Power-to-Methanol: The different scenarios, detailed breakdown of the TEA, inventory table, Life Cycle Impact Assessment and characterization graphs.

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1. Goal and scope – all compared processes

This LCA has been conducted to obtain the environmental impact of the Power-to-Methanol processes up to the end of the production line, covering the system from cradle to gate. This means that the LCA will only focus on the environmental impact of the system from mostly raw materials till the production of the methanol. In Table S1 a list of the production methods with electricity sources and the according EcoInvent processes are presented.

Table S1: *All compared MeOH processes and corresponding electricity processes*

MeOH production process	Electricity source	EcoInvent electricity processes
MeOH from CCU: Methanol produced from CO_2, resulting from biogas upgrading, and green H_2 produced from water electrolysis	Wind	electricity production, wind, 1-3MW turbine, offshore
	Solar	electricity production, photovoltaic, 570kWp open ground installation, multi-Si
	Hydro	electricity production, hydro, run-of-river
	Nuclear	electricity production, nuclear, pressure water reactor
	Fossil	electricity production, natural gas, conventional power plant
		electricity production, oil
		electricity production, hard coal
MeOH from DMR: Methanol produced from syngas, resulting from Dry Methane Reforming of biogas	Wind	electricity production, wind, 1-3MW turbine, offshore
	Solar	electricity production, photovoltaic, 570kWp open ground installation, multi-Si
	Hydro	electricity production, hydro, run-of-river
	Nuclear	electricity production, nuclear, pressure water reactor
	Fossil	electricity production, natural gas, conventional power plant
		electricity production, oil
		electricity production, hard coal

Although hydropower plays only a small role in the Dutch electricity mix, it was included in this

study as a scenario to broaden the comparison across renewable sources. According to data from 2022 the electricity in the Dutch electricity grid comes for 40% from NG, 14% from coal and 1% from oil, which sums up the electricity from fossil fuel. The green sources take up the leftover electricity, consisting for 18% from wind, 15% from solar, 7% from biomethane and 3% from nuclear energy (Figure S1) [1].

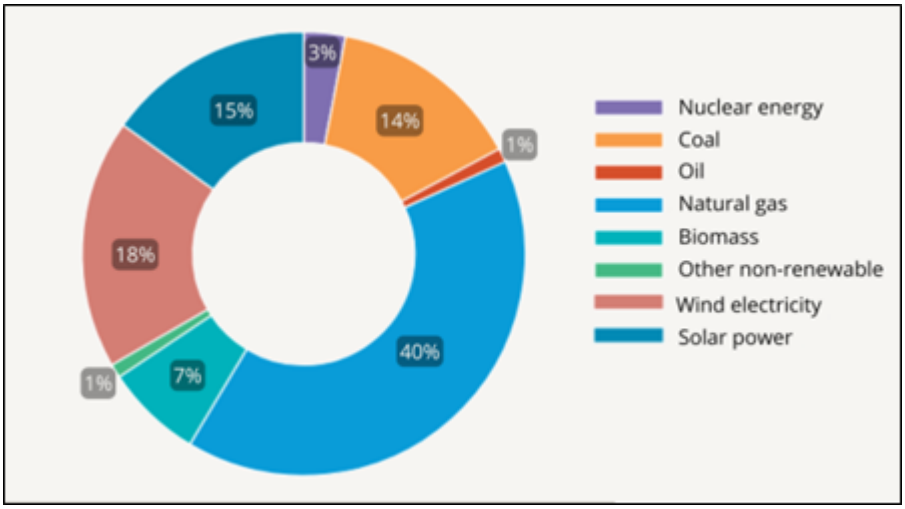


Figure S1: *Sources of Dutch electricity in 2022.*

The major steps for both processes are included in the LCA research, resulting in the following specific sub-processes: biogas membrane separation, alkaline electrolysis, dry methane reforming, compression, pump, G/L separation vessel, MeOH plug flow reactor and distillation column. Excluded from the LCA research is the water purification as raw material for the alkaline electrolysis.

2. Supplementary results Techno-Economic Analysis

Following the methodology of Turton the TEA is divided into CAPEX and OPEX, where the latter is sub-divided into direct-, fixed- and general costs [2], [3]. Figure 3 in the main file follows these four categories, however each category can be broken down further:

- CAPEX is build up by the general investment costs of the equipment and the corresponding installation cost for the total process.
- Direct OPEX are costs which are depending on the total production and is build up by the following factors: raw materials, waste treatment, utilities, operating labor, direct supervision, maintenance & repair, operating supplies, laboratory charges and patents & royalties.
- Fixed OPEX costs are independent of production rate and consists of the following aspects: depreciation, local taxes & insurance and plant overhead costs.
- General OPEX are general manufacturing expenses like administration costs, distribution & selling costs and research & development.

