEDT GJ/t t _{CH₃OH}	34.2	20.6	20.5	14.6	14.3	24	23.9

For the process evaluation, the industrial wastewater COD has been considered to consist of acetate (cf. 3.11. main paper). Furthermore, in the allocation of aeration electricity in the WWTP Reference System (cf. S6) the same assumption has been made. However, for the

municipal wastewater treatment process, the validity of this assumption is less justified than for the industrial wastewater. As described in S6, the chemical composition of COD has an effect on Eq. S10, in exact: on the COD that is removed via bacterial biomass growth.

In the calculations of S6, a different oxidation state of the wastewater carbon (resulting in a different COD per carbon atom) leads to more or less COD consumption by bacterial biomass growth (via the incorporation of carbon atoms in bacterial biomass). Thereby, in the partitioning allocation of aeration electricity to COD/TN (cf. S6), a different wastewater carbon species leads to a different share of electricity being allocated to COD/TN oxidation. As the *BioMethanol* System primarily treats COD, a different credit results via the substitution of conventional wastewater treatment (in the LCA “avoided burden approach”). In order to check on the sensitivity of LCA results on the assumption of wastewater carbon species being acetate, the following consideration, leading to sensitivity analysis have been made:

- The carbon atoms in acetate depict an oxidation state of zero
- In order to investigate the sensitivity of the acetate assumption, two extreme cases with a carbon oxidation state of -4 (CH₄) and +3 (CO) have been calculated and their effect on LCA results checked
- In this investigation the operation of the *BioMethanol* System and WWTP Reference System has been modeled with renewable electricity mix e2

The results can be found in

Table S16 &

Table S17. As can be observed the results only have a minor influence on LCA results. The small change in impact results primarily from the low overall impact of the renewable electricity source e2 for wastewater treatment.

S12 Life Cycle Inventory

In the following the life cycle inventory for the *BioMethanol* System is listed (base case). The components in light gray have not been considered in the LCA model. Some values contain many decimals for the calculation of mass balances.

BioMethanol: Wastewater pump			
Input	Value	Unit	Source
Wastewater	336.5	Mt/a	Project data
Electricity	46.75	MWh/a	cf. S7
Market for pump, 4W [GLO]	6.9	Units	Ecoinvent v.3.4
Output	Value	Unit	Source
Wastewater	336.5	Mt/a	Project data

BioMethanol: Sludge pump 1			
Input	Value	Unit	Source
Sludge (99%H ₂ O)	2,230	t/a	cf. S4
Electricity	0.29	MWh/a	cf. S7
Market for pump,40W [GLO]	6.9	Units	Ecoinvent v.3.4
Output	Value	Unit	Source
Sludge (99%H ₂ O)	2,230	t/a	cf. S4

BioMethanol: Sludge pump 2			
Input	Value	Unit	Source
Sludge (98.5%H ₂ O)	1,490	t/a	cf. S4 (dewatered)

Electricity	0.29	MWh/a	cf. S7
Market for pump,40W [GLO]	6.9	Units	Ecoinvent v.3.4
Output	Value	Unit	Source
Sludge (98.5%H ₂ O)	1,490	t/a	cf. S4 (dewatered)

BioMethanol: Power electronics for microbial electrolysis cell			
Input	Value	Unit	Source
Electricity	428	MWh/a	Efficiency according to Supplier Data ¹²
Output	Value	Unit	Source
Electricity	385	MWh/a	cf. 3.1.2 (main paper)

BioMethanol: Power electronics hardware			
Input	Value	Unit	Source
Rectifier	0.925	Units/a	Market for inverter, 2.5kW [GLO]; Ecoinvent v.3.4
Transformer	293.2	kg/a	Market for transformer, 2.5kW [GLO]; Ecoinvent v.3.4

Microbial electrolysis cell: Hardware			
Input	Value	Unit	Source
Polypropylene	3.1	t/a	cf. S7
Stainless steel mesh	1.24	t/a	
Carbon Nanotubes	0.06	t/a	
Molybdenum	3	kg/a	
Membrane1:Polysulfone	0.4	t/a	
Membrane2: PTFE	0.11	t/a	

