Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Electronic supplementary information – Economic and life-cycle assessment of $OME_{3\text{-}5}$ as transport fuel: A comparison of production pathways

Daniel F. Rodríguez-Vallejo,[a] Antonio Valente,[b,c] Gonzalo Guillén-Gosálbez,*[b] and Benoît Chachuat[a]

Received Date
Accepted Date

DOI: 00.0000/xxxxxxxxxx

Number of pages: 15

Number of tables: 14

Number of figures: 2

This electronic supplementary information (ESI) includes the data used to conduct the environmental and economic assessment of the $OME_{3\text{-}5}$ fuels, namely the life-cycle inventories (Section A), monetization factors of endpoint protection areas (Section B), and production costs (Section C). Following the $OME_{3\text{-}5}$ infrastructure presented in Fig. 2 of the manuscript, the inventory tables S1–S12 correspond to the CO_2 procurement (SS1), H_2 procurement (SS2), $OME_{3\text{-}5}$ production (SS3), and fuel distribution (SS4) subsystems. This ESI also presents additional results regarding the midpoint impact categories of the main inputs in the OME infrastructure and the sensitivity of CO_2 economic allocation factors on the predicted environmental impacts.

[a] *Centre for Process Systems Engineering, Imperial College London, Exhibition Rd SW7-2AZ London, United Kingdom.*
[b] *Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland. E-mail:gonzalo.guillen.gosalbez@chem.ethz.ch*
[c] *European Commission, Joint Research Centre, Directorate D, Via Enrico Fermi 2749, 21027, Ispra, Italy.*

A. Life cycle inventories and complementary results

Table S1 LCI for H_2 from electrolysis. Values per kg H_2.[1]

Input	**Value**	**Unit**
Water, deionised	18.04	kg
Electricity*	52.26	kWh
Output	**Value**	**Unit**
H_2	1.00	kg
O_2	8.00	kg

*In this case the electricity comes either from nuclear, solar or wind resources.

Table S2 LCI for CO_2 captured directly from air (DAC). Values per kg CO_2 captured.[2]

Input	**Value**	**Unit**
Air	1968.61	kg
Natural gas	0.19	m^3
Calcium carbonate, precipitated	0.02	kg
Electricity	0.37	kWh
Output	**Value**	**Unit**
CO_2	1.00	kg

Table S3 LCI for CO_2 captured from biogas. Values per kg CO_2 captured[3].

Input	**Value**	**Unit**
Biogas	1.15	m^3
Electricity	0.24	kWh
Activated carbon, granular	3.37E-4	kg
Output	**Value**	**Unit**
CO_2 (4 bar)	1.00	kg
Methane	0.60	Nm^3
Hydrogen sulfide	1.24E-5	kg
Methane slip, non-fossil	8.23E-5	kg

Table S4 LCI for CO_2 captured from ammonia production. Values per kg CO_2 captured.[3]

Input	**Value**	**Unit**
Natural gas	0.49	kg
Heavy fuel oil	0.16	kg
Cooling water	0.11	kg
Electricity	0.06	kg
Water	7.32E-4	kg
Nickel	2.85E-4	kg
Solvent, organic	2.44E-5	kg
Output	**Value**	**Unit**
CO_2 (1 bar)	1.00	kg
Ammonia, liquid	0.81	kg
Acetaldehyde	1.01E-6	kg
Acetic acid	6.80E-6	kg
Acetone	9.84E-7	kg
Ammonia	6.59E-8	kg
Arsenic	8.70E-8	kg
Benzene	7.61E-6	kg
Benzo(a)pyrene	3.75E-10	kg
Butane	1.33E-5	kg
Cadmium	2.17E-7	kg
Calcium	5.27E-7	kg
Carbon dioxide	1.19	kg
Carbon monoxide	6.83E-5	kg
Chromium	1.04E-7	kg
Chromium VI	1.06E-9	kg
Cobalt	2.17E-7	kg
Copper	3.23E-7	kg
Dinitrogen monoxide	1.24E-5	kg
Dioxins as 2,3,7,8-tetrachlorodibenzeno-p-dioxin	3.54E-15	kg
Ethanol	1.98E-6	kg
Formaldehyde	4.87E-6	kg
Hydrocarbons, apliphatic alkenes	3.95E-6	kg
Hydrocarbons, apliphatic unsaturated	1.98E-7	kg
Hydrocarbons, aromatic	9.84E-7	kg
Hydrogen chloride	9.51E-6	kg
Hydrogen fluoride	9.51E-7	kg
iron	1.19E-6	kg
Lead	3.46E-7	kg
Mercury	1.56E-9	kg
Methane	9.76E-6	kg