For both processes the detailed cost-breakdown of CAPEX and OPEX is given in Figure S3 below,

following the discussion and conclusion of the main article.

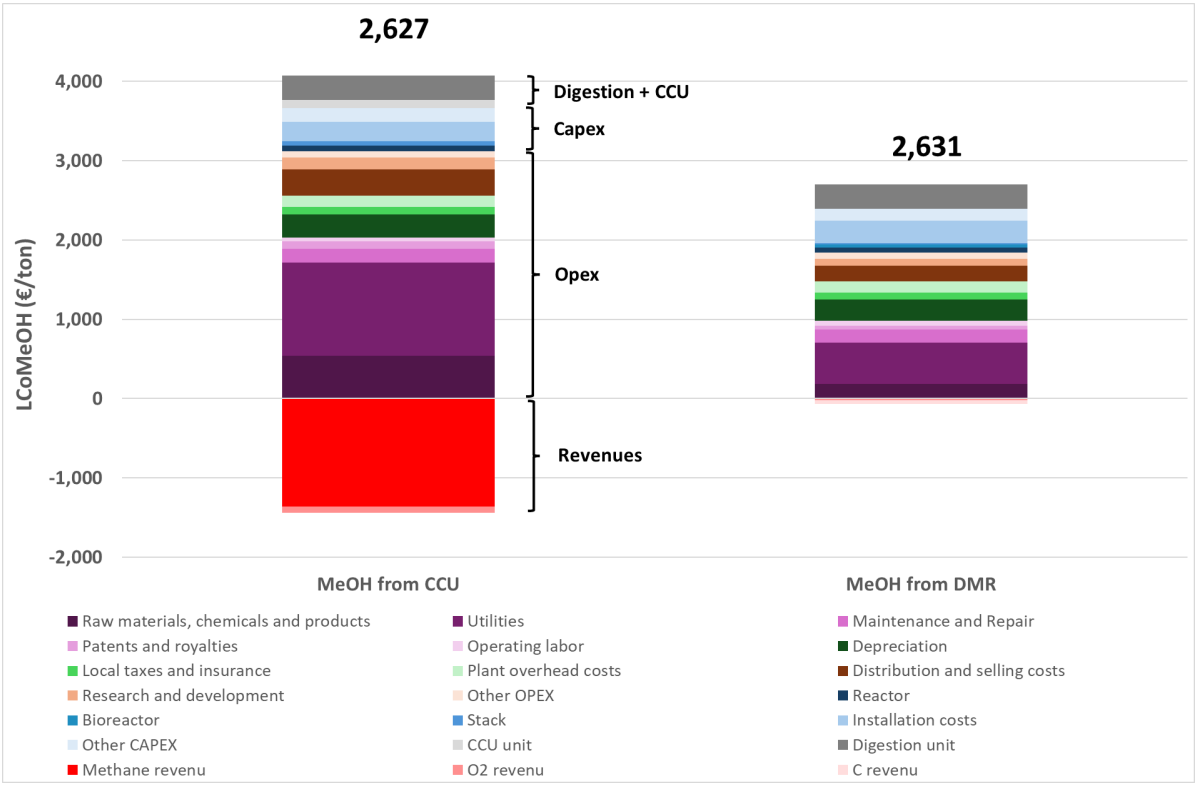


Figure S2. *Detailed cost-breakdown of TEA of Methanol from CCU and Methanol from DMR processes*

In graph S2 the blue bars represent the CAPEX costs, while the OPEX is divided in the three mentioned parts: direct costs (purple bars), fixed costs (green bars) and general expenses (brown bars). The two grey bars at the top represents the cost of digestion and biogas upgrading per tonne of produced methanol.

The given number above the columns represents the net LCoMeOH; the difference between costs and revenues. For the MeOH from CCU process the total costs are 4,070 €/t and the total revenues are 1,443 €/t. For the MeOH from DMR process these numbers are 2,702 and 71 €/t, respectively.

3. Process Inventory Data

Process inventory data for the process models are provided in Table S2. The inventory is build up with the major steps of the two processes, MeOH from CCU and MeOH from DMR and is scaled with known data from literature.