Microbial electrolysis cell: Operation			
Input	Value	Unit	Source
COD	1,312.188	t/a	Project data
Total Nitrogen	140.976	t/a	Project data
Water	336,458.333	t/a	Project data
Electricity from electricity source	375.5	MWh/a	cf. 3.1.2 (main paper)
Electricity from CHP	9.6	MWh/a	cf. 3.1.6 (main paper)
Output	Value	Unit	Source
COD	524.875	t/a	60% COD removal assumed
Total Nitrogen	139.884	t/a	7% N in biomass assumed ³
Water	336,015.077	t/a	Stoichiometric calculation
Hydrogen	35.711	t/a	cf. Eq. 10 (main paper)
Carbon Dioxide	1,054.954	t/a	cf. Eq. 13 (main paper)
Protons _{aq}	30.927	t/a	Stoichiometric calculation
Sludge (99%H ₂ O)	22.289	t dry matter /a	cf. S4
Input mass	337,911.5	t/a	
Output mass	337,823.7	t/a	
Difference	0.03%	Of input mass	

BioMethanol: Gas cleaning			
Input	Value	Unit	Source
Activated Carbon	310	kg/a	Supplier Data ¹³
Electricity	21	kWh/a	Estimation cf. S7

BioMethanol: Sludge storage			
Input	Value	Unit	Source
Sludge (99% H_2O)	2,230	t/a	cf. S4
Output	Value	Unit	Source
Sludge (98,5% H_2O)	1,490	t/a	cf. S4 (1.5% dry matter after storage assumed)
Water	740	t/a	Difference of the above

BioMethanol: Biogas digester			
Input	Value	Unit	Source
Sludge (98,5% H_2O)	1,485.914	t/a	cf. S4 (dewatered)
Electricity	1.93	MWh/a	cf. 3.1.5 (main paper)
Mild steel	675.7	kg/a	cf. S7
Stainless steel	16	kg/a	cf. S7
Output	Value	Unit	Source
Sludge (97% H_2O)	482.922	t/a	cf. S4 (dewatered)
Methane	2.775	t/a	cf. 3.1.5 (main paper)
Carbon Dioxide	6.329	t/a	cf. Eq. 16 (main paper) (stoichiometric CO_2 formation in CH_4 oxidation subtracted)
Water	993.888	t/a	Difference sludge mass input and sludge, methane, carbon dioxide output

BioMethanol: Sludge press			
Input	Value	Unit	Source
Sludge (97% H_2O)	482.922	t/a	cf. Eq. S9
Electricity	0.12	MWh/a	Based on data from ⁶
Stainless steel	2.24	kg/a	cf. S7
Output	Value	Unit	Source
Sludge (72,5% H_2O)	52.682	t/a	cf. Eq. S9 (dewatered)
Water	430.24	t/a	Difference in sludge mass

BioMethanol: Transport of excess sludge to sludge treatment			
Input	Value	Unit	Source
Sludge (72,5% H_2O)	52.7	t/a	cf. Eq. S9 (dewatered)
Transport	1,300	t*km/a	Distance (maps) x weight
Output	Value	Unit	Source
Sludge (72,5% H_2O)	52.7	t/a	cf. Eq. S9 (dewatered)

BioMethanol: Methane burning in combined heat & power plant			
Input	Value	Unit	Source
Methane	2.8	t/a	cf. 3.1.5 (main paper)
Oxygen from air	11	t/a	Stoichiometric calculation
Output	Value	Unit	Source
Electricity	12.8	MWh/a	cf. 3.1.6 (main paper)
Carbon Dioxide	7.6	t/a	Stoichiometric calculation
Water	6.2	t/a	Stoichiometric calculation

Input mass	13.8	t/a	
Output mass	13.8	t/a	
Difference	0%	Of input mass	

BioMethanol: Sludge treatment after microbial electrolysis cell			
Input	Value	Unit	Source
Sludge (72,5%H ₂ O)	52.7	t/a	cf. Eq. S9 (dewatered)
Electricity from German Grid	4.2	MWh/a	3.1.10 (main paper)
Output	Value	Unit	Source
Sludge (15%H ₂ O)	17	t/a	Eq. S9 (dewatered)
Water	35.7	t/a	Difference in sludge mass

BioMethanol: Transport of excess sludge from sludge treatment to incineration			
Input	Value	Unit	Source
Sludge (15%H ₂ O)	17	t/a	cf. Eq. S9 (dewatered)
Transport	3,409	t*km/a	200 km transport assumed
Output	Value	Unit	Source
Sludge (15%H ₂ O)	17	t/a	cf. Eq. S9 (dewatered)