Methanol	3.36E-6	kg
Molybdenum	1.06E-7	kg
Municipal solid waste	1.63E-4	kg
Nickel	4.28E-6	kg
Nitrogen	8.13E-5	kg
Nitrogen oxides	8.13E-4	kg
Polycyclic aromatic hydrocarbons	1.94E-7	kg
Particulates, $< 2.5\ \mu$ m	2.34E-4	kg
Particulates, $> 2.5\ \mu$ m	6.59E-5	kg
Particulates, $> 10\ \mu$ m	3.29E-5	kg
Pentane	2.28E-5	kg
Propane	4.00E-6	kg
Propionic acid	3.80E-7	kg
Selenium	7.90E-8	kg
Sodium	4.94E-6	kg
Sulfur dioxide	8.13E-6	kg
Toluene	4.00E-6	kg
Vanadium	1.72E-5	kg
Water	0.04	kg
Water (water)	0.07	kg
Zinc	2.63E-8	kg

Table S5 LCI for CO_2 captured from a coal-based power plant. Values per kg CO_2 captured.[1]

Input	**Value**	**Unit**
Coal	0.52	kg
Limestone	0.04	kg
Light fuel oil	6.20E-3	kg
Natural gas	7.80E-4	m^3
Monoethanolamine	1.55E-3	kg
Sodium hydroxide	1.20E-4	kg
Ammonia	1.15E-3	kg
Output	**Value**	**Unit**
CO_2 (1 bar)	1.00	kg
Electricity	0.78	kWh
CO_2 (air)	0.05	kg
Sulphur dioxide	7.00E-3	kg
Nitrogen oxide	1.60E-3	kg
Particulates, unspecified (air)	1.10E-4	kg
Ammonia	2.70E-4	kg
Monoethanolamine	9.00E-5	kg
Municipal solid waste to sanitary landfill	4.06E-3	kg

Table S6 LCI for CO_2 captured from a natural gas-based power plant. Values per kg CO_2 captured.[4]

Input	Value	Unit
Natural gas	0.62	Nm^3
Monoethanolamine	1.50E-3	kg
Sodium hydroxide	1.30E-4	kg
Activated carbon	7.50E-5	kg
Water	8.00E-4	m^3
Output	**Value**	**Unit**
CO_2 (1 bar)	1.00	kg
Electricity	2.75	kWh
CO_2 (air)	0.11	kg
Monoethanolamine	6.30E-5	kg
Ammonia	3.50E-5	kg
Formaldehyde	2.62E-4	g
Acetaldehyde	1.67E-4	g
Toxic solid waste to landfill	1.65E-3	kg

Table S7 LCI for methanol production from H_2 and CO_2. Values per kg methanol.[1]

Input	Value	Unit
CO_2	1.46	kg
H_2	0.20	kg
Electricity	0.21	kWh
Cooling water	0.08	m^3
Copper oxide	2.11E-5	kg
Zinc oxide	7.93E-6	kg
Aluminium oxide	3.96E-6	kg
Output	**Value**	**Unit**
Methanol	1.00	kg
CO_2 (air)	0.08	kg
NO_2 (air)	1.78E-4	kg
Methanol (air)	0.01	kg
Wastewater	5.71E-4	m^3

