Appendices

Appendices

The appendices include relevant background materials for the research performed in this project. Most text is less refined as it hasn't made the cut in the full report. If any material from these appendices are used, please contact the author. If any data of the ZEF system is used, please contact the corresponding expert.

Table Contents

A. Mass flows in the microplant

The mass flows included in this section were the first received from Zero Emission Fuels B.V. It is an overview of the mass flows between the subsystems and the internal parts within the subsystems. The bold flows are the main in- and outputs of the subsystems.
Important: some flows are different than the unit process data in this report and in the main model. Some flows were corrected to close the mass balance. This included an additional MS reactor requirement of around 0.102 kg CO_2 per day and a slight correction of the hydrogen in the non-continuous purge flow.

Sub-system	Subsystem Flow number	Air mass flow (kg/d)	Amine (TEPA) mass flow (kg/d)	Diluent (PEG200) mass flow (kg/d)	Water Mass Flow (kg/d)	CO2 Mass Flow (kg/d)	O2 mass flow (kg/d)	H2 mass flow (kg/d)	CO mass flow(kg/d)	MeOH mass flow (kg/d)
DAC	Air inlet	1.60E+04								
DAC	Air exit	1.60E+04	2.74E-04	2.74E-04						
DAC	Sorbent Recycle		5.45E+03	1.36E+04	1.66E+03	8.39E+02				
DAC	**Rich feed**		2.08E+01	5.21E+01	6.34E+00	**2.75E+00**				
DAC	CO2 production				7.56E-02	3.58E+00				
DAC	Lean return		2.08E+01	5.21E+01	2.89E+00	4.58E-01				
DAC	DAC water tank exit				3.38E+00	5.78E-03				
FM	Wet CO2 return				3.38E+00	8.25E-01				
FM	Dry CO2 return					8.25E-01				
FM	Dry CO2 main stream					3.58E+00				
FM	1st stage CO2					2.75E+00				
FM	**2nd stage CO2**					**2.75E+00**				
MS	CO2 entry to MS					2.75E+00				
MS	Top Left Condenser				1.24E+00	1.08E+01		2.54E+00	1.90E+00	2.88E+00
MS	Exit reactor bed				1.24E+00	6.80E+00		2.54E+00	1.90E+00	2.88E+00
MS	To purge				1.38E-03	1.07E-01		2.54E-02	1.90E-02	9.42E-03
MS	**Final MeOH/water stream**				**1.11E+00**	**6.05E-02**		**3.93E-04**	**2.98E-04**	**1.95E+00**
AEC	O2 to Degasser						3.00E+00			
AEC	O2 purge				9.67E-02	4.33E-03	3.00E+00			
AEC	H2 production							3.76E-01		
AEC	KOH filling entry point									
AEC	**Water Feed**				**3.38E+00**		1.02E-05			
DS	**Water output**				**1.11E+00**					3.33E-03
DS	purge dissolved gases					6.05E-02		3.93E-04	2.98E-04	
DS	**Methanol grade AA**				3.89E-03					**1.95E+00**

B. Impact totals

The tables below contain the impact scores of the impact assessment using the ILCD 2018 impact method. The values were calculated using foreground microplant scenarios, foreground PV scenarios, and background future database scenarios.

Totals (microplant + PV burdens)	ST-P	ST-N	ST-O	MT-P	MT-N	MT-O
CC - climate change total	-9.19E-01	-1.03E+0	-1.05E+00	-1.04E+00	-1.07E+00	-1.09E+00
EQ - freshwater and terrestrial acidification	4.23E-03	2.09E-03	1.96E-03	2.13E-03	1.80E-03	1.58E-03
EQ - freshwater ecotoxicity	1.74E+00	1.49E+00	1.40E+00	1.50E+00	1.38E+00	1.25E+00
EQ - freshwater eutrophication	1.68E-04	1.36E-04	1.30E-04	1.31E-04	1.23E-04	1.14E-04
EQ - marine eutrophication	6.57E-04	4.04E-04	3.76E-04	4.23E-04	3.68E-04	3.23E-04
EQ - terrestrial eutrophication	1.17E-02	4.41E-03	4.03E-03	5.29E-03	4.09E-03	3.35E-03
HH - carcinogenic effects	6.02E-08	5.19E-08	4.96E-08	5.16E-08	4.87E-08	4.54E-08
HH - ionising radiation	4.05E-02	2.57E-02	2.44E-02	3.21E-02	2.88E-02	2.60E-02
HH - non-carcinogenic effects	2.02E-07	1.75E-07	1.64E-07	1.76E-07	1.62E-07	1.47E-07
HH - ozone layer depletion	4.79E-08	3.86E-08	3.70E-08	3.88E-08	3.63E-08	3.39E-08
HH - photochemical ozone creation	1.85E-03	1.50E-03	1.44E-03	1.49E-03	1.40E-03	1.31E-03
HH - respiratory effects, inorganics	3.04E-08	1.68E-08	1.56E-08	1.81E-08	1.55E-08	1.34E-08
Resources - land use	4.06E+00	3.37E+00	3.17E+00	3.66E+00	3.37E+00	3.05E+00
Resources - minerals and metals	5.35E-05	4.79E-05	4.64E-05	4.81E-05	4.60E-05	4.37E-05
Resources - fossils	5.95E+00	3.75E+00	3.52E+00	3.83E+00	3.37E+00	3.00E+00
Resources - dissipated water	8.33E+00	7.22E+00	6.66E+00	7.35E+00	6.65E+00	5.84E+00

No PV burdens (and no carbon uptake)	ST-P	ST-N	ST-O	MT-P	MT-N	MT-O
CC - climate change total	2.51E-01	1.64E-01	1.62E-01	1.65E-01	1.54E-01	1.49E-01
EQ - freshwater and terrestrial acidification	3.02E-03	1.04E-03	9.90E-04	1.12E-03	8.90E-04	7.76E-04
EQ - freshwater ecotoxicity	4.47E-01	3.63E-01	3.62E-01	3.53E-01	3.47E-01	3.44E-01
EQ - freshwater eutrophication	9.21E-05	6.91E-05	6.87E-05	6.54E-05	6.32E-05	6.22E-05
EQ - marine eutrophication	3.33E-04	1.21E-04	1.16E-04	1.41E-04	1.13E-04	9.88E-05
EQ - terrestrial eutrophication	8.94E-03	2.00E-03	1.80E-03	2.89E-03	1.92E-03	1.43E-03
HH - carcinogenic effects	2.76E-08	2.35E-08	2.34E-08	2.28E-08	2.26E-08	2.25E-08
HH - ionising radiation	2.48E-02	1.21E-02	1.18E-02	1.44E-02	1.28E-02	1.20E-02
HH - non-carcinogenic effects	4.41E-08	3.73E-08	3.71E-08	3.68E-08	3.62E-08	3.59E-08
HH - ozone layer depletion	2.68E-08	2.02E-08	2.00E-08	2.03E-08	1.95E-08	1.92E-08
HH - photochemical ozone creation	1.06E-03	8.13E-04	8.08E-04	8.04E-04	7.79E-04	7.67E-04
HH - respiratory effects, inorganics	1.75E-08	5.53E-09	5.22E-09	6.81E-09	5.21E-09	4.42E-09
Resources - land use	1.19E+00	8.74E-01	8.68E-01	1.00E+00	9.62E-01	9.42E-01
Resources - minerals and metals	3.17E-05	2.89E-05	2.88E-05	2.87E-05	2.85E-05	2.84E-05
Resources - fossils	3.22E+00	1.37E+00	1.32E+00	1.47E+00	1.24E+00	1.13E+00
Resources - dissipated water	9.11E-02	3.94E-02	3.81E-02	4.38E-02	3.74E-02	3.43E-02

Reference – Natural gas based methanol (ecoinvent 3.7.1.)	NG-MeOH 2025	NG-MeOH 2030
CC - climate change total	0.637482935	0.628516961
EQ - freshwater and terrestrial acidification	2.06E-03	2.02E-03
EQ - freshwater ecotoxicity	6.07E-01	6.04E-01
EQ - freshwater eutrophication	4.91E-05	4.34E-05
EQ - marine eutrophication	3.64E-04	3.58E-04
EQ - terrestrial eutrophication	3.86E-03	3.81E-03
HH - carcinogenic effects	9.14E-09	9.09E-09
HH - ionising radiation	2.05E-02	2.29E-02
HH - non-carcinogenic effects	2.79E-08	2.76E-08
HH - ozone layer depletion	2.19E-07	2.18E-07
HH - photochemical ozone creation	1.85E-03	1.84E-03
HH - respiratory effects, inorganics	7.03E-09	6.93E-09
Resources - land use	8.62E-01	1.09E+00
Resources - minerals and metals	8.42E-06	8.44E-06
Resources - fossils	3.15E+01	3.14E+01
Resources - dissipated water	1.87E-01	1.88E-01

C. Maintenance unit process data

In theory, a central system keeps track of the performance of the microplants in the methanol farm. When the system notices that a microplant performs badly, it would be marked for maintenance. Some machinery use will be necessary to detach the microplant from the structure. To keep the performance of the methanol-plant as high as possible, a new or refurbished microplant will immediately replace the decommissioned plant. The decommissioned microplant is then sent to a maintenance facility where, depending on the complexity of the required repair the microplant, it is either repaired locally, sent back to the original manufacturer, or decommissioned altogether.

The impact of maintenance is not expected to be very relevant for the overall assessment, and unfortunately no estimations about the relative shares of the beforementioned scenarios in the total amount of maintenance cases are currently available. Therefore the strongly simplified assumption is made that every year 1% of the microplants is sent back to the original manufacturer (OEM), 1.5% is repaired locally, and 0.5% is decommissioned.

To keep the modelling fully transparent, clear and to reduce the need for additional parameters, the maintenance is modelled as a separate activity that produces 'one year of microplant maintenance'. The following assumptions / modelling steps are made to ensure that the maintenance of the methanol plant is accounted for:

- Parameters:
  - Maintenance-local-repair (Mrepair) = 1.5%, 0.015
  - Maintenance-to-OEM (Moem) = 1%, 0.01
  - Maintenance-to-decommissioning (Mdecommissioned) = 0.5%, 0.005
- All vehicle movements and machinery requirements related to the microplant instalment are multiplied by the total replacement rate (1+(Mrepair-1)+(Moem-1)+(Mdecomissioned-1)) = 1.03
- For the sake of data manageability, consistency and transparency, the additional material input required for:
  - Repair, is assumed to be 20% of the weight of a microplant. This is modelled by multiplying the total material input by that factor (Mrepair)*0.2 = 0.003.
  - Maintenance to OEM, is assumed to be 40% of the weight of a microplant. This is modelled by multiplying the total material input by that factor (Moem)*0.4 = 0.004.
  - Maintenance to decommissioning requires a 100% replacement of the micro-plant = 0.005
  - The total material input required for maintenance is therefore 0.012 or 1.2%
- LCI modelling of maintenance goes beyond taking a simple percentage of the total material input because this assumption cannot be made for all inputs. Steel and steel parts for example, will far outlast the lifetime of other parts and will only be replaced if steel is an integral part of more vulnerable parts.
  The same assumption is applied to some other material inputs.
- Steel for parts that are likely to be swapped all together is included in the maintenance activity
- The maintenance activity is highly uncertain and should not weigh heavily in the final interpretation of the results.
- Transport is modelled based on the distance to the Original Equiment Manufacturer and the distance to the decommissioning site. Transport is simplified and overestimated slightly because the total empty weight for the microplant is assumed times the occurrence of the transport per year.

The overview of the unit process for maintenance can be viewed in the table below.

Exchange name	amount	unit
Microplant maintenance	**1**	**year**
AEC stack production	0.013	unit
cable production, ribbon cable, 20-pin, with plugs	0.0065	kilogram
cable production, three-conductor cable	0.013	meter
ceramic tile production	0.0026	kilogram
chromium steel pipe production	0.13	kilogram
copper oxide production	4.55E-05	kilogram
flat glass production, uncoated	0.1378	kilogram
inverter production, 2.5kW	0.00065	unit
market for aluminium oxide, non-metallurgical	0.00585	kilogram
market for aluminium, cast alloy	0.052	kilogram
market for transport, freight, sea, container ship	0	ton kilometer
market for transport, freight, sea, container ship	0.784	ton kilometer
market for waste aluminium	-0.05785	kilogram
market for waste mineral wool	-0.026	kilogram
market for waste polyethylene	-0.1573	kilogram
market group for waste polypropylene	-0.0013	kilogram
polyester fibre production, finished, adapted from ecoinvent	0.052	kilogram
polyethylene production, high density, granulate	0.078	kilogram
polypropylene production, granulate	0.08606	kilogram
printed wiring board production, surface mounted, unspecified, Pb free	0.0026	kilogram
steel production, 316	0.075	kilogram
stone wool production	0.026	kilogram
transport, freight, lorry 16-32 metric ton, EURO5	0.0784	ton kilometer
transport, freight, lorry 16-32 metric ton, EURO5	0.0147	ton kilometer
treatment of scrap printed wiring boards, shredding and separation	-0.0026	kilogram
treatment of used cable	-0.00195	kilogram
treatment of waste glass, municipal incineration	-0.01378	kilogram
treatment of waste plastic, mixture, municipal incineration	-0.01729	kilogram
zinc oxide production	0.000195	kilogram

D. Embodiment of the microplant

The embodiment of the microplant includes an approximation of electric components, steel pipes for internal methanol transport, polyethylene for the external housing, and all transport movements for between production in China and farm construction in Oman.
From a model perspective, the burdens of this process are added to the final methanol stream from the microplant in a function that includes microplant lifetime and production volume.