BioMethanol: Sludge incineration			
Input	Value	Unit	Source
Sludge (15%H ₂ O)	17	t/a	cf. Eq. S9 (dewatered)
Oxygen from air	11.077	t/a	Corresponding to COD _{Biomass}
Output	Value	Unit	Source
Electricity	9.2	MWh/a	cf. 3.1.8 (main paper)
Incineration Ash	6.687	t/a	Non-organic sludge components cf. S5
Carbon Dioxide	13.941	t/a	Stoichiometric relation in oxidation of biomass cf. 3.1.9
Water	6.566	t/a	Stoichiometric calculation cf. 3.1.9
NO ₂ (filtered, not emitted)	2.915	t/a	Stoichiometric calculation cf. 3.1.9
Input mass	28.1	t/a	
Output mass	30.1	t/a	
Difference	6.6%	Of input mass	

BioMethanol: Hydrogen compression			
Input	Value	Unit	Source
Hydrogen @ 1 bar	35.7	t/a	cf. Eq. 8 (main paper)
Electricity	74.03	MWh/a	CHEMCAD simulation
Output	Value	Unit	Source
Hydrogen @ 50 bar	35.7	t/a	cf. Eq. 8 (main paper)

Heat	53.9	MWh/a	CHEMCAD simulation
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BioMethanol: Carbon dioxide compression from 1 bar			
Input	Value	Unit	Source
Carbon Dioxide @ 1 bar	286.5	t/a	CHEMCAD simulation
Electricity	24.5	MWh/a	CHEMCAD simulation
Output	Value	Unit	Source
Carbon Dioxide @ 50 bar	286.5	t/a	CHEMCAD simulation
Heat	19.4	MWh/a	CHEMCAD simulation

BioMethanol: Carbon dioxide compression from 9 bar			
Input	Value	Unit	Source
Carbon Dioxide @ 9 bar	286.5	t/a	CHEMCAD simulation
Electricity	29.8	MWh/a	CHEMCAD simulation
Output	Value	Unit	Source
Carbon Dioxide @ 50 bar	286.5	t/a	CHEMCAD simulation
Heat	24.7	MWh/a	CHEMCAD simulation

BioMethanol: Compression hardware			
Input	Value	Unit	Source
Hydrogen Compressor	0.11	Units/a	Market for air compressor, screw-type compressor, 4kW [GLO]; Ecoinvent v.3.4
Carbon Dioxide Compressor	0.04		

BioMethanol: Methanol synthesis & distillation: operation			
Input	Value	Unit	Source
Hydrogen @ 50 bar	35.7	t/a	cf. Eq. 10 (main paper)
Carbon Dioxide @ 50 bar	286.5	t/a	CHEMCAD simulation
Electricity recirc. compressor	3.8	MWh/a	CHEMCAD simulation
Output	Value	Unit	Source
Methanol (99.85wt%)	185.255	t/a	CHEMCAD simulation
Water	106.014	t/a	CHEMCAD simulation
Methanol in purge	3.886	t/a	CHEMCAD simulation
Hydrogen in purge	0.064	t/a	CHEMCAD simulation
Carbon dioxide in purge	26.644	t/a	CHEMCAD simulation
Water in purge & methanol	0.332	t/a	CHEMCAD simulation
Heat	136	MWh/a	CHEMCAD simulation
Input mass	322.2	t/a	
Output mass	322.2	t/a	
Difference	0%	Of input mass	

BioMethanol: Methanol synthesis & distillation hardware			
Input	Value	Unit	Source
CuO	5.7	kg/a	cf. S7
ZnO	1.9	kg/a	cf. S7
AlO ₃	0.75	kg/a	cf. S7
Methanol factory	6.85*10 ⁻⁶	Units/a	Market for methanol factory [GLO]; Ecoinvent 3.4

BioMethanol cooling: case CO ₂ from microbial electrolysis			
Input	Value	Unit	Source
Heat	209.3	MWh/a	CHEMCAD simulation
Electricity	1.87	MWh/a	cf. 3.1.7 (main paper)
Output	Value	Unit	Source
Heat	209.3	MWh/a	CHEMCAD simulation