Table S8 LCI for methanol production from natural gas via SMR.[5]

Input	Value	Unit
Natural gas	0.65	m^3
Electricity	0.07	kWh
Steam	6.93	MJ
Cooling water	8.16E-03	m^3
Water, deionised	0.85	kg
Copper oxide	9.00E-5	kg
Molybdenum	1.00E-5	kg
Zinc	3.00E-5	kg
Aluminium oxide	2.40E-04	kg
Nickel	2.00E-05	kg
Output	**Value**	**Unit**
Methanol	1.00	kg
Methane	9.80E-04	kg
CO_2	0.08	kg
NO_2	1.78E-04	kg
NO_X	1.50E-04	kg
Sulfur dioxide	1.38E-05	kg
AOX, Adsorbable Organic Halogen as Cl, water	1.00E-06	kg
BOD5, Biological Oxygen Demand, water	1.80E-04	kg
Chloride, water	2.00E-06	kg
COD, Chemical Oxygen Demand, water	4.90E-04	kg
DOC, Dissolved Organic Carbon, water	2.40E-04	kg
Formaldehyde, water	1.00E-04	kg
Methanol, water	3.00E-05	kg
Phenol, water	1.00E-05	kg
Phosphorus, water	1.00E-05	kg
Suspended solids, water	2.00E-05	kg
Total organic carbon, water	2.40E-04	kg
Wastewater	5.67E-03	m^3

Table S9 LCI for methanol production from biomass-based syngas.[5]

Input	Value	Unit
Wood chips dry	0.72	kg
Wood chips wet	2.60	kg
Electricity	0.28	kWh
Steam	6.93	MJ
Cooling water	8.16E-03	m^3
Water, deionised	0.85	kg
Copper oxide	9.00E-5	kg
Molybdenum	1.00E-5	kg
Zinc	3.00E-5	kg
Aluminium oxide	2.40E-04	kg
Nickel	2.00E-05	kg
Output	**Value**	**Unit**
Methanol	1.00	kg
Methane	9.80E-04	kg
CO_2, biogenic	2.76	kg
CO, biogenic	6.51E-06	kg
Methane, biogenic	6.20E-06	kg
NO_2	3.10E-07	kg
NO_X	2.06E-04	kg
Methanol	5.30E-04	kg
Acetaldehyde	3.10E-09	kg
Acetic acid	4.65E-07	kg
Benzene	1.24E-06	kg
Benzo(a)pyrene	3.10E-11	kg
Butane	2.17E-06	kg
Formaldehyde	3.10E-07	kg
Mercury	9.30E-11	kg
polycyclic aromatic hydrocarbons	3.10E-08	kg
Particulates, $< 2.5\ \mu m$	6.20E-07	kg
Pentane	3.72E-06	kg
Propane	6.20E-07	kg
Propionic acid	6.20E-08	kg
Sulfur dioxide	1.71E-06	kg
Toluene	6.20E-07	kg
AOX, Adsorbable Organic Halogen as Cl, water	1.00E-06	kg
BOD5, Biological Oxygen Demand, water	1.00E-06	kg
Chloride, water	2.00E-06	kg
COD, Chemical Oxygen Demand, water	4.90E-04	kg
DOC, Dissolved Organic Carbon, water	2.40E-04	kg
Formaldehyde, water	1.00E-04	kg
Methanol, water	3.00E-05	kg
Phenol, water	1.00E-05	kg
Phosphorus, water	1.00E-05	kg
Suspended solids, water	2.00E-05	kg
Total organic carbon, water	2.40E-04	kg
Wastewater	5.32E-03	m^3

Table S10 LCI for formaldehyde production from methanol. Values per kg formaldehyde.[5]

Input	**Value**	**Unit**
Methanol	1.20	kg
Electricity	0.15	MJ
Output	**Value**	**Unit**
Formaldehyde	1.00	kg
Steam[a]	6.60	MJ
CO_2	0.11	kg
Formaldehyde, air	2.50E-05	kg
Methanol, air	3.10E-05	kg
NO_X	3.80E-04	kg
NMVOC	3.00E-06	kg
Particulates, $< 2.5\ \mu m$ and $> 10\ \mu m$	5.00E-06	kg
BOD5, Biological Oxygen Demand, water	8.00E-06	kg
COD, Chemical Oxygen Demand, water	8.90E-06	kg
Catalyst waste	5.00E-05	kg

[a] In our case, this steam is transferred to $OME_{3\text{-}5}$ process in order to partially satisfy its heat requirement.