Exchange name	amount	unit
PLANT - microplant embodiment	**1**	**unit**
cable production, ribbon cable, 20-pin, with plugs	0.5	kilogram
cable production, three-conductor cable	1	meter
steel pipe production	10	kilogram
market for transport, freight, lorry 16-32 metric ton, EURO5	3.92	ton kilometer
market for transport, freight, lorry 16-32 metric ton, EURO5	2.94	ton kilometer
market for waste polyethylene	-0.6	kilogram
polyethylene production, high density, granulate	6	kilogram
printed wiring board production, surface mounted, unspecified, Pb free	0.2	kilogram
transport, freight, sea, container ship	980	ton kilometer
transport, freight, sea, container ship	156.8	ton kilometer
treatment of scrap printed wiring boards, shredding and separation	-0.2	kilogram
treatment of used cable	-1.5	kilogram

E. Farm construction

The farm construction unit process includes vehicle movements and electricity needs for the construction of roads, and the installation of the microplants under the photovoltaic panels. All other relevant energy-demanding construction flows are included in the construction of the photovoltaic plant according to the work by Frischknecht et al. (2020), which is a different unit process in the LCA model.

- The road is assumed to be around 25 kilometres.
- The liquid storage tank production, chemicals, organics, is a large storage facility consisting of four tanks. The requirement by the farm in this study is much smaller due to the expected frequent methanol collection by freight trucks. A set assumed storage volume is calculated and used for the approximation.

Exchange name	amount	unit
PLANT - Farm construction	**1**	**unit**
diesel, burned in building machine	3478205	megajoule
gravel production, crushed	82025395	kilogram
liquid storage tank production, chemicals, organics	0.15	unit
market for mastic asphalt	837648	kilogram
market for waste asphalt	-837648	kilogram
market group for electricity, low voltage	25039	kilowatt hour
transport, freight, lorry 16-32 metric ton, EURO5	8286200	ton kilometer

F. Production of the sorbent

Production of TEPA

Multiple routes of TEPA production are possible but few have detailed data and realistic production methods. In this study a patent from 2018 filed by Ten Kate et al. as part of the R&D by Akzo Nobel will be used to provide reasonably accurate data for the production of TEPA from widely available materials. The yield (efficiency) of this method is relatively low which is why it cannot immediately be assumed that this is the actual process that is used for the production of TEPA in industry. Still the production route provides a basis for inventory modelling using stoichiometry. The initial modelling will be done using the parameters from the patent.

Figure and table 10 provide the overview for the production of TEPA: DEA (12.1 g, 115 mmol), EDA (1.8 g, 30 mmol), and EU (9.90 g, 115 mmol) are added to a pressure reactor. The reactor is then put under an atmosphere of N2 and is heated to 270 00 during 1 h and kept at 270 00 for 4 h. The reactor is then cooled to ambient temperature.

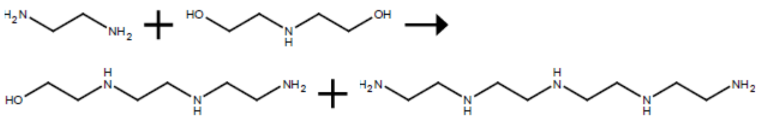


Table 1: Production data for the production of the sorbent

Before the reaction	After the reaction
66 mmol Diethanolamine (DEA)	<1 wt% DEA
67 mmol Ethylenediamine (EDA)	13 wt% EDA
200 mmol EthyleneUrea (EU)	29.9 wt% EU
	16.9 mmol Hydroxyethyldiethylenetriamine (HEDETA)
	17.2 mmol TEPA

Total weight % of these compounds is 67.7%. The remaining weight percentage is expected to consist of urea and derivatives of HEDETA and urea derivatives of TEPA (Ten Kate et al., 2018). A percentage of the remaining compounds is assumed to be recycled for the same process, this is included in the life cycle inventory as a reduced input of material.

In their LCA on DAC, Deutz and Bardow (2021) assume that the unreacted raw materials for PEI production are incinerated. The yield of the chemical reaction in that study was considerably higher than the yield for the production of TEPA. For that reason, it could be reasonable to incinerate the leftover reactants. The same assumption cannot be made for the case of TEPA production as the yield is much lower and incineration of the reactants would likely make the process uneconomical. Under a best case scenario approach it therefore is assumed that all identifiable unreacted reactants are recycled and that only derivatives of the main reaction products are incinerated (weight percentage approximately 30%).

The energy and heat requirements for the reaction will be based on industry averages as is recommended by Tsoy et al. (2018) in their LCA framework for the upscaling of the production of industrial chemicals. This includes therefore the total energy and heat requirements, including the separation step which is often a highly energy intensive process (Kim & Overcash, 2003). Similar to the inventory modelling by Deutz & Bardow, industry averages will come from the Gendorf Chemiepark which houses the Global Amines company, making it likely that TEPA is produced here. Gendorf publishes core indicators for environmental performance including all average exchanges with the environment (Gendorf, 2020). These averages were compiled, aggregated, normalised, and used as input for the TEPA production process. The averages from Gendorf were cross-checked with the averages from Kim & Overcash (2015). Average material exchanges from Gendorf were found to be slightly higher (e.g. energy requirement of 5.2 MJ vs. 0-4 MJ respectively).

Production of the diluent

To model the production of PEG-200, another patent is consulted. The process in the patent describes the polymerization of ethylene oxide in the presence of water, and ethylene glycol, di- or tri-ethylene glycol following the follow reaction:

$HOCH_2CH_2OH + n(CH_2CH_2O) \longrightarrow HO(CH_2CH_2O)_{n+1}H$

The result is a yield of 97% and all reported masses are copied to the LCI (Sakanoue, Sanchika & Yasukohchi, 2002). The same assumptions for the energy demand and demand for auxiliary materials are followed.

Allocation of TEPA and co-produced HEDETA

Scaled for the production of 1kg of TEPA, the process also produfileces 0.73kg of HEDETA. Both compounds are used in multiple processes. HEDETA is used in skincare products whereas TEPA could be deemed more valuable in general due to its use in a wider range of applications. Still, HEDETA can be purchased from Sigma-Aldrich for a market price of 70 EUR per kg whereas TEPA can be purchased for 61.20 EUR per kg. It should be noted that very large price optimizations are possible with higher quantities (e.g. in the range of 5 EUR per kg). In general, getting quotations for these products will result in widely ranging results.
The price difference between the two products, albeit small, could be explained by process optimizations as result of a higher demand of TEPA. In other words, the fact that the price of HEDETA is higher, does not necessarily mean that this compound would be the driving factor for the process and should therefore receive the largest allocation. Still, allocation based on other factors such as weight would be even less relevant.
The TEPA production process results in 1kg * 61.20 = 61.20 EUR worth TEPA, and 0.73*70 = 51.1 EUR worth of HEDETA. The allocation factors then become 0.55 for TEPA and 0.45 for HEDETA.
As a sensitivity analysis, the impacts are fully allocated to the production of TEPA due to low demand of HEDETA. Even though the modelled process is expected to overestimate the impacts, the full allocation of impacts to TEPA then provides a range of the potential impacts.

Unit process data for the Sorbent and Diluent

Sorbent	**amount**	**type**	**unit**
Carbon dioxide, fossil	0.00026	Emission	kilogram
NMVOC, non-methane volatile organic compounds, unspecified origin	7.87E-05	Emission	kilogram
Occupation, industrial area	0.00207	Emission	square meter-year
Particulates, > 2.5 um, and < 10um	6.39E-06	Emission	kilogram
Water	0.004639	Emission	cubic meter
Water	0.03391	Emission	cubic meter
Water, river	0.024021	Emission	cubic meter
Water, well, in ground	0.017134	Emission	cubic meter

MF - Production of Tetraethylenepentamine	1.7343	Product (unallocated)	unit
ethanolamine production	1.735853	Technosphere	kilogram
ethylenediamine production	0.110098	Technosphere	kilogram
imidazole production	2.237057	Technosphere	kilogram
market for electricity, medium voltage	0.996842	Technosphere	kilowatt hour
market for natural gas, high pressure	0.122759	Technosphere	cubic meter
market for wastewater, average	-0.05981	Technosphere	cubic meter
market group for tap water	0.059806	Technosphere	kilogram
treatment of spent solvent mixture, hazardous waste incineration, with energy recovery	-2.3487	Technosphere	kilogram

Diluent	amount	type	unit
Carbon dioxide, fossil	0.00015	Emission	kilogram
NMVOC, non-methane volatile organic compounds, unspecified origin	4.54E-05	Emission	kilogram
Occupation, industrial area	0.001195	Emission	square meter-year
Particulates, > 2.5 um, and < 10um	3.68E-06	Emission	kilogram
Water	0.000267	Emission	cubic meter
Water	0.01955	Emission	cubic meter
Water, river	0.01385	Emission	cubic meter
Water, well, in ground	0.009879	Emission	cubic meter
Production of PEG-200	**1**	**Product**	**kilogram**
ethylene glycol production	0.7693	Technosphere	kilogram
ethylene oxide production	0.261579	Technosphere	kilogram
market for electricity, medium voltage	0.5747	Technosphere	kilowatt hour
market for phosphoric acid, industrial grade, without water, in 85% solution state	0.000451	Technosphere	kilogram
market for wastewater, average	-0.00417	Technosphere	cubic meter
market group for tap water	0.034484	Technosphere	kilogram
natural gas production	0.070496	Technosphere	cubic meter
potassium hydroxide production	0.000451	Technosphere	kilogram
treatment of spent solvent mixture, hazardous waste incineration, with energy recovery	-0.03077	Technosphere	kilogram

G. Cross study analysis appendices

These appendices consist of all additional work that was not included in the main report. It consists of two main parts; the initial methodological analysis of all included papers, and the results and discussion of biomethanol. Biomethanol was not included in the main report because there appeared to be no consistency between papers, rendering the results less useful for the overall analysis.

1. Article selection

The initial filtering of the search results resulted in approximately 80 papers published between 2015 and 2021 that assessed the environmental impacts of various low-carbon methanol production pathways. A relatively large share of papers adopted consequential LCA modelling techniques to investigate the relationship between green methanol production and direct injection of renewable electricity in the grid (e.g. Qahtani et al. 2020; UUsitalo et al., 2017). Such papers were excluded from the cross-study comparison if no original data was provided for the synthesis of green methanol. Other studies predominantly relied on non-original data, meaning that the authors collected data from papers that that were already published and abstained from adding new calculations or experimental data. A keystone paper is the work by Artz et al. (2018) which was often cited by papers found in the initial search. Artz and co-authors in turn used data by Hoppe et al. (2018), Pérez-Fortes et al. (2016) and Sternberg et al. (2017) which were all also often cited in more recent publications such as Thonemann (2020) and Garcia-Garcia et al. (2021). It was not always possible to discern case-based studies from literature-based studies but generally many interconnections between papers were found linked to the aforementioned papers.

The majority of the biomethanol studies and some CO_2-based r-methanol studies did not use Life Cycle Assessment as core-methodology and instead opted for emission accounting using process simulation software combined with CC impacts for electricity generation, feedstock, and other parameters. Although the information in these studies may be a good starting point for an LCA, the CC results cannot be compared to studies that do make use of the full LCA methodology. Biomethanol papers were also more often very case-specific, sometimes detailing small scale production of methanol from smaller agricultural companies. Such studies were generally excluded and only studies that discussed the wider implementation of the assessed biomethanol route were included in this analysis.

Two studies (Ravikumar et al., 2020; Consalez-Garay, 2019) reported impact results in non-conventional ways, which removed the possibility to use quantitative values for understanding the environmental profile. Still, these studies were included in the analysis due to relevant insights in the source of carbon dioxide and hydrogen (Consalez-Garay, 2019) and the alternative use of renewable electricity (Ravikumar et al., 2020).
From the initial selection of 80 papers, 18 papers assessing CO_2-based e-methanol and 9 papers assessing bio-based methanol remained. Combined, these studies assess 50 alternative product systems, of which the majority is deemed useful for this analysis.