Table S2. *Overview of processes and flows of EcoInvent inventory data for both processes*

Process	Flow	EcoInvent provider
Electricity sources	i. Wind	i. electricity production, wind, 1-3MW turbine, offshore | electricity, high voltage | Consequential, U – NL
	ii. Solar	ii. electricity production, photovoltaic, 570kWp open ground installation, multi-Si | electricity, low voltage | Cutoff, U – NL
	iii. Hydro	iii. electricity production, hydro, run-of-river | electricity, high voltage | Consequential, U – NL
	iv. Nuclear	iv. electricity production, nuclear, pressure water reactor | electricity, high voltage | Consequential, U – NL
	v. Fossil	v. Electricity, from fossil fuel
Biogas membrane separation [(a)]	i. Biogas	i. anaerobic digestion of manure | biogas | Consequential, U – RoW
	ii. Polyimide fiber	ii. glass fibre reinforced plastic production, polyamide, injection moulded | glass fibre reinforced plastic, polyamide, injection moulded | Consequential, U – RER
	iii. Electricity	iii. see electricity sources
	iv. Compression	iv. see compression
	v. Steel	v. market for steel, chromium steel 18/8 | steel, chromium steel 18/8 | Consequential, U - GLO
Alkaline Electrolysis [(b)]	i. Acetic anhydride	i. acetic anhydride production, acetaldehyde oxidation | acetic anhydride | Consequential, U – RER
	ii. Aniline	ii. aniline production | aniline | Consequential, U – RER
	iii. Hydrochloric acid	iii. hydrochloric acid production, from the reaction of hydrogen with chlorine | hydrochloric acid, without water, in 30% solution state | Consequential, U – RER
	iv. Nitric acid	iv. nitric acid production, product in 50% solution state | nitric acid, without water, in 50% solution state | Consequential, U - Europe without Russia
	v. Terephthalic acid	v. purified terephthalic acid production | purified terephthalic acid | Consequential, U – RER
	vi. Steel	vi. steel production, converter, unalloyed | steel, unalloyed | Consequential, U – RER
	vii. Carbon monoxide	vii. carbon monoxide production, from synthesis gas, through absorption | carbon monoxide | Consequential, U – RER
	viii. Pyrrolidone	viii. N-methyl-2-pyrrolidone production | N-methyl-2-pyrrolidone | Consequential, U – RER
	ix. Phenylene sulfide	ix. polyphenylene sulfide production | polyphenylene sulfide | Consequential, U – GLO
	x. Polysulfone	x. polysulfone production, for membrane filtration production | polysulfone | Consequential, U – GLO
	xi. Zirconium oxide	xi. zirconium oxide production | zirconium oxide | Consequential, U – RoW
	xii. Copolymer	xii. acrylonitrile-butadiene-styrene copolymer production | acrylonitrile-butadiene-styrene copolymer | Consequential, U – RER

	xiii. Lubricating oil	xiii. lubricating oil production | lubricating oil | Consequential, U – RER
	xiv. Tetrafluoroethylene	xiv. tetrafluoroethylene production | tetrafluoroethylene | Consequential, U - RER
	xv. Electricity	xv. see electricity source
Dry Methane Reforming [c]	i. Biogas	i. anaerobic digestion of manure | biogas | Consequential, U – RoW
	ii. Cr-steel pipe	ii. market for chromium steel pipe | chromium steel pipe | Consequential, U – GLO
	iii. Electricity	iii. see electricity sources
	iv. Compression	iv. see compression
Compression [d]	i. Polymer	i. acrylonitrile-butadiene-styrene copolymer production | acrylonitrile-butadiene-styrene copolymer | Consequential, U - RER
	ii. Electric motor	ii. electric motor production, vehicle | electric motor, vehicle | Consequential, U - RER
	iii. Fibre	iii. polyester fibre production, finished | fibre, polyester | Cutoff, S – IN
	iv. Lubricating oil	iv. lubricating oil production | lubricating oil | Consequential, U – RER
	v. Nylon 6	v. market for nylon 6 | nylon 6 | Consequential, U – RER
	vi. Iron	vi. market for pig iron | pig iron | Consequential, U – RER
	vii. HD polyethylene	vii. polyethylene production, high density, granulate | polyethylene, high density, granulate | Consequential, U – RER
	viii. LD polyethylene	viii. polyethylene production, low density, granulate | polyethylene, low density, granulate | Consequential, U – RER
	ix. Polypropylene	ix. polypropylene production, granulate | polypropylene, granulate | Consequential, U – RER
	x. PVC	x. polyvinyl chloride production, unspecified polymerisation, weighted average | polyvinyl chloride, unspecified polymerisation, weighted average | Consequential, U – RER
	xi. Steel	xi. steel production, converter, low-alloyed | steel, low-alloyed | Consequential, U – RER
	xii. Electricity	xii. See electricity sources
Pump	i. Lubricating oil	i. market for lubricating oil | lubricating oil | Consequential, U – RER
	ii. Water pump, 22 kW	ii. market for water pump, 22kW | water pump, 22kW | Consequential, U – GLO
	iii. Electricity	iii. See electricity sources
G/L Separation vessel (Equicoll X 20L) [e]	i. AISI steel 304L	i. steel tank 304L process
	ii. Cast iron	ii. market for cast iron removed by turning, average, computer numerical controlled | cast iron removed by turning, average, computer numerical controlled | Consequential, U – GLO
	iii. Electricity	iii. See electricity sources