Table S11 LCI for distribution of $OME_{3\text{-}5}$. Values per kg $OME_{3\text{-}5}$.[3]

Input	**Value**	**Unit**
Transport, pipeline, onshore	0.56	tkm
Transport, freight, lorry	0.06	tkm
Transport, freight train	0.04	tkm
Transport, freight, inland waterways, barge tanker	0.03	tkm
Transport, freight, light commercial vehicle	1.80E-3	tkm
Water	6.89E-4	kg
Steam	5.84E-4	MJ
Electricity	6.70E-3	kWh
Output	**Value**	**Unit**
$OME_{3\text{-}5}$	1.00	kg
Water (air)	1.03E-7	m^3
Water (water)	5.86E-7	m^3
Municipal solid waste	6.27E-6	kg
Wastewater	6.89E-7	m^3

Table S12 LCI for Diesel[6] and $OME_{3\text{-}5}$[3] utilization phase. Values in kg per km driven.

Input	**Diesel**	**$OME_{3\text{-}5}$**
Fuel consumption	0.05	0.12
Output (emissions)	**Diesel**	**$OME_{3\text{-}5}$**
Carbon dioxide	0.17	0.20
Sulfur dioxide	1.06E-6	0.00
Cadmium	5.28E-10	0.00
Copper	8.98E-8	0.00
Chromium	2.64E-9	0.00
Nickel	3.70E-9	0.00
Zinc	5.28E-8	0.00
Lead	4.36E-15	0.00
Selenium	5.28E-10	0.00
Mercury	1.06E-12	0.00
Chromium IV	5.28E-12	0.00
Dinitrogen monoxide	2.64E-6	2.78E-6
Ammonia	8.45E-7	0.00
Polycyclic aromatic hydrocarbons	9.74E-9	1.03E-9
Carbon monoxide	6.07E-5	0.00
Nitrogen oxides	9.38E-6	6.77E-4
Particulates, $< 2.5\ \mu$m	4.02E-6	0.00
Methane	1.87E-6	1.87E-6
Ethane	8.22E-8	8.22E-8
Propane	2.74E-8	2.74E-8
Butane	2.74E-8	2.74E-8
Pentane	9.96E-9	9.96E-9
Heptane	4.98E-8	4.98E-8
Cyclohexane	1.62E-7	1.62E-7
Ethene	2.73E-6	2.73E-6
Propene	8.96E-7	8.96E-7
Formaldehyde	2.99E-6	0.00
Acetaldehyde	1.61E-6	1.61E-6
Acrolein	8.91E-7	8.91E-7
Benzaldehyde	2.14E-7	2.14E-7
Acetone	7.32E-7	7.32E-7
Methyl ethyl ketone	2.99E-7	2.99E-7
Toluene	1.72E-7	1.72E-7
m-Xylene	1.52E-7	1.52E-7
o-Xylene	6.72E-8	6.72E-8
Styrene	9.21E-8	9.21E-8
Benzene	4.93E-7	4.93E-7
others NMVOC from diesel	1.47E-5	1.32E-5

