

## **Towards Flexible Large-Scale Environmentally Sustainable Methanol and Ammonia Production using Industrial Symbiosis**

Joshua Magson<sup>a</sup>, Thérèse Lee Chan<sup>b</sup>, Akeem Mohammed<sup>b</sup>, Keeran Ward<sup>\*a</sup>

<sup>a</sup>School of Chemical and Process Engineering (SCAPE), University of Leeds, Leeds, LS2 9JT, U.K

<sup>b</sup>Department of Chemical Engineering, University of the West Indies, St. Augustine, Trinidad, WI.

\*Corresponding author; Email: [k.r.ward@leeds.ac.uk](mailto:k.r.ward@leeds.ac.uk);

### **Appendix A- Supplementary data**

## 1. Electrolyser capacity requirements for hydrogen production

Within one year of the introduction of the Clean Hydrogen Production Tax Credit in the United States, 9 GW of electrolyser projects were announced and at the end of 2022, the global installed electrolyser capacity reached approximately 700 MW.<sup>1</sup>

The electrolyser capacity was determined based on the methodology outlined by González-Garay *et al.*,<sup>2</sup> and a proton exchange membrane (PEM) type electrolyser was used since it has the highest technology readiness level (TRL) alongside alkaline electrolysers.<sup>3</sup> The value of the enthalpy for water electrolysis was assumed to be 65.83 kWh per kmol of water which equates to 32.92 kWh per kg of H<sub>2</sub> and the electrical efficiency of the PEM electrolyser was assumed to be 70.5%.<sup>2</sup>

Using the electrical efficiency and the equivalent enthalpy of water electrolysis in terms of hydrogen production, the real energy of water electrolysis was calculated:

$$\text{Real energy} = \frac{\text{Enthalpy of water electrolysis}}{\text{Electrolyser efficiency}} = \left( \frac{32.92}{0.705} \right) \text{ kWh kg}^{-1} \text{ H}_2 = 46.7 \text{ kWh kg}^{-1} \text{ H}_2.$$

Equation S1

The total amount of H<sub>2</sub> required for the 300,000 t y<sup>-1</sup> e-methanol plant was determined as 6849 kg H<sub>2</sub> h<sup>-1</sup>. The required size of the electrolyser was then calculated based on a solar capacity factor of 0.241 for Louisiana.<sup>4</sup>

$$\text{Size of the electrolyser} = \frac{\text{Real energy} \times \text{H}_2 \text{ Production Rate}}{\text{Solar Capacity Factor}} = \left( \frac{0.0467 \times 6849}{0.241} \right) \text{ MW} = 1327 \text{ MW}.$$

Equation S2

The current solar energy generation within Louisiana is 13,000 MW, thereby providing more than sufficient energy to be fed into water electrolysers for the co-production of ammonia and methanol. Although, the electrolyser capacity is almost twice the amount of the current globally installed capacity, it is anticipated that there will be a significant uptick in H<sub>2</sub> production via water electrolysis with a predicted installed capacity of 175 GW by 2030.<sup>1</sup> Therefore, if this were achieved, this co-production scheme would only require less than 1% of the global installed capacity.

## 2. LCI and LCIA results overview

Utilising the LCA methodology presented in Section X in the main article, **Table S1** gives the LCI inventories aligned to mass and energy balances for each co-production scheme, retrieved from Ecoinvent v3.7. The characterised impacts are shown in **Tables S2-S25**, calculated using ReCiPe midpoint and endpoint H 2016.

**Table S1.** LCI datasets retrieved from Ecoinvent v3.7 databases

Flow	Technology	Ecoinvent Database
Natural Gas for feedstock and heating	GHR <sub>MeOH</sub> , ATR <sub>MeOH</sub> , SMR <sub>MeOH</sub> ATR <sub>NH3</sub> , SMR <sub>NH3</sub> , Capture from Natural Gas Power Plant	Natural gas, high pressure {US}  market for   APOS, U
Water	GHR <sub>MeOH</sub> , ATR <sub>MeOH</sub> , SMR <sub>MeOH</sub> ATR <sub>NH3</sub> , SMR <sub>NH3</sub> , Green H <sub>2</sub> , E-methanol, CO <sub>2</sub> Capture from Natural Gas Power Plant	Water, deionised, from tap water, at user {RoW}  market for water, deionised, from tap water, at user   APOS, U
Electricity production from grid	GHR <sub>MeOH</sub> , ATR <sub>MeOH</sub> , SMR <sub>MeOH</sub> ATR <sub>NH3</sub> , SMR <sub>NH3</sub> , E-Methanol	Electricity, high voltage {SERC}  market for   APOS, U
Electricity production from solar power	Green H <sub>2</sub>	Electricity, low voltage {SERC}  electricity production, photovoltaic, 570kWp open ground installation, multi-Si   APOS, U
MEA	Capture from Natural Gas Power Plant	Monoethanolamine {GLO}  ethanolamine production   APOS, U
Process emissions	GHR <sub>MeOH</sub> , ATR <sub>MeOH</sub> , SMR <sub>MeOH</sub> ATR <sub>NH3</sub> , SMR <sub>NH3</sub> , E-Methanol	Carbon dioxide, fossil