	iv. Plastic extrusion	iv. market for extrusion of plastic sheets and thermoforming, inline | extrusion of plastic sheets and thermoforming, inline | Consequential, U – GLO
	v. Heat	v. market for heat, central or small-scale, natural gas | heat, central or small-scale, natural gas | Consequential, U - Europe without Switzerland
MeOH PFR	i. Cr-steel pipe	i. market for chromium steel pipe | chromium steel pipe | Consequential, U – GLO
	ii. Electricity	ii. See electricity sources
Destillation column [f]	i. AISI steel 304L	i. steel tank 304L process
	ii. Aluminium oxide	ii. market for aluminium oxide, metallurgical | aluminium oxide, metallurgical | Consequential, U - RoW
	iii. Electricity	iii. See electricity sources
	iv. Flat glass	iv. market for flat glass, coated | flat glass, coated | Consequential, U – RER
	v. Fe-Ni-Cr alloy	v. market for iron-nickel-chromium alloy | iron-nickel-chromium alloy | Consequential, U – GLO
	vi. Chromium steel	vi. steel production, electric, chromium steel 18/8 | steel, chromium steel 18/8 | Consequential, U – RER
	vii. Steel	vii. market for steel, unalloyed | steel, unalloyed | Consequential, U – GLO
	viii. Synthetic rubber	viii. market for synthetic rubber | synthetic rubber | Consequential, U – GLO

[a] Data taken from [4], [5], [6]
[b] Data taken from [7]
[c] Data taken from [8]
[d] Data taken from [9]
[e] Data taken from [10]
[f] Data taken from [11]

Minor process steps, such as mixers or valves, are neglected in the inventory, as well as the catalyst material in the MeOH reactor. Furthermore, transport between the different process steps is absent; the total process is considered on-site without significant transportation.

4. Life Cycle Impact Assessment

4.1 Environmental Footprint (EF) v3.0

With all inventory data ready and the simulation having been built during the LCI phase, the next step of the LCA is to calculate the environmental impact. The impact assessment method used in this paper is EF v3.0 [12], [13]. This method considers the impact categories: climate change, ozone depletion, toxicities, particulate matter, human health, land use, water scarcity, eutrophication, acidification and resource use. These impact categories are divided into sub-categories illustrated in Figure S3.

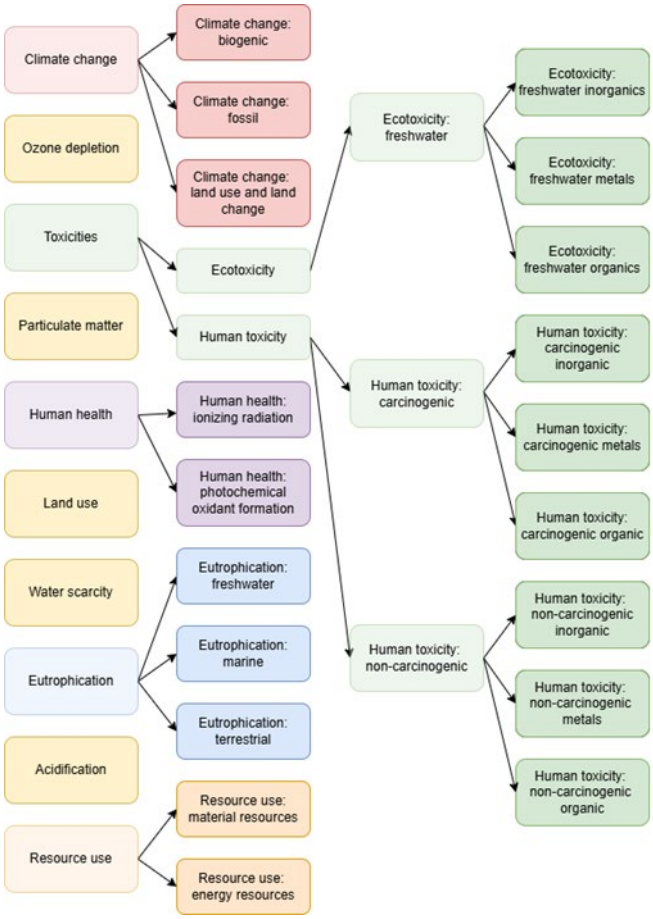


Figure S3. *Categories and sub-categories of the EF v3.0 impact assessment method*

4.2 Normalisation and weighting according to EF v3.0

Impact assessment calculations results in numbers for the different environmental impact categories, expressed in the specific unit (kg CO_2-eq, mol H^+-eq, CTUe, CTUh, kBq U235-Eq, kg NMVOC-Eq, m^3 world Eq deprived, MJ and kg Sb-Eq). Normalisation and weighting factors are taken from the European Commission to convert the specific units to Person Year (PY) and Points [14], [15]. These factors are given in Table S3 below:

Table S3. *Normalisation and weighting factors corresponding to the Environmental Footprint v3.0 (EF v3.0)*

Impact categories	Normalisation factor	Weighting factor
Ecotoxicity: freshwater	42,700	6.2
Eutrophication: freshwater	1.61	2.8
Energy resources: non-renewable	65,000	8.32
Material resources	0.0636	7.55
Acidification	55.6	6.2
Climate change	8,100	21.06
Human toxicity: carcinogenic	1.69e-5	2.13
Human toxicity: non-carcinogenic	2.30e-4	1.84
Ionising radiation	4,220	5.01

Land use	819,000	7.94
Ozone depletion	0.0536	6.31
Particulate matter formation	5.95e-4	8.96
Photochemical oxidant formation	40.6	4.78
Water use	11,500	8.51

4.3 Catalyst influence on environmental burden

Both processes include one or more reaction steps, where catalyst material is involved, but which is not included in the LCA inventory table. Justification of neglecting the environmental burden of the catalyst is calculated, based on mass balance of the processes and data reported by Robbins et al. (2024) [16]:

The following amount of catalyst is required to produce 50 kg of methanol, where reforming catalysts are typically Ni-based supported catalysts used in methane reforming processes.:

- Reformer catalyst (Ni-based): $1.17 \cdot 10^{-3}$ kg
- Methanol synthesis catalyst: $1.41 \cdot 10^{-5}$ kg

Mass balance for the simulated processes results in ~10.6 ton MeOH per year, resulting in 0.0234 kg/t reforming catalyst and 0.000282 kg/t MeOH synthesis catalyst. Total amount of catalyst is 0.0236 kg/t catalyst, mainly the Ni-based reforming catalyst. The composition of these Ni reforming catalysts typically contains:

- 10–30 wt % Ni
- supported on Al_2O_3 or $MgO–Al_2O_3$.

This results in ~0.00236 kg Ni and ~0.02124 kg Al_2O_3. From literature the Material Global Warming Potential (GWP) of Nickel and Alumina production equals ~15 kg CO_2-eq/kg and ~2 kg CO_2-eq/kg, respectively. This means that climate impact of catalyst production equals:

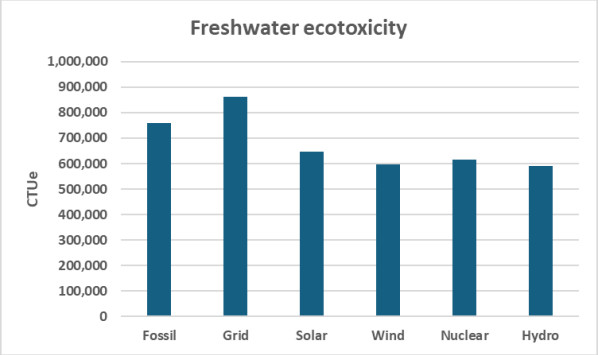
- Nickel = 0.035 kg CO_2-eq
- Alumina = 0.042 kg CO_2-eq

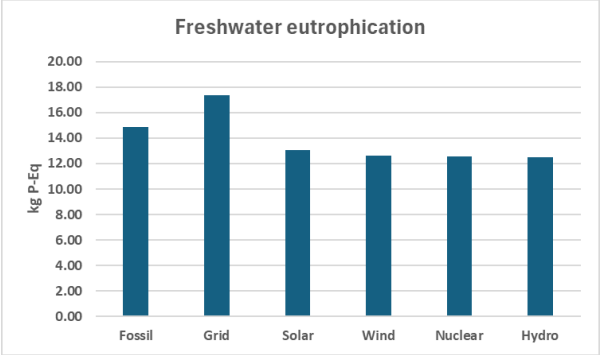
- Total catalyst impact: 0.035 + 0.042 = 0.077 kg CO_2-eq ≈ 0.08 kg CO_2-eq per ton methanol

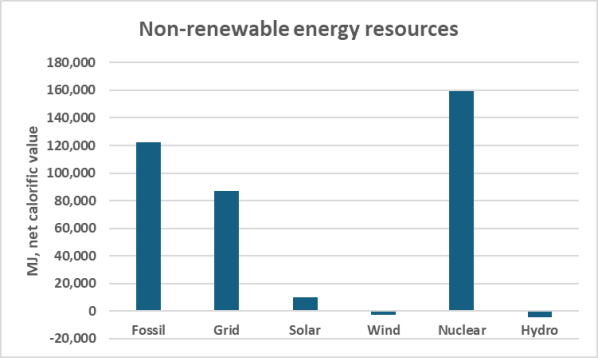
Typical cradle-to-gate GHG emissions for conventional methanol production are roughly: ~0.6–1.0 kg CO_2-eq per kg methanol (~600–1000 kg CO_2-eq per ton), resulting in a catalyst contribution of ~0.01 % of the total climate impact