Midpoint impact categories

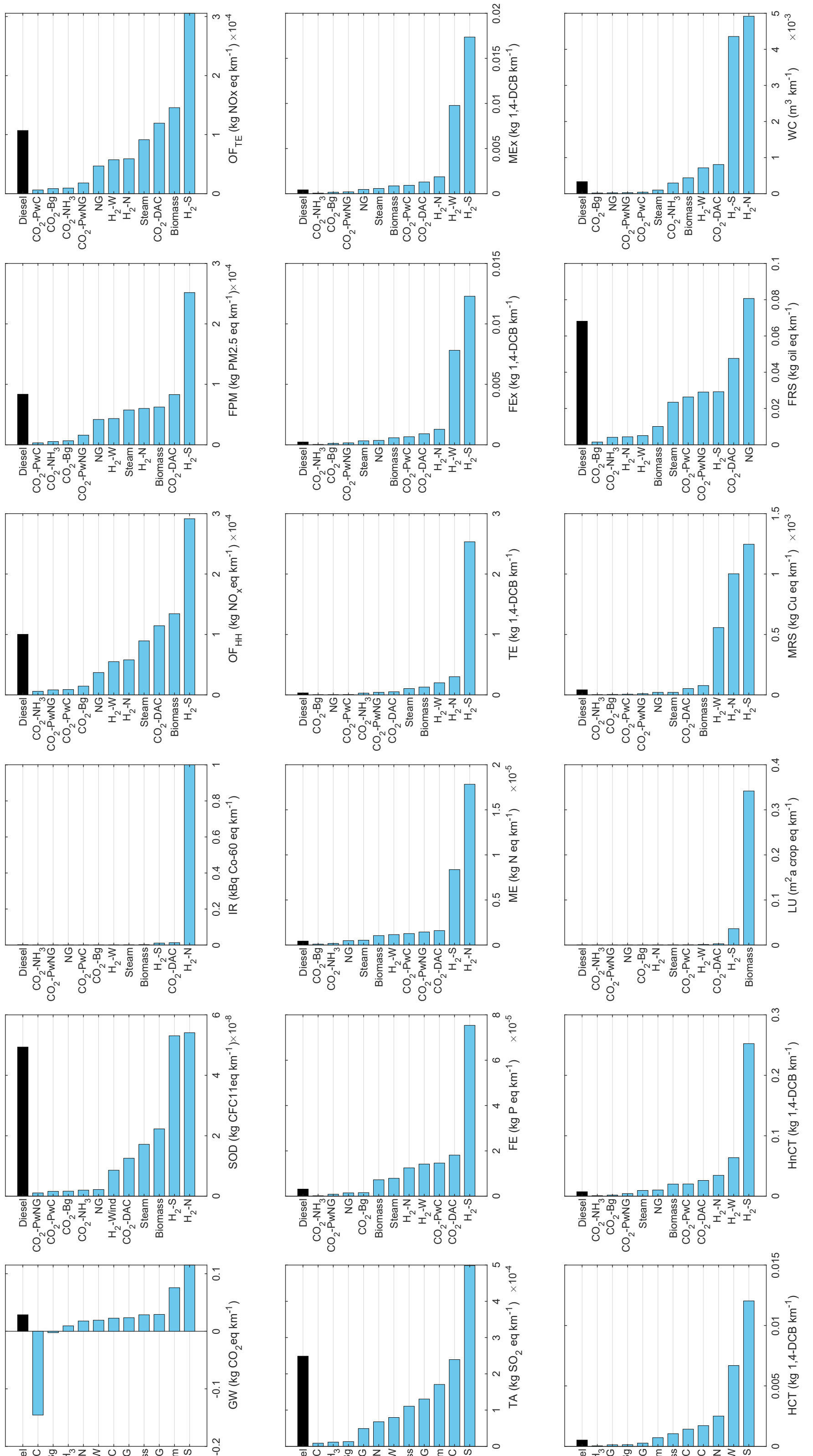

Fig. S1 Midpoint environmental impacts for the main inputs in the OME structure. GW:Global warming, SOD:Stratospheric ozone depletion, IR:Ionizing radiation, OF$_{HH}$:Ozone formation human health, FPM:Fine particulate matter formation, OF$_{TE}$:Ozone formation terrestrial ecosystem, TA:terrestrial acidification, FE:Fresh water eutrophication, ME:Marine eutrophication, TE:Terrestrial eutrophication, FEx:Fresh water ecotoxicity, MEx:Marine ecotoxicity, HCT:Human carcinogenic toxicity, HnCT:human non-carcinogenic toxicity, LU:land use, MRS:Mineral resource scarcity, FRS:fossil resource scarcity, WC: Water consumption.