BioMethanol cooling: case purchased CO ₂			
Input	Value	Unit	Source
Heat	214.6	MWh/a	CHEMCAD simulation
Electricity	1.92	MWh/a	cf. 3.1.7 (main paper)
Output	Value	Unit	Source
Heat	214.6	MWh/a	CHEMCAD simulation

Wastewater Treatment Plant Reference: Removal of chemical oxygen demand (COD)			
Input	Value	Unit	Source
COD	1,352.3	t/a	Project data
Electricity Aeration COD	198.7	MWh	cf. S6
Electricity Sludge Recirculation & Settler	64.2	MWh	cf. 3.1.10 (main paper)
Oxygen from air	907.2	t/a	Stoichiometric calculation
Output	Value	Unit	Source
COD	64.9	t/a	COD removal according to data from WWTP Project data
Carbon dioxide	1,247.73	t/a	cf. Eq. 13 (main paper)
Sludge (99%H ₂ O)	418	t dry matter/a	Cf. 3.1.4 (main paper)
Water	510.757	t/a	Stoichiometric calculation (acetate oxidation)
Input mass	2,259.5	t/a	
Output mass	2,241.4	t/a	
Difference	0.8%	Of input mass	

Wastewater Treatment Plant Reference: Removal of total nitrogen (TN)			
Input	Value	Unit	Source
Total Nitrogen (TN)	145.3	t/a	Project Data
Electricity Aeration TN	82.2	MWh	cf. S6
Output	Value	Unit	Source
Total Nitrogen	28.6	t/a	TN removal according to data from WWTP Project data

Nitrogen in sludge	20.5	t/a	7% N in sludge assumed ³
Nitrogen, molecular	96.2	t dry matter/a	Difference in TN mass

Wastewater Treatment Plant Reference: Biogas digestion & sludge drying			
Input	Value	Unit	Source
Sludge (99%H ₂ O)	41,801	t/a	cf. S4
Electricity	115.3	MWh	cf. 3.1.10 (main paper)
Output	Value	Unit	Source
Sludge (15%H ₂ O)	319.7	t/a	cf. Eq. S9
Methane	52	t/a	cf. Eq. 11 (main paper)
Carbon dioxide	118.7	t/a	cf. Eq. 16 (main paper); stoichiometric CO ₂ formation in CH ₄ oxidation subtracted)
Water	41,311	t/a	Difference sludge mass input and sludge, methane, carbon dioxide output

Wastewater Treatment Plant Reference: Methane burning in combined heat & power plant			
Input	Value	Unit	Source
Methane	52.044	t/a	cf. Eq. 11 (main paper)
Oxygen	207.614	t/a	Stoichiometric calculations
Output	Value	Unit	Source
Electricity	239.2	MWh/a	cf. Eq. 12 (main paper)
Carbon dioxide	142.772	t/a	Stoichiometric calculations
Water	116.887	t/a	Stoichiometric calculations
Input mass	259.7	t/a	
Output mass	259.7	t/a	
Difference	0 %	Of input mass	

Wastewater Treatment Plant Reference: Transport excess sludge to incineration			
Input	Value	Unit	Source
Sludge (15%H ₂ O)	319.7	t/a	cf. Eq. S9 (dewatered)
Transport	63,900	t*km/a	200 km transport assumed
Output	Value	Unit	Source
Sludge (15%H ₂ O)	319.7	t/a	cf. Eq. S9 (dewatered)

Wastewater Treatment Plant Reference: Sludge incineration			
Input	Value	Unit	Source
Sludge (15%H ₂ O)	319.66	t/a	cf. Eq. S9 (dewatered)
Oxygen	207.752	t/a	Corresponding to biomass COD
Output	Value	Unit	Source
Incineration Ash	125.403	t/a	Non-organic sludge components cf. S5
Electricity	172.5	MWh/a	cf. 3.1.8 (main paper)
Carbon dioxide	261.46	t/a	Stoichiometric calculation oxidation of biomass cf. 3.1.10
Water	123.14	t/a	Stoichiometric calculations cf. 3.1.10
NO ₂ (filtered, not emitted)	54.663	t/a	Stoichiometric calculations 3.1.10
Input mass	527.4	t/a	

Output mass	564.7	t/a	
Difference	6.6%	Of input mass	

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