2. Overview

Authors	*CO2 Source*	*CO2 capture technology*	*H2 source*	*Production route*	*Electricity Source*	*Heat source*
Sternberg, Jens, Bardow (2017)	Air, Power plant	Amine-based	Steam reforming, PEM electrolysis, excess hydrogen from chemical processes	Direct hydrogenation	Wind, Grid	Natural Gas (steam)
Hoppe et al. (2018)	Air, Biogas, Cement plant, Power plant, Waste plant	Amine-based	Alkaline Electrolysis	Direct hydrogenation, Syngas conversion	Wind, Grid (DE)	Heat integration, Natural Gas
Artz et al. (2018) (n=8)	Power plant and burden free CO2	Not considered	Alkaline Electrolysis	Direct hydrogenation, Syngas conversion (rWGS-based syngas, Co-Electrolysis-based syngas, Solar-based syngas)	EU mix & Wind	Natural gas & Power-to-Heat
Thoneman (2020) (n=13)	Market mix (Ammonia, biogas upgrading, fermentation)	Pure stream, and amine-based	PEM Electrolysis	Direct Hydrogenation	DE grid & Wind	Waste heat from chemical industry
Uusitalo et al. (2017)	Post combustion CO2	Amine-based	PEM electrolysis	Direct Hydrogenation	Wind	Natural gas and heat integration
Meunier et al. (2020)	Cement plant	Pure streams, and amine-based	Alkaline Electrolysis	Direct Hydrogenation	EU mix	Natural gas
*Nguyen, Zondervan (2019)**	Flue gas (no specification)	Not considered	Steam reforming, electrolysis, biomethane reforming, biomass gasification	Direct Hydrogenation, Bi/tri-reforming	Wind, PV, Hydro for hydrogen	Natural gas
Rumayor, Dominguez-Ramos, Irabien (2019)	Industrial Processes (burden free)	Not considered	Ecoinvent market	Direct Hydrogenation, Electro-reduction	PV solar	Steam (ecoinvent market)
Fernande-Dacosta (2019)	Post combustion	Amine-based	Alkaline Electrolysis	Direct Hydrogenation	PV & national mix	Natural gas
Biernacki et al. (2018)	CO2 from biogas upgrading to biomethane and DAC	Amine-based	PEM electrolysis	Direct Hydrogenation	Wind	Natural gas
Ravikumar, Keoleian, Miller (2020)	Post combustion	Amine-based	Alkaline Electrolysis	Direct Hydrogenation	Wind, PV, Nuclear	Nat mix
Consalez-Garay (2019)	Coal/NG power plants, DAC	Amine-based	AEC, PEM, SOEC electrolysis	Direct Hydrogenation	Solar, Wind, Nuclear	Heat integration, natural gas
Nabil et al. (2021)	Set values (no specification)	Amine-based	Steam methane reforming, AEC	Direct Hydrogenation, Electrochemical conversion	National mix (Canada)	Electric, national mix
Gul Ryoo et al. (2021)	Point source	Amine-based (MEA)	Alkaline Electrolysis	Direct Hydrogenation, Photocatalytic conversion	Solar, wind, Nuclear, nat mix (Korea)	Solar thermal, natural gas, steam
Eggeman et al. (2020)	Flue gas from biogas production	Pressure Swing Adsorption and recuperative afterburning	PEM electrolysis	Direct Hydrogenation	Wind (surplus)	Heat integration, Natural Gas
Delikonstantis et al. (2021) based on Chen et al. (2019)	Flue gas (no specification)	Amine-based (MEA)	Alkaline Electrolysis	Direct Hydrogenation	Wind	Heat integration, Heat pump
Chen et al. (2019)	Capture from internal biomass CHP plant	Amine-based	PEM Electrolysis	Direct Hydrogenation	PV and Biomass CHP	Biomass CHP
Adnan & Kibria (2020)	Not specified	Amine-based (von der Assen, 2013)	PEM electrolysis	Direct Hydrogenation, Syngas conversion, Direct synthesis	Wind, Solar, Nuclear	Not specified
Rosental, Fröhlich & Liebich (2020)	DAC, point source	Amine-based (MEA), Climeworks	Alkaline Electrolysis	Direct Hydrogenation	Wind	Electric heating

*Overview of the CO2-based methanol LCA studies published between 2017 and 2021. *= Results not included in the cross-study exercise due to irregular result reporting*

CO_2-based e/f-methanol

First and foremost the main source of variation between the collected studies can be found in the composition of the production chains. As summarised in previous sections, the production chains are mostly determined by the number of processing steps and the sources of feedstocks delivered to the production chain. Out of the 18 CO_2-based e/f-methanol LCAs, all considered direct hydrogenation (i.e. one-step approach) either as the primary product system (15/18) or as an alternative (3/18). Most authors explained that the reason for the focus on direct hydrogenation is its thermodynamically favourable position with respect to syngas conversion (i.e. two-step approach). Other arguments pointed at the strongly increasing research into direct hydrogenation of CO_2 for value-added products and the already existing pilot projects showing its technological feasibility.

Three out of 18 LCAs considered syngas conversion in addition to direct hydrogenation. Artz et al. (2018) used existing literature to assess the impact of syngas produced by rWGS, Co-electrolysis, and solar-thermal disassociation. Adnan & Kibria (2020) model the electrolysis of CO2 in addition to a low-TRL direct synthesis to methanol. Two out of the 18 LCAs include the electrochemical conversion of CO2 to CO and methanol using solid oxide electrolysis cells (Nabil et al. 2021; Rumayor et al. 2021). The photocatalytic direct conversion of CO2 to methanol was only assessed in a single study by Ryoo et al. (2021). Other methanol synthesis steps were included in the initial selection of articles but were excluded, mostly due to not following official LCA guidelines and opting for manual carbon footprint calculations. It is expected that especially early technologies tend to pick more convenient carbon footprint methods over LCA studies. Still, it is important to consider that it is likely that more LCAs on emerging technologies, such as the direct electrochemical synthesis of methanol, will be published in the near future.

Secondly, From an initial quick assessment of the contribution analyses in the collected studies it became clear that a few global choices regarding the supply chain primarily determine the environmental profile of the produced methanol. Especially the electricity source, heat source, hydrogen source, CO_2 source, and CO_2 capture technology were most relevant. All of these design choices are collected in table 18.
In terms of energy use it can be seen that the majority of studies used wind energy as main supplier of electricity (14/18), next is electricity from local grids (8/18), photovoltaic electricity (7/18), and nuclear electricity (4/18). Due to the reliance on hydrogen from electrolysis using PEM and AEC units, most studies assessed the relevance of multiple sources of electricity (12/18). Heat was mostly sourced from natural gas (9/18) though this was often coupled to heat integration to minimise heat-related impacts. Two studies assumed heat from power-to-heat technologies, another two considered waste heat from other industrial processes, only one study assumed solar thermal as main heat source.

The analysed product systems most often relied on CO_2 from point-source capture (12/18) and CO_2 from industrial chemical processes (4/18). Direct Air Capture was not often included (3/18), the lack of reliable data was reported as the most important reason. Data collection practices will be discussed in following sections. Hydrogen was most often produced in electrolysis cells with about an equal preference for PEM and AEC, only a few studies also considered other cell types such as SOEC or fossil routes via steam methane reforming.

The beforementioned aspects of the production system were often configured in alternatives that provided a stark contrast in their results, for example by comparing systems using fossil energy with those using renewable energy, or by opting for different synthesis pathways. The relation between this approach and the results will be elaborated in following sections.

Author	***Biomass source***	***Production route***	***Electricity source***	***Heat source***
Biernacki et al. (2018)	Wood residue (woodchips)	Gassification and syngas conversion	Grid (DE)	Natural gas (grid) and Biogas (internal)
Delikonstantis et al. (2021)	Not specified	Dry methane reforming + Water-Gas-Shift + Synthesis	Grid, natural gas combustion	Natural gas (grid)
Streeck et al. (2018)	Industrial wastewater (bio-based)	Wastewater to Microbial Electrolysis cell to direct hydrogenation	Grid (DE)	Natural gas (grid)
Yadav et al. (2020)	Wood residue (woodchips)	Gassification and syngas conversion	Grid (Sweden)	Wood-based Heat
Khoo et al. (2016)	Rice straw and sugar bagasse	Pre-treatment, Gassification, and Syngas conversion	Market, Internal biomass based Co-generation	Market, Internal biomass based Co-generation
Liu er al. (2020)	Surplus cotton stalks, wheat straw	Gassification and syngas conversion	Grid (China)	Steam, Heat integration
Renó et al. (2011)	Sugar bagasse	Gassification, WGS for conditioning, and standard syngas conversion	Internal biomass based Co-generation	Internal biomass based Co-generation
Fózer et al (2021)	Microalgae	Gassification and syngas conversion	Fluctuating Renewable electricity	Heat exchanger, (rest not known)
Da Silva (2021)	Rice straw	Gassification and syngas conversion	Grid (BR)	Natural gas (grid)

Bio-based methanol studies considered published between 2011-2021. Selected for the use of by-products as biomass feedstock

Biomethanol
The standard processes that are associated with biomethanol production were included in five out of the nine LCAs on biomethanol production, consisting of pre-treatment of the feedstock, gasification, gas conditioning/cleaning, and synthesis. Four LCAs examined other biomass conversion processes. Delikonstantis et al. (2021) analysed the use of plasma-based and thermochemical dry methane reforming for biogas conversion, rWGS and subsequent methanol synthesis. Streeck et al. (2018) considered the treatment of wastewater in a microbial electrolysis cell and downstream direct hydrogenation to methanol. Fózer et al. (2021) modelled the direct hydrothermal gasification of wet biomass at high temperatures and tri-reforming of the syngas to produce methanol, a technology that circumvents the need of drying wet biomass. Yadav et al. (2020) also deviated from the standard production chain by implementing a novel chemical pre-treatment process which was expected to lead to higher methanol conversion efficiencies.

In nearly all cases the feedstock for biomethanol was classified as a waste, residue or by-product. Wood residue from forestry, sugar bagasse from sugar production, and rice straw from rice cultivation were each assessed twice whereas wheat straw, surplus cotton stalks, industrial wastewater were assessed once. Microalgae form the only non-waste biomass source in the study by Fózer et al. (2021).

The relative abundance of a feedstock with a high energy content at the start of the fuel production stage and the often remote location of biomethanol plants makes it more attractive to produce electricity and heat from local biomass. Internal co-production from feedstock biomass or other waste flows formed the main energy inputs for 6 out of the 9 studies, the remainder being supplied via grid electricity and natural gas. The remaining four studies assessed biomethanol from a more abstract and national perspective, using larger plant designs that rely mainly on national energy mixes.

3. Methodology of the screened papers

Any literature-based comparison would be illogical if no attention would be given to the methodological foundation of the screened papers. Especially for the case of CCU projects, matters such as the system boundaries and approaching multifunctionality determine for a large part the impact results. Besides methodological considerations papers tend to differ in what is and what is not included in the Life Cycle Inventory. More importantly, the general data quality is another source of variation, though it can be challenging to assess data quality from just published material. Regardless, this section briefly discusses the methodological and technological choices in the screened papers with the aim to better support the comparative discussion.

CO2-based methanol	***LC foreground***	***LCI background***	***CO_2 feedstock considerations***	***Geographic location***	***Construction (foreground)***	***Transport (foreground)***	***System boundaries***	***Temporal coverage (+ scenarios)***	***Functional Unit***	***Multifunctionality***	***Impact method***	***Impact categories***
Sternberg, Jens, Bardow (2017)	Literature, manual calculations	Ecoinvent	Deducible, brief discussion	EU (DE)	Not included	Not included	Cradle-to-gate	Forecasted (2020)	Hydrogen utilisation	Not disclosed	ReCiPe	GWP, FD
Hoppe et al. (2017)	Literature, manual calculations	Ecoinvent 3.1	Deducible, no discussion	EU (DE)	Not included	Not included	Cradle-to-gate	Current	mass	Not disclosed	Not disclosed	GWP, RMI, TMR
Artz et al. (2018) (8 studies)	Literature (n=8), harmonized	Ecoinvent 3.5	Provided, brief discussion	EU (DE)	Not included	Not included	Cradle-to-gate	Forecasted (2020) and forecasted best-case	mass	Not disclosed	ReCiPe midpoint (h)	GWP
Thoneman (2020) (13 studies)	Literature (n=13), harmonized	Ecoinvent 3.5	Deducible, brief discussion	EU (DE)	Not included	Not included	Cradle-to-gate	Current	mass	Not disclosed	ILCD 2018 midpoint	GWP, ecosystem quality (all), Human Health (all), Resource use (land and minerals)
Uusitalo et al. (2017)	Literature	Gabi 6.0	Not deducible, no discussion	-	Not included	Not included	Cradle-to-gate	Current	LHV	Not disclosed	Not disclosed	GWP
Meunier et al. (2020)	Aspen Plus simulation	Ecoinvent v3	Not deducible, no discussion	-	Some considered	Not included	Gate-to-gate	Current	mass	Not disclosed	ReCiPe midpoint	GWP, FD, TA, FE, HT, WD, MD
Rumayor, Dominguez-Ramos, Irabien (2019)	Aspen Plus, manual calculations, Literature	Ecoinvent v3.3	Deducible, brief discussion	N.A.	Not included	Not included	Cradle-to-gate	Current	mass	Not disclosed	Not disclosed	GWP
Fernande-Dacosta (2019)	Literature, manual calculations	Ecoinvent (no version)	Deducible, thorough discussion	NL	Not included	Yes (Chemicals and waste)	Cradle-to-grave	Current	LHV	System expansion	Literature	GWP, NREU
Biernacki et al. (2018)	Aspen Plus simulation	Ecoinvent 3.3	Not deducible, limited discussion	DE	Yes, as scenario	Not included	Cradle-to-grave	Current	mass	Not disclosed	ILCD	GWP, FD, TA, FE, HT, WD, MD
Ravikumar, Keoleian, Miller (2020)	Literature, manual calculations	Simapro	Not deducible, included in expansion	-	Not included	Yes (intermediate transport)	Cradle-to-gate	Current and potential improvements	mass	System expansion	TRACI	GWP
Consalez-Garay (2019)	Literature, manual calculations	Ecoinvent	Not deducible, limited-discussion	-	Not included	Not included	Cradle-to-gate	Current and potential improvements	mass	Not disclosed	ReCiPe endpoint	Endpoints
Nabil et al. (2021)	Literature, manual calculations	Ecoinvent	-	-			Cradle-to-gate	Current	mass	Not disclosed	Literature	GWP, NREU
Gul Ryoo et al. (2021)	Literature, manual calculations	Ecoinvent	Deducible, no discussion	Korea	Included	Not included	Cradle-to-gate	Current	mass		ReCiPe midpoint (h) & endpoint	GWP, FE, TA, FD, PMF, WC
Eggeman et al. (2020)	Literature	Ecoinvent 3.5	Not deducible, limited discussion	DE	Not included	Not included	Cradle-to-gate	Current	mass	System expansion with crediting (n=5)	ReCiPe midpoint	GWP, FD, FE, ME, HT, POF, ODP, Ap
Delikonstantis et al. (2021)	Literature	Ecoinvent 3.6	Deducible, brief discussion	n.a.	Not included	Not included	Cradle-to-gate	Current and potential improvements	mass	Not disclosed	Environmental Footprint (EU)	GWP
Chen et al. (2019)	Literature, Aspen plus simulation	Gabi			Not included	Included	Cradle-to-gate	ex-ante	mass		CML 2001	GWP, AP, EP, POCP, ADP
Adnan & Kibria (2020)	Literature, Aspen plus simulation	Not disclosed	Deducible, no discussion		Not included	Not included	Cradle-to-gate	Current	mass	not disclosed	Not disclosed	GWP
Rosental, Fröhlich & Liebich (2020)	Literature	Ecoinvent	Deducible, limited discussion	EU (DE)	Included	Not included	Cradle-to-gate	2010 and 2050	mass	Allocation: mass	CML	GWP, AP, EP, ODP PMF, CED