Effect of CO_2 allocation factor

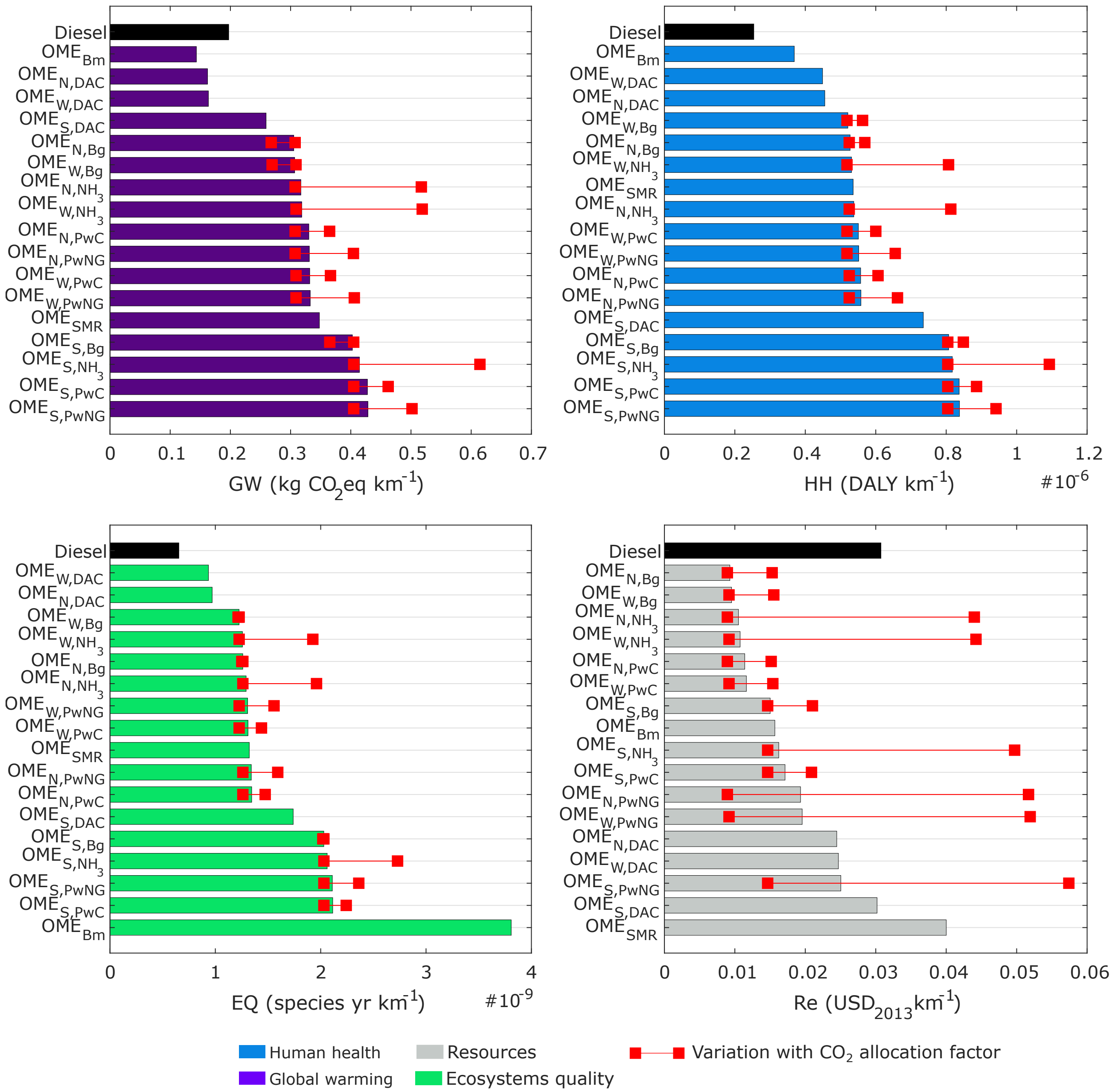

Fig. S2 Variation of GW and the endpoint protection areas (HH, EQ and Re) with the allocation factor used in the CO_2 subsystems presenting multifunctionality within the OME_{3-5} structure.

B. Monetary valuation

Monetary valuation is employed to express the environmental endpoint impacts into monetary values, which allow us to compare those impacts against each other and with the driving cost. Thus, making possible to express the environmental indicators into a single score. Table S13 includes the conversion factors employed in our study, which are based on the values reported in the work by Weidema[7] who compared the Eco-Indicator 99, Stepwise 2006 and ReCiPe 2008 life cycle impact assessments methods in an endpoint perspective.

Table S13 Monetary valuation factors for the three environmental endpoint impacts.[7]

Endpoint impact	Unit	Monetization factor
Human health	USD2019/DALY	116,345
Ecosystems quality	USD2019/Species·yr	14,936,175
Resources scarcity	USD2019/USD2013	1.10

C. Economic information

Table S14 Production costs employed to compute the driving cost in the $OME_{3\text{-}5}$ structure.

Component	Value	Unit
CO_2 direct air capture[1]	0.16	USD/kg
CO_2 biogas production[1]	0.02	USD/kg
CO_2 ammonia production[8]	0.01	USD/kg
CO_2 coal-based power plant[1]	0.05	USD/kg
CO_2 natural gas power plant[1]	0.08	USD/kg