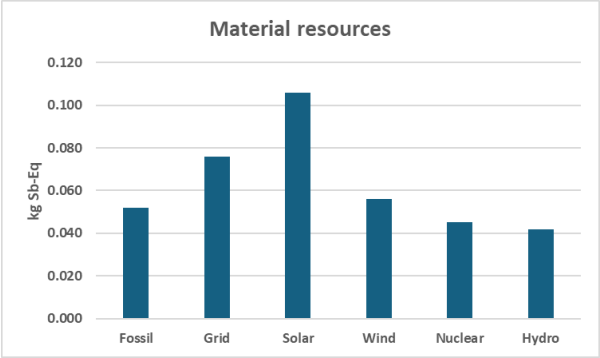
5. Supplementary results LCA

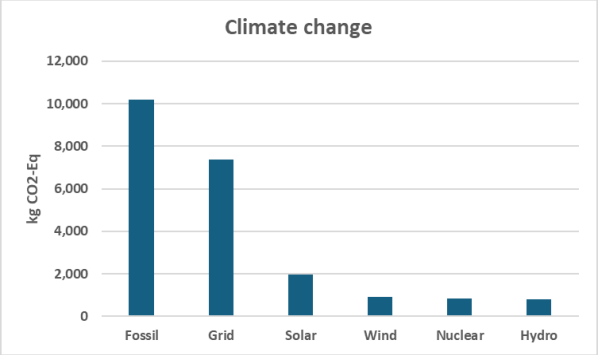
For all environmental impacts the absolute values in the specific corresponding unit are given in Figure S4 (MeOH from DMR) and Figure S5 (MeOH from CCU).

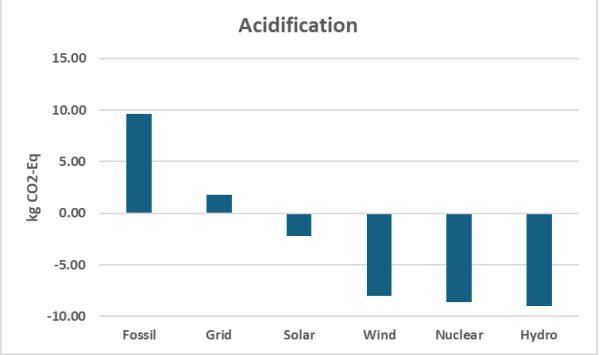

Freshwater ecotoxicity
CTUe
1,000,000
900,000
800,000
700,000
600,000
500,000
400,000
300,000
200,000
100,000
0
Fossil
Grid
Solar
Wind
Nuclear
Hydro

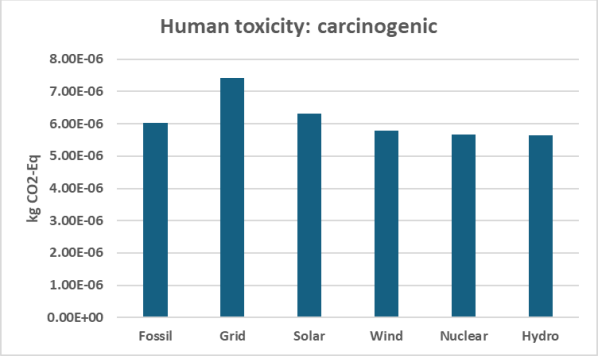

Freshwater eutrophication
kg P-Eq
20.00
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
Fossil
Grid
Solar
Wind
Nuclear
Hydro

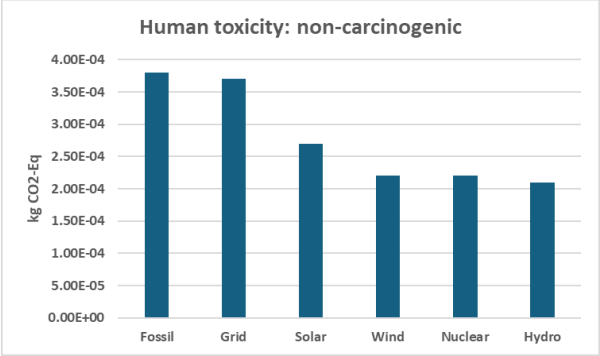

Non-renewable energy resources
MJ, net calorific value
180,000
160,000
140,000
120,000
100,000
80,000
60,000
40,000
20,000
0
-20,000
Fossil
Grid
Solar
Wind
Nuclear
Hydro