CO2-based methanol	LC foreground	LCI background	CO_2 feedstock considerations		Geographic location	Construction (foreground)	Transport (foreground)	System boundaries	Temporal coverage (+ scenarios)	Functional Unit	Multifunctionality	Impact method
Delkonstantis et al. (2021)	Literature	Ecoinvent 3.6	Deducible, brief discussion	n.a.	Not included	Not included	Cradle-to-gate	current	mass	Not disclosed	Not disclosed	GWP
Biernacki et al. (2018)	Aspen Plus Similation	Ecoinvent 3.3	Not deducible, no discussion		Yes, as scenario	Not included	Cradle-to-grave	current	mass	Not disclosed	ILCD	GWP, FD, TA, FE, HT, WD, MD
Streeck et al (2018)	Literature, Chemcad simulations	Ecoinvent 3.4	Not deducible, limited discussion	DE	Included	Not included	Cradle-to-gate	current	mass	System expansion	Recipe (H)	GWP, TAP, POF, MDP, FEP, CED-f, CED-r
Yadav et al. (2020)	Literature, experiments, SimaPro sumulations	Ecoinvent 3.5	Not deducible, no discussion	SE	Not included	Included	Cradle-to-gate	current	mass	Not applicable	CML 2001	GWP, HTP, AP, LCEC
Liu et al. (2020)	Literature, Aspen Plus	Gabi 9.2	Not decible, no discussion	CN	Not included	Included	Cradle-to-gate	current	mass	Not disclosed	CML 2001	GWP, AP, HTP
Renó et al. (2011)	Literature	NREL, Ecoinvent, others	Deducible, brief discussion	CN, NL, etc.	Not included	Not included	Cradle-to-gate	current	mass	Allocation: energy content	CML 2001	GWP, AP, ET, OLD, HT, et. (most included)
Fózer et al. (2021)	Literature, simulations	Not disclosed	Not deducible, no discussion	BR	Not included	Not included	Cradle-to-gate	ex-ante	mass	Not disclosed	IMPACT2002+ v2.14	GWP, AP, ET, OLD, HT, etc. (most included)
khoo et al. (2016)	Literature, Artificial Neural Networks, Aspen plus	Ecoinvent	Not deducible, limited discussion		Not included	Included	Cradle-to-gate	current	mass	Allocation: mass	Not disclosed	GWP, AP, EP, HT, POCP, Water use
da Silva et al. (2021)	Experimental, Literature, Aspen Plus	None (full LCI)	All biogenic CO2 considered neutral	BR	Not included	Included	Cradle-to-gate	current	mass	Allocation: economic	Calculated (IPCC GWP's)	GWP

Tables showing all methodological parameters of the collected papers

Goal & Scope definition

The temporal scale defined in the collected LCA studies show in practice the challenges that were identified in the literature review of ex-ante LCAs in chapter 5. As van der Giesen et al. (2020) pointed out, a temporal mismatch between the foreground and background system can be problematic and should be avoided. However, in 11 out of the 18 LCAs on CO_2-based methanol no special attention was given to the temporal scale while the compilation of the Life Cycle Inventory mostly relied on experimental or simulated data. The result is that the foreground system details a future expectation of a technology whilst all background data, including energy mixes, stems from databases that are at best only slightly outdated. In defence for the disregard for temporal scale is the fact that CO_2-based methanol projects already exist, limiting foreground systems to mimic these cases reduces the discrepancy between the fore- and background system to only a couple of years. Still, it is concerning that especially for lower TRL technologies (e.g. DAC, or electro/photochemical methanol synthesis) so few studies give the temporal relevance of the LCI the attention it deserves.

In some studies, such as the work by Artz et al. (2018) and Sternberg et al. (2017), the temporal scale was covered in scenarios. Yet, the scenario by Artz et al. was limited to global assumptions about the carbon intensity of important feedstocks and energy inputs, disregarding the relevance of the background system. 2050 was set as a global time horizon but the authors failed to take into account the role of technological improvements (i.e. scale-up) in the foreground system. Rosental et al. (2020) were the only to consider both the role of a future background system by implementing technological improvements for key background processes, and foreground system scenarios using future technological expectations.

Other authors showcased temporal awareness by performing sensitivity analyses in line with expected future improvements. Though not disclosing a certain time horizon. Papers by Ravikumar et al. (2020), Consalez-Garay (2019), and Delikonstantis et al. (2021) do provide the reader with an idea about potential future states of the assessed methanol systems. It could be argued that reporting technological improvements without a temporal aspect at least prevents unjust and highly specific technological expectations by a set date.
Developments in the reference system were not accounted for by any study, meaning that the comparison was often performed between a futuristic product system and an outdated conventional system. In studies were impact results between alternatives were only marginally different, this could lead to the drawing of incomplete conclusions.

In terms of geographical coverage most CO_2-based methanol studies focus on the European setting, thereby also relying on the respective national energy mixes and the presence of renewable energy technologies. Biobased methanol studies tended to be non-European with exception of forestry residue valorisation projects. The obvious consequences of the geographical location were generally discussed at length in biobased methanol studies whereas CO_2-based methanol studies focused more on the technological aspects of the study.

Functional units showed little variation across the collected studies, though it is expected that this is also a result of the initial search queries and article selection. The focus of this research project is the assessment of CO_2-based methanol but other goals such as the finding of the most preferable means of CO_2 valorisation could also be defined. The studies that had the latter orientation were automatically excluded from the search results as their impact results would not directly prove useful for the goal of this cross-literature analysis.

System boundaries and the methodological consideration of feedstock CO_2 for CO_2-based methanol

Of particular importance for CCU LCAs is the definition of the system boundaries, as these partially determine how the feedstock CO_2 is viewed. As nearly all studies follow the ISO 14040/14044 guidelines for LCA the system boundaries nearly always receive attention in the methodological section. However, the system boundaries are not always well-explained and tend to focus more on the direct lifecycle of the produced methanol from its cradle and not the origin of the feedstocks. Only two studies by Fernández-Dacosta et al. (2019) and Meunier et al. (2020) included a thorough discussion on the origin of the feedstocks in a gate-to-grave approach. All studies assumed a cradle-to-gate approach with the exception of Biernacki et al. (2018), Rosental et al. (2020) and Fernández-Dacosta et al. (2019) who also explicitly addressed the end-of-life of the produced chemicals in a cradle-to-grave approach as to prevent the drawing of incorrect conclusions.

Besides system boundaries, the methodological treatment of the CO_2 feedstock appears to be a major source of variation between studies. Practically, this leads to 1) Differences in the provision of credits to the CO_2 feedstock, and 2) the inclusion or exclusion of carbon capture processes from the product system. Direct Air Capture is an exception to the challenges imposed by these two points (Ramírez Ramírez et al. 2020); the capture of CO_2 receives a carbon credit of -1 kg CO_2 eq./kg CO_2, and the entire capture process is included within the system boundaries.

For the case of point capture however, additional consideration is required, as there is a moment when CO_2 is converted from a waste into a primary product. These cases are first and foremost cases of multifunctionality, as capture processes provide both a function to the emitting system and to the system making use of the emitted CO_2. According to the ISO 14040/44 guidelines such multifunctionality issues should be solved first by subdivision or system expansion and only if this is not feasible, by allocation. In the screened papers three strategies to deal with the issue of multifunctionality could be identified.

A first strategy that was applied in three of the reviewed papers is the 'cut-off' approach, in which the first (emitter) and second (user) product systems are considered separately. The intermediate value chain between systems consists of the capture, compression, and transport of the CO2. The placement of the 'cut' in this intermediate value chain is then the most important methodological consideration because this determines how the impacts of the CO2 feedstock are divided over both systems. In the reviewed literature the point of cut-off differs, either including or excluding the capture and compression processes. When the system boundaries are defined this still leaves the issue of CO2 credits or burdens, which are commonly provided in LCA studies for the temporary carbon sequestration potential of CO2-based products. In the cut-off approach, CO2 crediting or burdening is not methodologically constrained and tends to be a source of academic debate (Fernández-Dacosta, 2019). Indeed, the provision of credits to the CO2-utilising system is another source of variation in the reviewed papers. Meunier et al. (2020), whose earlier work is often cited by other papers, include the capture and compression within the system boundaries but do not seem to take into account credits. The result is a net-positive cradle-to-gate CC impact score. Rosental et al. (2020) model point source capture and DAC within the system boundaries and state that they assume a carbon credit of -1 for the uptake of carbon in both cases though this is not reflected in the results which are also net positive. The cut-off approach was adopted by multiple papers but the discussion of the carbon feedstock was often too limited to determine the place of the cut-off and its implications.

The second strategy is adopted by the majority of screened papers and circumvents part of the complexity of CCU LCAs by assigning a set GWP to the CO_2 feedstock based on earlier reports or estimations. In essence, this leaves the CCU part of the foreground systems to other authors and instead focuses on the utilisation side of the total system. Examples are Artz et al. (2018) who assign a value of -0.87 and -1.0 kg CO_2 eq. / kg CO_2 depending on technological expectations of carbon capture in 2020 and 2050. This approach is copied by other authors such as Sternberg et al. (2017) who refer to their earlier work which found a carbon intensity of -0.701 kg CO_2 eq. / kg CO_2. Nabil et al. (2021) similarly follow the -0.8 CO_2 eq. / kg CO_2 reported by Müller et al. (2020b) who studied and published the carbon footprints of feedstock CO_2 for that purpose. Studies published before 2021 often cite Von der Assen et al. (2013) and their contribution to the carbon intensity of CO_2 feedstocks (e.g. Adnan & Kibria, 2020) whereas the work by Müller et al. is more popular for recent publications.
Some studies (e.g. Ryoo et al., 2021) argue for the exclusion feedstock CO_2 impacts altogether to provide more easily interpretable results without spending considerable efforts understanding the variability of CO_2 sources. Such papers then often result in net-positive cradle-to-gate CC impacts.

Clearly the reliance on set values for the carbon intensity of feedstock CO_2 is a popular method of mitigating the complexity of CCU LCAs. When assessing CCU projects from a more abstract level this could be a valuable tool, especially when used carbon intensities originate from elaborate reviews such as Müller et al., (2020b). Yet, as Ramírez Ramírez et al. (2019) explain, there is a need of case-by-case analysis if authors attempt to provide case-specific conclusions from a higher level approach. For that reason, the third strategy seen in screened papers is system expansion, meaning that both the emitter and the utiliser are considered in a single system. The expansion of the system boundaries allows authors to more closely examine the relation between the two systems and paves the way for a more consequential modelling approach in which broader questions can be answered. Eggeman (2020) and colleagues for example, study a complex system of combined heat and power generation from biogas and methanol synthesis from CO_2 captured from the raw biogas. The authors then study scenarios with various assumptions including avoided emissions / credits for substitution in the local electrical grid. The results and discussion show the use of the system for a local case but due to the awarding of credits become difficult to interpret for the case of methanol production. Ravikumar et al. (2020) use system expansion to attempt to answer whether it is better to use renewable energy sources for grid replacement plus conventional methanol production or instead to use renewable energy sources for the production of CO_2-based r-methanol. As is the case for Eggeman et al., the results of a consequential modelling approach are not easily interpreted for attributional purposes. Yet, the use of system expansion proves a deeper understanding of how CO_2 emissions should be counted.

Due to different reporting methods the treatment of CO_2 as a feedstock could not be analysed in all reviewed papers. Some papers discussed the nature of the feedstock before entry in the system, others discussed its characteristics after capture within the system boundaries. The results of this exercise are shown in the appendices, showing the findings of the carbon intensity of the feedstock CO_2 as reported in the papers or calculated from values in the papers. The reader is advised to be careful when reading these results as errors could easily have been made in the review of the papers.