H_2 nuclear-based electrolysis[1]	4.63	USD/kg
H_2 solar-based electrolysis[1]	8.87	USD/kg
H_2 wind-based electrolysis[1]	5.24	USD/kg
Natural gas[?]	0.33	USD/m^3
Biomass (wood chips)[?]	0.17	USD/kg
Steam[9]	4.77	USD/MJ
Electricity[1]	0.10	USD/kWh
Cooling water[9]	0.02	USD/m^3
Wastewater[9]	0.04	USD/m^3
Driving cost diesel[*] [?]	0.06	USD/km

[*]Driving cost considers an oil price of 60 USD per bbl.

Notes and references

1 A. González-Garay, M. S. Frei, A. Al-Qahtani, C. Mondelli, G. Guillén-Gosálbez and J. Pérez-Ramírez, *En. Env. Sc.*, 2019, **12**, 3425–3436.

2 D. W. Keith, G. Holmes, D. S. Angelo and K. Heidel, *Joule*, 2018, **2**, 1573–1594.

3 C. Hank, L. Lazar, F. Mantei, M. Ouda, R. J. White, T. Smolinka, A. Schaadt, C. Hebling and H.-M. Henning, *Sust. En. Fuels*, 2019, **3**, 3219–3233.

4 B. Singh, A. H. Strømman and E. Hertwich, *Int. J. Greenhouse Gas Cont.*, 2011, **5**, 457–466.

5 G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz and B. Weidema, *Int. J. Life Cycle Assess.*, 2016, **21**, 1218–1230.

6 A. Simons, *Int. J. Life Cycle Assess.*, 2016, **21**, 1299–1313.

7 B. P. Weidema, *J. Ind. Ecol.*, 2015, **19**, 20–26.

8 P. Bains, P. Psarras and J. Wilcox, *Prog. En. Comb. Sc.*, 2017, **63**, 146–172.

9 R. Turton, R. C. Bailie, W. B. Whiting and J. A. Shaeiwitz, *Analysis, Synthesis and Design of Chemical Processes*, Pearson Education, New Jersey, 2008.