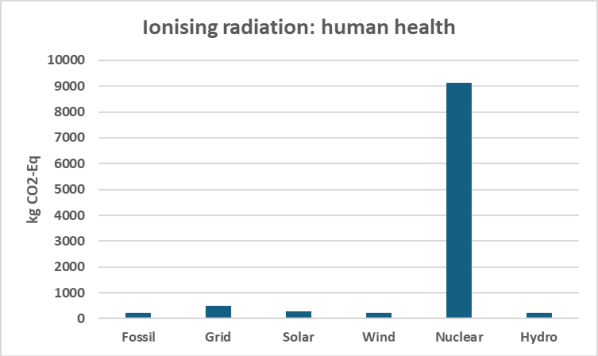

Material resources
kg Sb-Eq
0.120
0.100
0.080
0.060
0.040
0.020
0.000
Fossil
Grid
Solar
Wind
Nuclear
Hydro

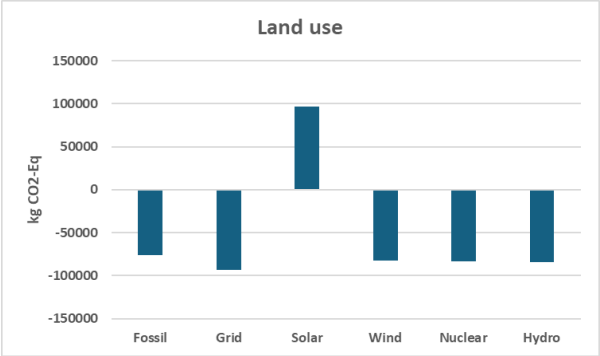

Climate change
kg CO2-Eq
12,000
10,000
8,000
6,000
4,000
2,000
0
Fossil
Grid
Solar
Wind
Nuclear
Hydro


Acidification
kg CO2-Eq
15.00
10.00
5.00
0.00
-5.00
-10.00
Fossil
Grid
Solar
Wind
Nuclear
Hydro


Human toxicity: carcinogenic
kg CO2-Eq
8.00E-06
7.00E-06
6.00E-06
5.00E-06
4.00E-06
3.00E-06
2.00E-06
1.00E-06
0.00E+00
Fossil
Grid
Solar
Wind
Nuclear
Hydro


Human toxicity: non-carcinogenic
kg CO2-Eq
4.00E-04
3.50E-04
3.00E-04
2.50E-04
2.00E-04
1.50E-04
1.00E-04
5.00E-05
0.00E+00
Fossil
Grid
Solar
Wind
Nuclear
Hydro


Ionising radiation: human health
kg CO2-Eq
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
Fossil
Grid
Solar
Wind
Nuclear
Hydro


Land use
kg CO2-Eq
150000
100000
50000
0
-50000
-100000
-150000
Fossil
Grid
Solar
Wind
Nuclear
Hydro