Other credits or avoided burdens
Avoided burdens are a common practice in LCAs and are applied when a co-produced product has the potential to displace the same product produced by a dedicated conventional process.
The electrolysis of water, besides hydrogen, yields oxygen which can be compressed and sold on the market or injected in other parallel processes in cases of Industrial Symbiosis. Multiple studies consider the by-product O_2 as mitigating factor for the overall impact score by allocating the benefits of avoided burdens to the product system (e.g. Rumayor et al., 2019, Biernacki et al., 2018). Whether surplus oxygen

from the large scale implementation of electrolysis should be included in the main product system and not in a sensitivity analysis is open for debate. The use of avoided burdens could also be seen in the work by Eggeman et al. (2020) who provide the avoided burdens for co-produced electricity and resulting grid replacement. For the case of biomethanol, Streeck et al. (2019) give avoided burdens to the system for its processing of wastewater as opposed to conventional wastewater treatment.
In the screened papers, the application of credits/avoided burdens majorly impacted the total impact assessment and caused the overall results to be non-comparable to other studies. Any supplementary materials furthermore failed to list results without the avoided burdens.

Foreground data collection and background systems

Of particular importance to this exercise is the origin of the data that describes the CO_2-based r/f-methanol and bio-based methanol production systems. For the modelling of the methanol synthesis process and carbon capture process, an equal preference in the screened papers was found for computer simulation of key processes with dedicated software, and the manual calculation. Computer simulation (using Aspen Plus) often relied on data inputs from the software's databases, only sometimes using kinetics from experimental testing. Authors typically applied full software-based system design to approximate the entire process (e.g. Meunier et al., 2020). Manual calculations were found to more often make use of earlier LCA work, non-LCA footprint calculations, experiments or advanced topic-specific literature. Sticking to the hierarchy of LCI data collection from Parvatker & Eckelman (2019), only a couple of papers actually used data from pilot projects or lab-experiments and most used stoichiometry and proxies to compile the data for the foreground system, resulting in a lower overall data quality.

The supply of heat and electricity to the major processes was most often done using background processes from LCI databases. Only in some cases authors actually engaged in the modelling of power systems such as wind turbines. In these cases the inventory for these processes were very limited and only included a couple of major material and energy inputs (e.g. Meunier et al., 2020). In some papers the energy delivering system was integrated and more complex due to vague system boundaries. Authors tended to then include full inventories of important energy and material flows but generally did not include material for construction. Only a few authors actually considered material and energy inputs for the construction of carbon capture and methanol synthesis plants (e.g. Rosental et al., 2020; Biernacki et al., 2018; Meunier et al., 2020). Even fewer included major transportation processes for key material inputs and exchanges (e.g. Chen et al., 2019; Fernandez-Dacosta et al. 2019).

19 out of the 27 studies used the ecoinvent database for the background system, others used the Gabi software and included databases or the databases in SimaPro without specifying exactly which databases were used. The ecoinvent v3+ database was most frequently used, though often authors failed to specify exactly which version was used in the research. In a rare occasion the entire product system was modelled in the foreground system due to the isolated case study (da Silva et al., 2021). The consulted databases were relatively up to date and no cases of older databases (ecoinvent v1-v2) could be found.

Impact methods and impact categories

All papers included the Climate Change impact category in the impact assessment with the exception of the work by Consalez-Garay (2019) who used endpoint indicators in their assessment. Only seven out of the 18 studies on CO_2-based r/f-methanol included other relevant environmental impact categories regarding impacts on ecosystem quality or human health. Another four included indicators regarding the efficiency of used energy and the use of fossil resources. Bio-based methanol studies tended to include the entire environmental profile with seven out of the total of nine studies.

The impact methods used by the authors to calculate the impact indicators were most often the ReCiPe (7/27), CML 2001 (5/27) and ILCD methods (4/27). Some authors included single sources for specific impact categories, most often from collaborative workshops organised by relevant institutions (3/27). Multiple studies failed to explicitly address the impact assessment methods. This lack of attention could also be noticed in the type of methods used for the climate change impact assessment, as there was rarely a discussion on the temporal aspect of the global warming potential calculations (i.e. GWP 20/100).

Overview

As can be deduced from the previous sections, the variation between studies is large. Still, some consistencies can also be found, for example in the approach to the modelling of the foreground system, the use of background databases, LCA software, and impact assessment methods. With caution, it should therefore be possible to map the results of these papers and assessing the relation of the LCA performed in this study to the reported results.

H. Biomethanol results

The biomethanol part was included in the report in earlier versions but excluded in the final version due to too large differences between assessed studies. Results here are only as good as the reporting style of the included papers and prone to interpretation errors.

Climate change impacts - Biomethanol

Because there are far fewer similarities between biomethanol systems and the ZEF microplant system, the discussion on the reported results in biomethanol LCA studies is approached a bit differently. In this section, the results are described in the context of each individual study, without much detail on inter-study comparison.

Table 2: Reported CC impacts of Biomethanol. Biomass burdens are sometimes excluded

Author	***Biomass burden***	***Biomass treatment***	***CC impact***
Biernacki et al. (2018)	Included	Included	0.75
Delikonstantis et al. (2021)	Burden-free	Included	5.58
	Burden-free	Included	2.05
Streeck et al. (2019)	Burden-free	Included	-0.8 to -1.01
Yadav et al. (2020)	Burden-free	Included	6.31E-2
	Burden-free	Included	
	Burden-free	Included	0.46
	Burden-free	Included	0.44
Khoo et al. (2016)	Included		4.70
	Included		0.77
Renó et al. (2011)	Included	Included, allocated	-2.28
Liu et al. (2020)	Included	Included	-3.26
da Silva et al. (2021)	Included		0.81
Fózer et al. (2021)	Included	Included	-0.44
	Included	Included	-0.73

Reported CC impacts for bio-methanol

The most recent paper by Delikonstantis et al. (2021) assessed methanol synthesised from syngas produced by plasma-assisted and electrically heated dry methane reforming (DMR). Delikontsantis et al. furthermore compared their DMR-based methanol routes with CO_2-based methanol (using renewable electricity for hydrogen production). The comparison unequivocally showed that it is highly probable that CO_2-based methanol significantly outperforms bio-based methanol via the DMR route in the climate change impact category. The use of biogas in the electrified methanol synthesis route led to CC impacts of between 7.46 kg CO_2 eq. for plasma-assisted- and 2.82 kg CO_2 eq. for electrically heated thermo-catalytic DMR. Full electrification and supplying the full energy demand with PV or wind electricity reduced the impacts with approximately 55 to 66%, though this was only calculated for natural gas based processes.

Da Silva et al. (2021) found that the CC impact of methanol from rice straw came to 0.809 CO_2 kg eq. / kg MeOH. The site-specific contributions to the CC IC included the emissions from diesel burning for biomass collection and transport (43% and 15% respectively), showing how the design of the cultivation area and the supply chain plays an important role in the total CC impact of rice straw-based methanol. Da Silva et al. (2021) considered all direct emissions of biomass processing and methanol synthesis to be carbon neutral due to its biogenic nature. The authors did not consider methanol as temporary carbon sink and therefore did not include the carbon uptake by the biomass. If these would be included, the cradle-to-gate CC impact would likely drop below zero.

One of four papers that did report negative impact scores in the climate change impact category was the work by Renó et al. (2011) on the use of sugar bagasse (-2.284 kg CO_2 eq./FU). In part the negative impact scores can be attributed to the inclusion of an integrated co-generation plant, which supplies heat and electricity from biomass. However, the authors seem to have assumed carbon credits for carbon sequestration in plant growth without taking into account other upstream impacts. In addition, the first steps of the biomass treatment process were allocated on the basis of energy content in a near 1:1 ratio between the juice and bagasse flows, thus leading to lower impacts.

The paper by Liu et al. (2020) reported strongly negative CC impact scores as well; -3.26 kg CO_2 eq. / kg MeOH. Due to a non-conventional way of reporting the LCI, the reader is left to guess how this impact score was achieved. In theory, it should not be possible to achieve this score without awarding credits for the product system or without preventing downstream emissions of the captured biogenic CO_2 . It is expected that the authors did not model key downstream processes for the treatment of by-products from feedstock processing, thereby omitting sources of CO_2 emissions. Liu et al. (2020) did find that the biomethanol performed similar to coal-based methanol in the Human toxicity and Acidification potential impact categories.

An interesting case can be found in the ex-ante work of Fózer et al. (2021) who modelled the hydrothermal gasification of wet biomass at high temperatures and the subsequent tri-reforming of the syngas to produce methanol. The authors considered the boosting of the syngas by renewably produced hydrogen to enable optimal syngas ratios for methanol synthesis. Hydrogen was assumed to be produced in an AEC with electricity from variable renewable energy sources. The most significant impacts were coupled to the hydrothermal gasification process and the alkali metal catalyst production. The negative emissions were attributable to the high carbon uptake of the microalgae strain. In total, the low carbon intensity of the energy supply to the total system resulted in negative cradle-to-gate emissions of -0.44 and -0.73 kg CO_2 eq. / kg MeOH. No major inconsistencies in the methodology and LCI could be identified which indicates that this particular route might be a potential competitor for CO_2-based methanol.
Streeck et al fixme

Overall, the reported CC impacts of biomethanol studies seem to largely depend on case-specific parameters and are perhaps even more vulnerable to methodological variation than CO_2-based methanol studies. It is hoped that the previous introduction into the case studies offers some help with the interpretation of the results. Yet, for the purpose of this study it is not required to elaborate case-specific details, instead the results should give an introductory overview of the performance of biomethanol in relation to CO_2-based methanol. This is elaborated in the following sections.

Biomethanol – other impact categories

The purpose of this particular section is to validate if biomethanol could be desirable over CO_2-based methanol taking other impact categories in consideration than Climate Change. Unfortunately a lack of reporting on the used LCIA methods makes it practically impossible to perform a side-by-side comparison of the LCA results of this study with literature results of biomethanol. To still partially adhere to the goal of this section, the biomethanol literature is scanned on comparative studies with conventional fossil-based methanol as this is the common denominator between life cycle assessments of CO_2-based methanol and of bio-based methanol.

All studies that include other impact categories clearly show that biomethanol is associated with higher impacts in acidification and eutrophication impact categories. These higher impacts are mostly related to the use of fertilisers in cases of biomass from agricultural businesses (Fózer et al., 2021; Khoo et al., 2016; Reno et al., 2011), but is also found in a study of biomass valorisation from waste-water treatment (Streeck et al., 2018) and biomass from micro-algae (Fózer et al., 2021). Impacts in these categories are furthermore aggravated by all processes surrounding the upgrading of biomass, including the biomass preparation, gasification, gas cleaning, and conditioning (Biernacki et al., 2018; Fózer et al., 2021). NOx emissions from fertiliser use furthermore caused higher impacts in photochemical ozone creation categories (Khoo et al., 2016; Biernacki et al., 2018), though this category does not show a large difference in the work by Streeck et al. (2018) and Liu et al. (2020). There is not a single study that reports lower impacts in acidification, eutrophication and photochemical ozone creation impact categories compared to conventional methanol. Impacts of bio-based methanol are often a factor of two or more higher in these categories.

Ecotoxicity and human toxicity categories were found to show slightly lower impacts compared to conventional methanol in the studies by Khoo et al. (2016), Liu et al. (2020), though Khoo et al. warned for the use of herbicides and pesticides and their implications for toxicity impacts. Biernacki et al. (2018) on the other hand, found that bio-based methanol was more impactful due to emissions of combustion products from syngas conversion.

Similar to the results found in this study, the ozone layer depletion potential of natural gas-based methanol was found to be much higher than bio-based methanol in collected works. In all the collected studies, climate change and ozone layer depletion categories are the only areas where biomethanol seems to significantly outperform conventional methanol.

I. Full LCI comparative overview

The LCI comparison with other comparable works was done on the basis of the data below. Not all data could be gathered from the assessed works, hence some own calculations filled in the blanks. Although effort has been put into collecting the correct data, it is not recommended to blindly use this data for continued research and instead verify the values independently.

Study	H_2 IN	CO_2 In	H_2 elec. (kWh/kg)	CO_2 elec (kwh/kg)	CO_2 heat (mJ/kg)	H_2 elec total (kWh)	CO_2 elec total (kWh)	CO_2 heat total (MJ)	MSR total (kWh)	MSR heat (MJ)	Total energy (no steam)	Total energy (total) kWh	Authors, comment, source
Aresta et al. (2002)	0.19	1.37	54.00	0.13	1.06	10.28	0.16	1.36	0.89		11.33	11.70	From Thonemann (2020)
Biernacki et al. (2018)	0.19	1.40	54.00	0.13	1.06	10.37	0.18	1.49	0.34	0.14	10.89	11.34	From Thonemann (2020)
Kim et al. (2011)		1.84	54.00	0.13	1.06	0.00	0.24	1.96	2.46	3.59	2.70	4.24	From Thonemann (2020)
Meunier et al. (2019)	0.20	1.44	54.00	0.13	1.06	11.08	0.19	1.53	0.33	-1.40	11.60	12.03	Not considering heat integratio
Sternberg & Bardow (2015)	0.20	1.44	54.00	0.13	1.06	10.70	0.19	1.53	1.33		12.22	12.64	From Thonemann (2020)
Sternberg et al. (2017) (1)	0.20	1.44	54.00	0.13	1.06	10.76	0.18	1.53	1.34		12.28	12.71	From Thonemann (2020)
Sternberg et al. (2017) (2)	0.20	1.48	54.00	0.13	1.06	11.14	0.19	1.58	0.69		12.02	12.46	From Thonemann (2020)
Sternberg et al. (2017) (3)	0.19	1.38	54.00	0.13	1.06	10.32	0.18	1.47	0.67	1.33	11.17	11.94	From Thonemann (2020)
Uustitalo et al. (2017)	0.19	1.38	54.00	0.13	1.06	10.37	0.18	1.47	1.33	-1.23	11.88	12.29	Not considering heat integratio
Fernández-Dacosta et al. (2019)	0.20	1.45	54.00	0.13	1.06	10.95	0.19	1.55	0.14	3.32	11.28	12.64	From Thonemann (2020)
von der Assen et al. (2015) (1)	0.19	1.38	54.00	0.13	1.06	10.24	0.18	1.46	1.27	2.20	11.68	12.70	From Thonemann (2020)
Rosental et al. (2021) (DAC)	0.20	1.44	45.50	1.98	6.84	9.23	0.79	9.85	0.33	-1.40	10.35	13.09	Not considering heat integratio
Rosental et al. (2021) (PS)	0.20	1.44	45.50	0.05	3.13	9.23	0.02	4.51	0.33	-1.40	9.58	10.84	Not considering heat integratio
Nabil (one-step)	0.20	1.40	50.00	0.35		10.00	0.50		42.01		52.51	52.51	Electrochemical
Nabil (two-step)	0.20	1.40	50.00	0.35		10.00	0.50		37.77		48.27	48.27	Electrochemical
Rumayor (DH)	0.19	1.38				n.a.	n.a.				11.90	11.90	Direct hydrogenation
Rumayor (ER)	0.22	1.38				n.a.	n.a.				50.50	50.50	Electrochemical
Hoppe (DAC)	0.19	1.37	54.80	0.25	1.65	10.40	0.34	0.63	1.27		12.01	12.19	Direct air capture
Hoppe (PS)	0.19	1.37	54.80	0.16		10.40	0.22		1.27		11.89	11.89	Point source capture
Pérez-Fortes (2016)	0.20	1.46	50.00	n.a.	n.a.	10.00			0.17	0.44	10.17	10.29	High purity co2 from ethanol production (no capture energy)
Kalbani (DH)				1.11		22.89						24.61	Direct hydrogenation
Kalbani (SOEC)				1.11								12.61	Electrochemical (SOEC)

J. Additional PV panel data

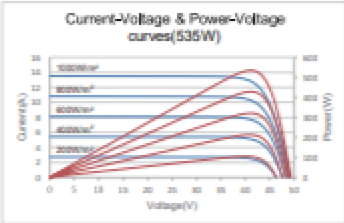
The PV panels in this study were based as much as possible on the panels in these data sheets. All LCI information was sourced from Frischknecht et al., (2020), and a variety of additional LCI studies (See main report)

ELECTRICAL SPECIFICATIONS

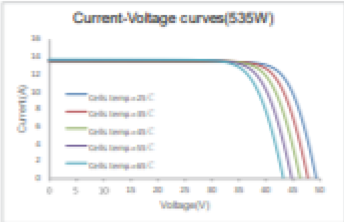
Power rating (front)	525 Wp		530 Wp		535 Wp		540 Wp		545 Wp	
Testing Condition	Front	Back	Front	Back	Front	Back	Front	Back	Front	Back
STC rated output (P_{mpp}/Wp)	525	368	530	371	535	375	540	378	545	382
Rated voltage (V_{mpp}/V) at STC	41.43	41.48	41.60	41.65	41.76	41.81	41.93	41.98	42.10	42.15
Rated current (I_{mpp}/A) at STC	12.67	8.87	12.74	8.92	12.81	8.97	12.88	9.01	12.95	9.06
Open circuit voltage (V_{oc}/V) at STC	49.30	49.25	49.50	49.45	49.70	49.65	49.90	49.85	50.10	50.05
Short circuit current (I_{sc}/A) at STC	13.40	9.27	13.48	9.33	13.57	9.39	13.66	9.45	13.75	9.52
Module efficiency	20.5%	14.4%	20.7%	14.5%	20.9%	14.7%	21.1%	14.8%	21.3%	14.9%
Temperature coefficient (P_{max})	- 0.35%/°C									
Temperature coefficient (I_{sc})	+0.045%/°C									
Temperature coefficient (V_{oc})	- 0.27%/°C									
Nominal module operating temperature (NMOT)	41±2°C									
Maximum system voltage (IEC/UL)	1500V_{DC}									
Number of diodes	3									
Junction box IP rating	IP 68									
Maximum series fuse rating	30 A									

STC: Irradiance 1000W/m², Cell Temperature 25°C, AM=1.5

CURVE



Current-Voltage & Power-Voltage curves(535W)



Current-Voltage curves(535W)

ELECTRICAL SPECIFICATIONS (Integrated power)

P_{mpp} gain	P_{mpp}	V_{mpp}	I_{mpp}	V_{oc}	I_{sc}
5%	562 Wp	41.76 V	13.45 A	49.70 V	14.25 A
10%	589 Wp	41.76 V	14.09 A	49.70 V	14.93 A
15%	615 Wp	41.77 V	14.73 A	49.71 V	15.61 A
20%	642 Wp	41.77 V	15.37 A	49.71 V	16.29 A
25%	669 Wp	41.78 V	16.01 A	49.72 V	16.96 A

Electrical characteristics with different rear power gain (reference to 535 W)

MECHANICAL SPECIFICATIONS

Outer dimensions (L x W x H)	2256 x 1133 x 35 mm
Frame technology	Aluminum, silver anodized
Glass thickness	2.0 mm
Cable length (IEC/UL)	Portrait: 300 mm Landscape: 1400 mm
Cable diameter (IEC/UL)	4 mm² / 12 AWG
[1] Maximum mechanical test load	5400 Pa (front) / 2400 Pa (back)
Connector type (IEC/UL)	HCB40 / MC4-EVO2

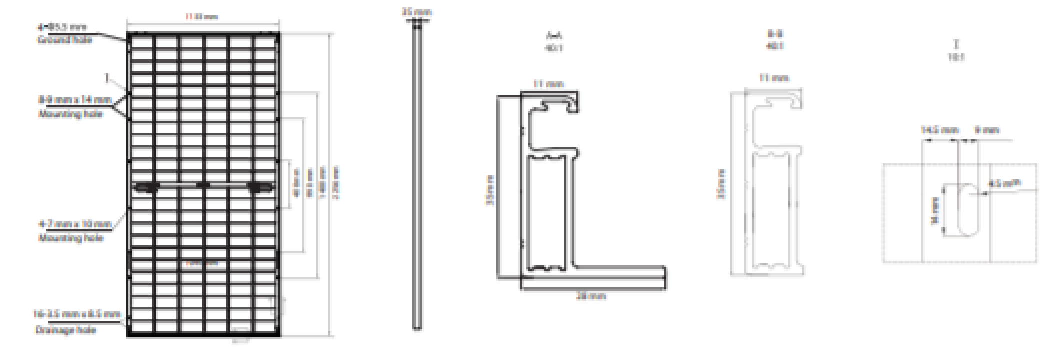
[1] Refer to Astronergy crystalline installation manual or contact technical department.
Maximum Mechanical Test Load=1.5×Maximum Mechanical Design Load.

PACKING SPECIFICATIONS

[1] Module Weight	32.3 kg
[2] Packing unit	31 pcs / box
Weight of packing unit (for 40'HQ container)	1040 kg
Number of modules per 40'HQ container	620 pcs

[1] Tolerance +/- 1.0kg
[2] Subject to sales contract

MODULE DIMENSION DETAILS



K. PV panel unit process data

Exchange	Value	Unit	Comment
photovoltaic cell, single-Si, at plant	0.94	m2	Frischknecht et al. (2020); for single-si monofacial
Aluminium, wrought alloy {GLO}| market | Cut-off, U	1.24	kg	Own calculation Méndez et al. (2021): Frame Updated Industrial Tier 1 producers (1.374kg), assumed that bifacial panels contain 90% of the aluminium of monofacial panels due to a smaller aluminium bevel on the backside (source: Chint Solar personal communication)
Silicone product {RER}| market silicone product | Cut-off, U	0.20	kg	Méndez et al. (2021): Industrial Tier 1 producers
Solar glass, low-iron {GLO}| market | Cut-off, U	7.77	kg	Méndez et al. (2021): For 3.2 mm (frontside)
Solar glass, low-iron {GLO}| market | Cut-off, U	6.80	kg	Own calculation / assumption: 2.8 mm (backside) (Jiu et al., 2019; PV supplier)
Tempering, flat glass	14.57	kg	Frischknecht et al. (2020); Sum of glass inputs
Ethylvinylacetate, foil {GLO}| market | Cut-off, U	0.88	kg	Méndez et al. (2021): EVA Encapsulant updated Industrial Tier 1 producers, EVA requirements are not assumed to be higher for bifacial panels
Ethylene vinyl acetate copolymer {RER}| market ethylene vinyl acetate copolymer | Cut-off, U	2.23E-02	kg	Méndez et al. (2021): Electric connectors
Copper {GLO}| market | Cut-off, U	3.96E-02	kg	Méndez et al. (2021): Electric connectors
Glass fibre reinforced plastic, polyamide, injection moulded {GLO}| market | Cut-off, U	0.19	kg	Méndez et al. (2021): Connection box
Silicon capacitor (diode)	2.51E-03	kg	Méndez et al. (2021): Updated
Corrugated board box {RER}| market | Cut-off, U	1.10	kg	Méndez et al. (2021): Packaging
Copper {GLO}| market | Cut-off, U	0.10	kg	Frischknecht et al. (2020); for single-si monofacial
Wire drawing, copper {GLO}| market | Cut-off, U	0.10	kg	Frischknecht et al. (2020); for single-si monofacial
polyethylene terephthalate, granulate, amorphous, at plant	0.35	kg	Frischknecht et al. (2020); for single-si monofacial
polyethylene, HDPE, granulate, at plant	2.38E-02	kg	Frischknecht et al. (2020); for single-si monofacial
tap water, water balance according to MoeK 2013, at user	5.03	kg	Frischknecht et al. (2020); for single-si monofacial
hydrogen fluoride, at plant	6.24E-02	kg	Frischknecht et al. (2020); for single-si monofacial
1-propanol, at plant	1.59E-02	kg	Frischknecht et al. (2020); for single-si monofacial
isopropanol, at plant	1.47E-04	kg	Frischknecht et al. (2020); for single-si monofacial
potassium hydroxide, at regional storage	5.14E-02	kg	Frischknecht et al. (2020); for single-si monofacial
soap, at plant	1.16E-02	kg	Frischknecht et al. (2020); for single-si monofacial
EUR-flat pallet	5.00E-02	unit	Frischknecht et al. (2020); for single-si monofacial
Electricity, medium voltage,	1.41	kWh	Méndez et al. (2021); For poly-Si monofacial
Heat, central or small-scale, natural gas {Europe w/o CH}| market | Cut-off, U	5.41	MJ	Méndez et al. (2021); For poly-Si monofacial
photovoltaic panel factory	4.00E-06	unit	Frischknecht et al. (2020); for single-si monofacial
transport, freight, lorry, fleet average	2.77	tkm	Frischknecht et al. (2020); for single-si monofacial
transport, freight, rail	16.64	tkm	Frischknecht et al. (2020); for single-si monofacial
disposal, municipal solid waste, 22.9% water, to municipal incineration	3.00E-02	kg	Frischknecht et al. (2020); for single-si monofacial
disposal, polyvinylfluoride, 0.2% water, to municipal incineration	4.29E-03	kg	Frischknecht et al. (2020); for single-si monofacial
disposal, plastics, mixture, 15.3% water, to municipal incineration	2.81E-02	kg	Frischknecht et al. (2020); for single-si monofacial
disposal, used mineral oil, 10% water, to hazardous waste incineration	1.61E-03	kg	Frischknecht et al. (2020); for single-si monofacial
treatment, sewage, residence, to wastewater treatment, class 2	4.53E-03	m3	Frischknecht et al. (2020); for single-si monofacial
Carbon dioxide	2.18E-02	kg	Frischknecht et al. (2020); for single-si monofacial
Heat, waste	5.03E+01	MJ	Frischknecht et al. (2020); for single-si monofacial

NMVOC, non-methane volatile organic compounds, unspecified origin	8.06E-03	kg	Frischknecht et al. (2020); for single-si monofacial
Water	5.03E-01	m3	Frischknecht et al. (2020); for single-si monofacial