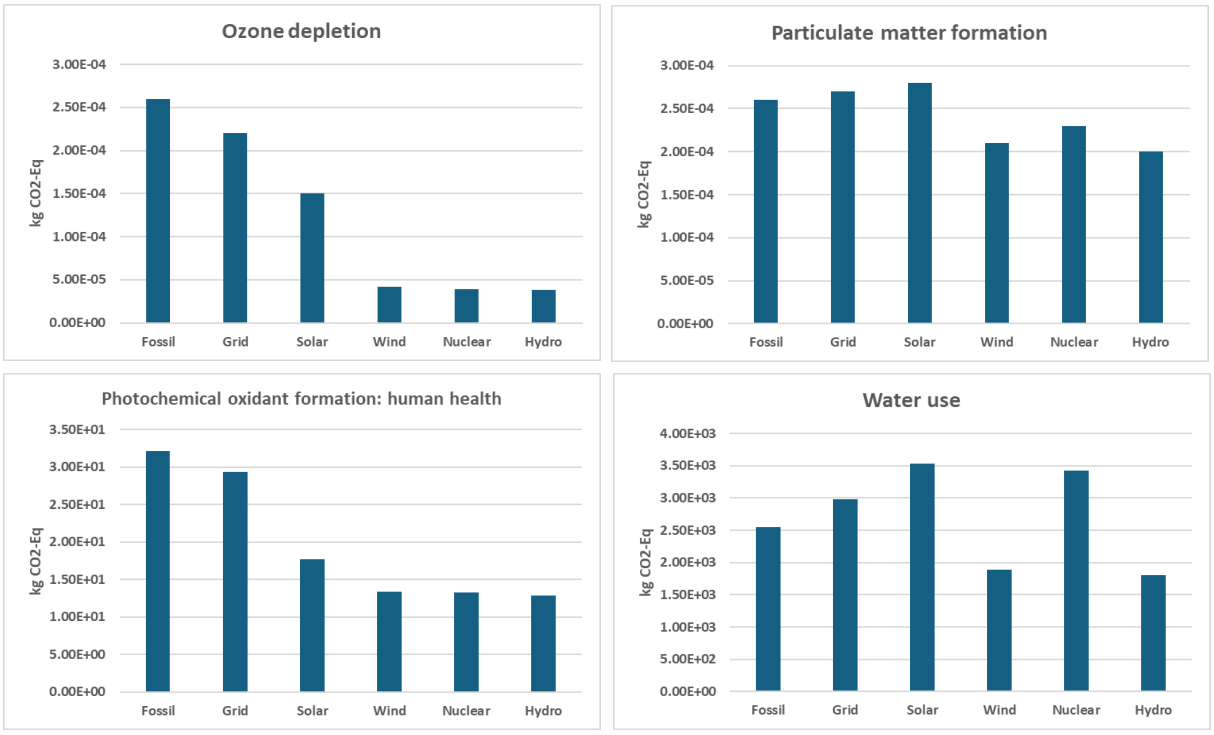


Figure S4. *Absolute results for freshwater ecotoxicity, freshwater eutrophication, non-renewable energy resources, material resources and climate change for the process MeOH from DMR*

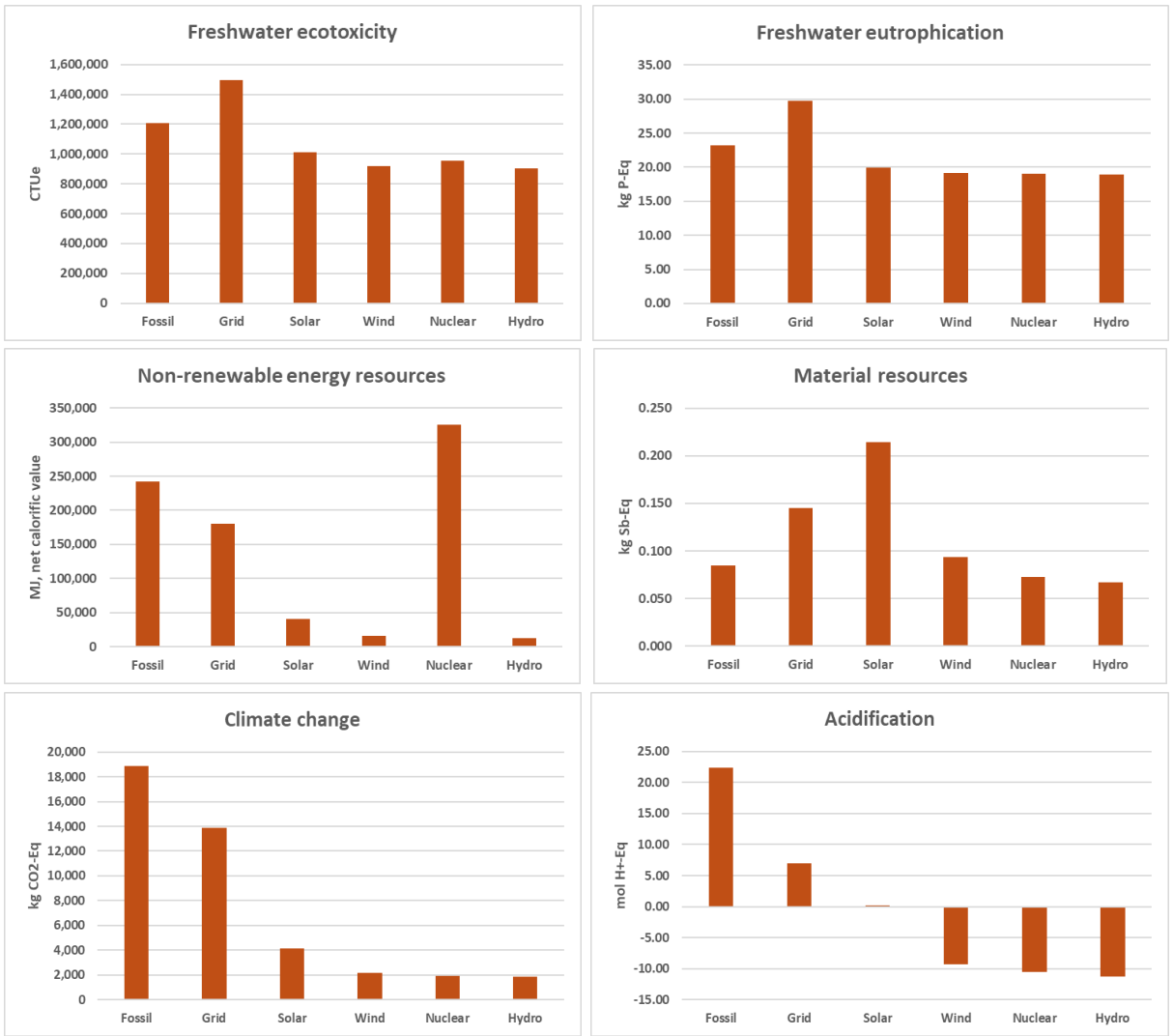




Figure S5. *Absolute results for all environmental impacts for the process MeOH from CCU*

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