L. Extended ex-ante literature review

1. Prospective / Ex-ante LCAs

Since the introduction of Life Cycle Assessment and the drafting of ISO guidelines LCA has solidified its reputation as scientific tool for the analysis and assessment of environmental impacts associated with products, services, or systems. The relative success with which LCA practitioners facilitate discussions on the sustainability of complex systems then spawned a wider interest in applications of LCA beyond its conventional use. To this date most LCA studies are performed on an ex post basis, meaning that the analysed system is already in place and the needed data can be extracted by observing its processes (Cucurachi et al., 2020). Yet, it is well known amongst technology developers and LCA practitioners alike that the power to influence and improve the environmental impact of a product system is greater earlier in its development process rather than later (Arvidsson et al., 2017).
The mismatch between the typical application of LCA and the application of the tool for those cases that could benefit most from it, led to a large variety of case studies where Life Cycle Assessment was performed in an ex-ante fashion as opposed to ex-post (e.g. as analysed by Arvidsson et al., 2018; Cucurachi et al., 2018). Most ex-ante LCA's typically study 'emerging' technologies that are in an early phase of development but extrapolate and model this technology in a theoretical future and more developed phase. Modelling an emerging technology in an 'emerged' phase inevitably requires a consideration about how the performance aspects of the technology can and will change, for example through the increased economies of scale. Similarly, in a comparative assessment with an incumbent technology the analyst should also take into account the development of the analysed alternative. In that sense the studies cannot be said to predict the future but instead to explore scenarios in which the technology may operate in order to guide R&D decisions (Cucurachi et al., 2018; van der Giesen et al., 2020).
Whereas conventional LCA has already benefitted from a steep learning curve since 1970, the same cannot yet be said for ex-ante LCA. This is reflected in the strongly varying terminology used to denote such LCA studies, such as 'prospective' (Arvidsson et al., 2018; Moni et al., 2019), ex-ante (Cucurachi et al., 2018, van der Giesen et al., 2020), early stage, anticipatory, explorative, and scenario-based (Bergerson et al., 2020). There are differences in the modes of LCA between these types, though both 'ex-ante' and 'prospective' may be seen as the umbrella terms (van der Giesen et al., 2020). The definition as used by van der Giesen et al. (2020) limits the scope of ex-ante LCA's by stating that it serves as decision-support for R&D, while some future-assessment LCA's also focus on more wide-scale impacts (e.g. Berril et al., 2016).
It furthermore appears that the research and modelling approach in ex-ante LCA is not consistent across case studies and that there is a lack of clear guidelines as to what methods are appropriate for such studies (Moni et al., 2019; Bergerson et al., 2020). Regardless, multiple (meta-analysis) papers have been published in the attempt to contribute to identifying and potentially solving some of the main challenges associated with the assessment of emerging technologies (examples). The next section reviews some key articles with the goal to identify the main challenges that need to be tackled in this thesis project.

2. Challenges of framing ex-ante LCA

Goal & scope definition: Defining the future

Naturally the temporal aspect of the scope definition plays a significantly larger role in ex-ante LCA as compared to conventional LCA. The extent to which the LCA practitioner wishes to extrapolate the development of an emerging technology impacts all other choices that directly influence the LCA results. Multiple temporal effects can be identified. For one, the analysed emerging technology will have a unique development trajectory that is influenced by internal and external drivers and barriers. In turn, the possibility exists that the emerging technology influences its direct and indirect market which furthermore complicates the prediction of its development (Cooper & Gytowksi, 2018; van der

Giesen et al. 2020). Bergerson et al. (2020) note how LCA analysts often do not include a distinction between technology and market maturity and mostly focus on emerging technology in mature markets, therefore omitting the effects of new markets. The authors of both papers therefore argue that it is crucial to explicitly define the technology's level of technological and market maturity in order to secure a proper scope definition.

The general approach towards defining the future of an emerging technology differ, Arvidsson et al. (2017) and Cucurachi et al. (2018) explain how ex-ante LCA can make use of multiple scenarios, representing a range of future states of the both the emerging technology and the incumbent technology. The inclusion of multiple scenarios in the goal and scope definition could allow the LCA practitioner to better communicate the range of results that an uncertain future can bring. Other authors omit the necessity for constructing multiple scenarios by first thoroughly analysing the future of the technology and sticking to a single future scenario. The approach towards the definition of a future context is still one of the main challenges of ex-ante LCA (van der Giesen et al., 2020).

Functional unit definition and choice of alternatives for comparative LCA

The true basis of assessment and comparison in LCA lies in the careful consideration of what functions a product, service or system actually provides, as opposed to a focus on a particular quantity of the product or service. The impact assessment then provides an idea about which option provides the service most effectively from an environmental perspective. The prediction of the service that an emerging technology may provide can be challenging. In some cases the technology developers may not be certain which market they will tend to (Cucurachi et al., 2018), whereas in other cases the emerging technology may be introduced into multiple markets thus providing multiple services (Ramírez Ramírez et al., 2019; e.g. van der Giesen et al., 2014). For both situations the definition of the functional unit remains a deliberate choice that includes an implicit assumption about the future of the technology. Such choice then impacts the choice of an incumbent technology for a comparative assessment, making it challenging to execute a proper comparative assessment (Hetherington et al., 2014). The establishment of a functional unit that is in line with the services that the emerging technology provides, and that is appropriate for the research objectives is a clear challenge of ex-ante LCA and requires thorough consideration (Cucurachi et al., 2018; Moni et al., 2019; van der Giesen et al., 2020).

Data collection; Missing data

Similar to ex-post LCA, required data for ex-ante LCA can be divided into the data that are directly relatable to the emerging technology (i.e. foreground data) and the data that are indirectly related to the emerging technology, for example as the result of material and energy requirements further upstream from the core processes of the emerging technology (i.e. background data) (Arvidson et al. 2017). For the latter, conventional LCA makes thankful use of existing LCI databases that have been compiled through real-life historic analysis of the respective processes. It takes time to build and verify these databases which is why these databases are not always up to date (Cucurachi et al., 2018). Conventional ex-post LCA also has the advantage of being able to observe real life process data for the foreground system, thereby providing the LCA analyst with enough sources of data.

Naturally, the analysis of a technology in a future context does not allow a LCA analyst to make use of conventional sources of data. The added problem of data availability in ex-ante LCA is widely recognized (Hetherington et al., 2014; Arvidsson et al. 2017; Cucurachi et al. 2018, Moni et al., 2019; Bergerson et al. 2020; van der Giesen et al., 2020). The available data for the modelling of the foreground system is often based on specific experiments and cases on lab-scale and can therefore not be used to model the foreground system in an operational context (Cucurachi et al. 2018; van der Giesen et al., 2020). Whereas missing data is otherwise supplemented by data from repositories this is more difficult for ex-ante LCA because such databases are non-existent or incomplete for the materials used in the emerging technology (Moni et al., 2019). Other secondary inventory data from scientific articles, patents, or from expert interviews suffers from the same problem; there either is a lack of appropriate data or data only describes the technology aspects under specific conditions (van der Giesen et al. 2020). In cases where technology developers can provide an estimation of operational data, data is likely to be in the form of probability distributions instead of point values which furthermore complicates the use of data for the Life Cycle Inventory (LCI) (Cooper & Gutowski, 2018).

Besides missing, incomplete, or non-representative data future-oriented LCAs have to deal with the challenge of scale-up. In practice, important process improvements occur when a technology moves to a more mature phase which has an enormous effect on its environmental performance and LCA practitioners have to take these effects into account (Moni et al., 2019). The process of manipulating available data to fit a future scenario is often found to lead to the further aggravation of the model uncertainties (Hetherington et al., 2014; Arvidsson et al. 2017; Cucurachi et al. 2018, Moni et al., 2019; Bergerson et al. 2020; van der Giesen et al., 2020). Although LCA analysts can rely on available theories and methods to project the data in a future timeframe it seems impossible to do so without using assumptions, thus further adding to the uncertainty (Cucurachi et al., 2018; van der Giesen et al., 2020).

Impact assessment

Life cycle assessment aggregates a large sum of in- and outflows into comprehensible impact categories. In the conversion from the life cycle inventory to the impact assessment values are assigned to the inventory data based upon the method of choice for the impact assessment. The translation values are the work of (explanation the ReCiPe method).
As is the case for the approach in modelling the background system, the approach for impact assessment cannot blindly be copied from conventional LCA. The reason is that it is possible that certain characterization factors for new materials are not included in the available characterization models which could lead to the omittance of certain materials that, by nature, are important for the assessment of novel technologies (Cucurachi et al., 2018, Moni et al. 2019, van der Giesen et al., 2020). The lack of coverage of new materials by existing impact categories could therefore mask a part of the environmental profile of an emerging technology, making it look more favourable in a comparative assessment with an incumbent technology.

Interpretation: Uncertainty

The compounded uncertainty of assumptions and data/scenario modelling leads to numerous uncertainties in the interpretation of the LCA results. According to Hetherington et al. (2014) and Cucurachi et al. (2018) a proper communication of the variability and uncertainty of the results are crucial for the usefulness of LCA for technology development. Uncertainty analysis in conventional LCAs allows open communication about the uncertainties that are associated with the assessment. Because the life cycle inventory and characterization factors are known, the confidence of the results can be calculated. However, ex-ante LCA adds a new layer to the uncertainty of LCA results because there is a lack of knowledge about the uncertainties due to a lack of data or simply because predictions of the future are inherently uncertain (van der Giesen et al. 2020). Uncertainty analyses in ex-ante LCAs are therefore prone to providing an incomplete picture of the certainty of the results by only addressing the 'certain uncertainties'. The differences in 'types of uncertainties' are captured by the typology of van der Giesen et al. (2020). Based on the typology by Wynne (1992) the authors make a distinction between; "a) risk, (system parameters and probabilities are known), b) uncertainty (system parameters are known, but not the probability distributions), c) ignorance (neither system parameters or probabilities are known, and d) (the future development is inherently undetermined)". The analysis of emerging technologies, especially those with low technology readiness levels, should therefore be paired with an additional discussion focused on identifying overseen impacts and disadvantages of the technology (Moni et al., 2019).

3. Towards solving the challenges of ex-ante LCA

Now that the main challenges of ex-ante LCA have been briefly visited, it is possible to analyse literature on its contribution to solving these challenges. Relevant literature is aimed predominantly on the issue of data collection (e.g.), data scale-up (e.g.), uncertainty communication (), or on the attempt to construct more general frameworks and approaches to LCA (e.g. Bergerson et al., 2020; van der Giesen et al. 2020). To review the all relevant and available literature falls hardly within the scope of this proposal. Yet, a brief visitation of some of the key concepts will allow a discussion regarding the approach of this project.

Two keystone articles by Bergerson et al. (2020) and Van der Giesen et al. (2020) attempt to capture the most important hurdles and barriers to ex-ante LCA in a set of questions that guides the LCA practitioner through the research efforts.

Fore- and background data collection and modelling

As explained, the challenge of data collection and manipulation represent one of the key challenges of ex-ante LCA. A significant part of the data collection is, off course, related to the modelling of the incumbent technology for a comparative assessment. The necessity to be clear about the intended application (i.e. service or function) of the emerging technology is stressed by most reviewed papers (Hetherington et al. 2014; Cucurachi et al. 2018; Moni et al. 2019; van der Giesen et al. 2020). Only then will the LCA analyst be presented with search areas for relevant secondary data. For the modelling of the incumbent technology (i.e. alternative) analysts can use industry roadmaps, technology learning curves and expert consultation. Be it under the condition that the incumbent is at a higher manufacturing readiness level (Moni et al. 2019; van der Giesen et al. 2020).

For the emerging technology, in addition to the previously mentioned sources of data, proxy data or simulation data can also be used (Moni et al. 2020). Van der Giesen et al. (2020) review the work by Parvatker & Eckelman (2019) to provide a hierarchy overview of methods of all these types of LCI data generation. Although Parvatker & Eckelman worked on LCA methodology for chemical engineering, the framework allows the LCA analyst to rank the available options when working with missing data. Even when data for the emerging technology can be provided, the analyst will have to make a subjective choice about how to propagate the found data in the LCA model.

Arvidsson et al. (2018) argue that an extreme condition scenario approach can be used to model the range of data points. In other words, to account for the still uncertain data, worst and best case data can be calculated and used to gather impact results for multiple scenarios. Ramírez Ramírez et al. (2020) agree with this method of supplementing missing data, though the authors explain that worst case results should be preferred in order to prevent green washing.

Other authors mention that instead of point-values, it is possible to capture data in a range of values based on a probability curve (Cooper & Gutowski, 2017; Cucurachi et al., 2018). Such an approach is called a 'probabilistic' approach to LCA and allows LCA analysts to construct a workable LCA model while not being dependent on precise data from technology developers (e.g. Blanco et al. 2020). A Monte-Carlo simulation can then be used to gather impact results in a probability function, thus allowing the LCA analysts to also communicate the ambiguity of the results.

Another approach relies on the iterative nature of LCA, in which consecutive sensitivity analyses lead to an understanding about which parameters in the LCA determine the future environmental impacts. Knowledge about the most important aspects of the model then allow the LCA analysts to focus their efforts on refining data, therefore streamlining the process of data collection and saving resources (Cucurachi et al. 2018; Bergerson et al. 2020).

As previously addressed, learning curves may be used to model the emerging technology in a future state (Hetherington et al., 2014; Arvidsson et al. 2017; Cucurachi et al. 2018, Moni et al., 2019; Bergerson et al. 2020; van der Giesen et al., 2020). Based on knowledge about similar technologies, and with the aid of close expert interviews, it is possible to estimate the learning curves of an emerging technology (van der Giesen et al. 2020). Van der Giesen et al. (2020) go on to conclude that structured discussions with experts in combination with the establishment of multiple hypothetic scenarios is the only way to approach scaling up data when scale-up methods specific to the field of the emerging technology are not available. Bergerson et al (2020) argue that learning curves could be estimated and supplemented by also taking into account the market maturity within which the emerging technology will operate. The available principles of diffusion of innovation can then help in determining the improvement rate of the technology (Bergerson et al., 2020). Tsoy et al. (2020) review 18 ex-ante LCA articles on the use of scale-up method and provide recommendations and a framework for the upscaling of emerging technologies. The authors add that most upscaling methods are applied to chemical engineering which, to some extent, can be regarded to as more of an abstract science than upscaling manufacturing processes of complex product systems. The use of proxy processes therefore seems to be the most viable option for the scale-up of manufacturable products (Tsoy et al., 2020).

Arvidsson & Molander (2016) compared the contribution of foreground scale-up techniques and background scenario techniques in the assessment of epitaxial graphene production and found that the upscaling of the foreground processes were insignificant compared to the impacts of the background system. Besides manipulation of the foreground system, the background system therefore plays an instrumental role in the total assessment of emerging technologies. Van der Giesen et al (2020) cite the success by Menoza et al. (2018) to model technology scenarios using an Integrated Assessment model (IAM) for a future background electricity mix. Menoza et al. (2018) thus allow the analysis of a technology (e.g. electric vehicles) in a future context, which drastically influences the results. Unfortunately, although significant, the energy mix used for most processes in a LCA model only accounts for a portion of the background system. Other relevant sectors that provide the upstream requirements for the foreground system can be more difficult to model. Rosenthal, Fröhlich and Liebich (2020) use a scenario approach to exchange database background processes related to infrastructure materials such as aluminium, copper, and steel, with future processes that are less resource intensive. The analysts use a conventional database but subdivide the relevant processes into processes that can be optimized using the future scenario assumptions. Depending on the outcomes of a sensitivity analysis, further detailing of the background system could be realized by first tackling the major impact-defining factors in the background system, i.e. the energy mix and key raw material supply. If no other means of scenario building are available, the shortcomings of a temporal mismatch between the fore- and background system should at least be thoroughly discussed (van der Giesen et al. 2020).

Calculating, communicating and managing uncertainty

Proper calculation and communication of uncertainty in LCA and ex-ante LCA has been at the focus of research efforts for a long time (Moni et al. 2019). As such there are numerous tools and approaches that can be used for 1) the propagation of uncertainty in the inventory data, 2) the calculation of the compounded uncertainties as result of impact calculations, and 3) the communication of uncertainty towards the stakeholders of the project. The variety of literature on this subject provides enough material for a separate literature review, which will be part of the wider research approach in this project. For now this topic will only be addressed minimally.

Moni et al. (2019) provide a list of common indicators for the quantitative determination of model and context uncertainties; intervals (lower and upper bond), variance, probability distribution and possibility distribution, or fuzzy intervals (Igos et al., 2018, as cited by Moni et al. 2019). However, these fit with the uncertainty types of ‘risk’ and ‘uncertainties’ in the typology of van der Giesen et al. (2020) and can generally be approached with currently existing methodologies, for example via Monte-Carlo simulations or the relatively new Pedigree Analysis. Ramírez Ramírez et al. (2020) provide an overview of available tools for the management of uncertainties which include not only quantitative but also qualitative approaches such as the ‘Expert elicitation’ process.

Concluding remark

In al reviewed literature and LCA case studies, LCA analysts found similar ways to deal with the ambiguous result of various assumptions, missing data and data scale-up. Although slightly differing amongst case studies, the most used approach can best be described at scenario-building. Authors use or recommend scenario building to provide upper and lower bounds for predictions in the background system (Liu et al., 2020; Menoza et al., 2018), for the filling of data gaps in the form of best and worst case scenarios (recommended in Ramírez Ramírez et al., 2020), or for the general scale-up or trajectory of the emerging technology (Arvidsson et al., 2018; Tsoy et al. 2020). It is this use of scenarios that makes the challenges of ex-ante LCA manageable.

M. Recycling in this LCA study

Recycling in LCA - theory

In a typical open loop recycling situation, one product system produces a ‘waste’ that is recycled and used by a second product system. A persistent issue in the modelling of recycling in LCA is how to distribute the total impacts of two supply chains over both chains as they are clearly interlinked by the recycling activity.

Ecoinvent

Ecoinvent, the database that is used for this project, makes a distinction between several modelling philosophies. The one currently preferred by most LCA practitioners is the cut-off system model. In this database and approach, all impacts related to the primary production of materials are allocated towards the product system that uses these primary materials. All impacts of waste treatment processes necessary for the end-of-life phase of the product system that are *not* recycling processes are also allocated towards this first product system as well.
All recycling activities, including the collection of the scraps, sorting, processing, and further transporting are allocated to the second product system. Before the secondary material ends up in the recycling phase, it is ‘cut-off’ from the previous product system, meaning that it becomes completely free of the burdens of the previous product system and only carries with it the burdens of the recycling activity.
If the same philosophy would be used for the modelling of recycling in LCA it would entail that activity A, which has primary material as input and a waste material output, has two outputs depending on the recycling factor of the material. Under a 90% recycling scenario, activity A has an output to a waste treatment activity of 10% of the total material input. All of these burdens are then allocated towards the product system that activity A is part of. The other 90% of the total material input is linked to an empty activity called ‘recycling’. This activity is empty because of the cut-off philosophy where all further burdens of recycling are allocated to the second product system that is not part of the system under study.
Intuitively, this approach has a fault. One could argue that it is unrealistic or unfair to give the second product system the advantage of an almost burden-free material input while assigning most impacts to the first product system. It seems like this is a subjective choice for the LCA practitioner which has drastic consequences for the assessment. However, in practice the boundaries are not as well defined and the primary input for the first product system often already has recycled content while the second product system also relies on new material input to make its product. The cut-off system model is a way to set clear rules for the modelling of an LCA database. When the philosophy is applied consistently and knowledgeably, it provides a valuable and simple solution to the recycling issue.

Economic allocation (lifecyclecenter.se)

In the handbook on LCA by Guinée et al. (2002) economic allocation is advised for most cases of allocation. Similarly to the cut-off approach, economic allocation seeks to separate the two product systems at the activity where the material is reprocessed. However, instead of hard boundary in the form of cut-off between the product systems, economic allocation uses the economic value of the waste output of activity A and the economic value of the secondary material after reprocessing to assess how the burdens of the recycling activity should be divided across the product systems. If the waste output of activity A is worth 20 euros while the output of the recycling process is worth 80 euros, then 20% of the impacts of the recycling process are allocated towards the first product system and 80% to the second.
A clear disadvantage is the highly fluctuating economic value of wastes and secondary materials due to market dynamics but also as result of regulations, this could lead to a wrongly identified economic value and to a less time-resistant LCA study. Additionally, compared to the cut-off approach the economic allocation approach would lead to an even higher impact of activity A whereas the overall impacts of the second product system decrease.

ISO

The ISO guidelines express a preference for system expansion, meaning that the product system should be expanded to include all other relevant processes until a 'closed' system is realised. For the previously introduced example, system expansion would entail that the downstream processes of activity A are included in the system boundaries. The second product system that uses the 'waste' of activity A as primary input for a recycling process now falls within the system boundaries of the studied product system. Besides the obvious disadvantage that the system may become increasingly complex, the approach of system expansion also introduces new allocation issues due to the presence of multiple functional outputs from all included product systems.

Substitution approach

The substitution or avoided impact philosophy puts an emphasis on the benefits of recycling and considers that substitution of primary materials by the recycled secondary material at the end of life stage.
The substitution approach envisions the product system as a theoretical semi-closed loop system where the materials retrieved in the end-of-life phase form new materials for the same product system. In such a system the only primary inputs are those materials that cannot be recovered at the end-of-life phase and therefore need to be 'replenished' in a new cycle.
The limitation of this method rests in the assumption that the material quality after reprocessing is the same as the primary material, and can therefore replace part of the primary material input for the new cycle.
It seems that in practice, the substitution approach is most preferred in product systems that include a focus on the end-of-life phase.

Approach to recycling in this study

Cut-off approach

Even within the cut-off modelling philosophy, exists discussion on its application, such as where to place the point of cut-off.

Arguments for the cut-off approach:

- In the current study the end of life phase is a necessary step but it is not expected to be of critical importance. The reason being that the recycling should be modelled not for the product produced by the product system (methanol) but for the equipment producing it after a service lifetime of roughly twenty years.
- The cut-off approach tends to work well for cases with well-established waste treatment and recovery processes, such as aluminium, copper, and steel. For such well-known materials current data from LCI datasets is likely to be sufficient. Only relatively new materials demand additional scrutiny due to lacking datasets.

Arguments for the placement of the cut-off point

- The point of cut-off is an often debated topic as this is where the first and second product chains can overlap after which allocation may be necessary. It is rarely the case that an E.o.L. material output consists solely of recyclable material, a significant portion of the material will need to be treated in waste management processes. Such processes are almost always attributed to the product system that causes the primary need for the waste treatment, i.e. the first product system. The cut-off point is then often situated at the point where material flows separate, meaning that collection and sorting of the materials is still attributed to the former product system.
- Guinée et al. (2002) argue for the economic allocation of processes at the end-of-life. The philosophy rests on the idea that a recycling chain provides both the service of treating waste flows and recovering materials. The impacts of the recycling activity are then allocated based on the economic value of these services or material flows. In general, economic allocation for

recycling processes seeks to identify the point of zero value as the point of cut-off. However, a problem arises when a material flow has a positive economic value at the very start of the E.o.L. phase, as economic allocation based on a negative economic input and a positive economic output is no longer possible. Guinée et al. (2002) explain that in this case, the use phase itself becomes a multi-functional output and therefore needs to be allocated.
It can be argued that allocation in the use phase should be avoided because of its direct and significant impact on the impact results.

- Nordelöf et al. (2019) talk about the convention to set the cut-off point at before or at the point where recyclables and non-recyclables are separated. The motivation for the convention is that other product systems create the demand for recyclable material and should receive part or all of the burdens associated with the recycling process.

How to approach recycling with Ecoinvent

The ecoinvent database takes the recycled content into account by using average market mixes for common materials/metals such as steel, aluminium and copper. Ecoinvent is based on the cut-off approach and can therefore be used flawlessly for attributional models using the cut-off method.

Materials in Ecoinvent and their recycling

The table below includes the materials that are part of this study, and their respective recycling treatment approach. If the material has recycled content in ecoinvent (i.e. a portion of its production is based on secondary materials) than it can be ruled out that the avoided burden approach is required.

Material	*Ecoinvent recycled content*	*Separation efficiency*	*Real world E.o.L. recovery rate*	*Ecoinvent waste treatment process*	*Comment*
Polypropylene	No		3-5%	100% Municipal incineration (without fly ash extraction)	Recycled PP can be mixed with virgin PP in a 50/50 ratio. This is not a widely practised mix. Because PP is not an important factor it will not be modelled according to this 50/50 ratio due to the additional modelling requirements for the secondary material input.
Polyethylene	Yes, average market mix for PE		90%	100% municipal incineration	Recovery rate is an estimation, PE is used for the encapsulation of the microplant and is expected to be easily sortable
Polyester	No, new process (65% virgin, 35% rPET)		0%	100% Municipal incineration	US market share (in USD) in 2018 of recycled rPET was about 34% (grandviewresearch.com)
Nylon	No		0%	100% municipal incineration	Nylon is not commonly recycled, thus also no input of secondary material in the production process
Glass	No		90%	100% municipal incineration	No proper data can be found for the specific type of glass use in this product system. Roughly 10% loss of glass is assumed, which needs to be processed in a treatment process.
SS316	Yes, about 55%		99% for larger parts 80% for smaller parts	100% Municipal incineration	Some smaller parts account for a small share of the weight of the microplant, these are not easily recyclable.

Mineral wool	No		90%	Market for waste mineral wool. (100%)	Estimation. Due to its low density and non-restrictive material requirements, stone wool can be assumed to be recycled effectively. 100% to market for waste mineral wool as that is modelled in ecoinvent according to the cut-off approach
Aluminium	Yes, about 40%		99% for larger parts	-	
PSU	No		0%	Waste plastic, municipal incineration	The PSU is sandwiched in the product and not likely to be recovered
Ceramics	No		0%	Municipal solid waste, incineration	Ceramics also occur in only in small quantities. It is not likely that these materials are recovered. Neither is it likely that new ceramic production makes use of secondary materials.
Electronic parts	Yes, varying per material		99% for metals. 0% for wire plastic	Waste plastic, industrial electronics, municipal incineration	
Electronic cables	Yes, varying per material		99% for metals, 0% for wire plastic	Waste plastic, industrial electronics, municipal incineration	
Catalyst from MS subsystem	Yes, varying per material			None	Ecoinvent has processes such as 'precious material recovery from waste electronics' which suits the E.o.L. of the catalyst best. These recovery processes however, are not part of the former product system and therefore fall outside of the system boundaries.
TEPA	No		0%	Chemical / hazardous waste incineration	
KOH	No		0%	Chemical / hazardous waste incineration	
Lubrication oil	No		0%	Chemical / hazardous waste incineration	