**Table S2.** BAU GHR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO2 eq	1.13E+00	6.96E-01	2.49E-01	3.41E-04	1.86E-01
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.86E-07	0.00E+00	2.14E-07	2.94E-10	7.21E-08
Ionizing radiation	kBq Co-60 eq	6.33E-02	0.00E+00	3.10E-03	4.19E-05	6.02E-02
Ozone formation, Human health	kg NOx eq	6.01E-04	0.00E+00	4.02E-04	7.60E-07	1.98E-04
Fine particulate matter formation	kg PM2.5 eq	7.04E-04	0.00E+00	3.15E-04	7.61E-07	3.89E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	6.48E-04	0.00E+00	4.46E-04	7.75E-07	2.02E-04
Terrestrial acidification	kg SO2 eq	1.36E-03	0.00E+00	9.62E-04	1.13E-06	3.94E-04
Freshwater eutrophication	kg P eq	1.41E-04	0.00E+00	1.12E-05	1.80E-07	1.29E-04
Marine eutrophication	kg N eq	1.34E-05	0.00E+00	4.09E-06	1.91E-08	9.34E-06
Terrestrial ecotoxicity	kg 1,4-DCB	9.23E-02	0.00E+00	3.03E-02	5.83E-04	6.15E-02
Freshwater ecotoxicity	kg 1,4-DCB	6.29E-03	0.00E+00	2.25E-03	1.51E-05	4.02E-03
Marine ecotoxicity	kg 1,4-DCB	8.36E-03	0.00E+00	2.82E-03	2.03E-05	5.52E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.98E-02	0.00E+00	1.03E-02	1.70E-04	9.30E-03
Human non-carcinogenic toxicity	kg 1,4-DCB	2.13E-01	0.00E+00	4.79E-02	3.45E-04	1.65E-01
Land use	m2a crop eq	9.13E-03	0.00E+00	1.01E-03	1.30E-05	8.11E-03
Mineral resource scarcity	kg Cu eq	3.05E-04	0.00E+00	1.93E-04	2.61E-06	1.09E-04
Fossil resource scarcity	kg oil eq	5.00E-01	0.00E+00	4.50E-01	8.73E-05	5.00E-02
Water consumption	m3	1.42E-03	0.00E+00	1.98E-04	3.15E-04	9.05E-04

**Table S3.** Hybrid GHR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2
Global warming	kg CO2 eq	1.00E+00	5.16E-01	2.25E-01	3.29E-04	1.80E-01	8.11E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	3.00E-07	0.00E+00	1.93E-07	2.84E-10	6.95E-08	3.67E-08
Ionizing radiation	kBq Co-60 eq	6.70E-02	0.00E+00	2.80E-03	4.05E-05	5.81E-02	6.13E-03
Ozone formation, Human health	kg NOx eq	7.70E-04	0.00E+00	3.63E-04	7.34E-07	1.91E-04	2.15E-04
Fine particulate matter formation	kg PM2.5 eq	8.22E-04	0.00E+00	2.85E-04	7.36E-07	3.75E-04	1.62E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	8.23E-04	0.00E+00	4.03E-04	7.49E-07	1.95E-04	2.25E-04
Terrestrial acidification	kg SO2 eq	1.57E-03	0.00E+00	8.69E-04	1.09E-06	3.80E-04	3.17E-04
Freshwater eutrophication	kg P eq	1.77E-04	0.00E+00	1.01E-05	1.74E-07	1.25E-04	4.15E-05
Marine eutrophication	kg N eq	1.87E-05	0.00E+00	3.69E-06	1.84E-08	9.01E-06	6.02E-06
Terrestrial ecotoxicity	kg 1,4-DCB	1.60E+00	0.00E+00	2.73E-02	5.63E-04	5.93E-02	1.51E+00
Freshwater ecotoxicity	kg 1,4-DCB	2.01E-02	0.00E+00	2.03E-03	1.46E-05	3.88E-03	1.42E-02
Marine ecotoxicity	kg 1,4-DCB	2.68E-02	0.00E+00	2.55E-03	1.97E-05	5.32E-03	1.89E-02
Human carcinogenic toxicity	kg 1,4-DCB	3.77E-02	0.00E+00	9.32E-03	1.64E-04	8.97E-03	1.93E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	4.03E-01	0.00E+00	4.33E-02	3.34E-04	1.59E-01	2.00E-01
Land use	m2a crop eq	4.14E-02	0.00E+00	9.09E-04	1.25E-05	7.82E-03	3.27E-02
Mineral resource scarcity	kg Cu eq	1.27E-03	0.00E+00	1.75E-04	2.52E-06	1.05E-04	9.89E-04
Fossil resource scarcity	kg oil eq	4.76E-01	0.00E+00	4.06E-01	8.44E-05	4.82E-02	2.11E-02
Water consumption	m3	4.19E-03	0.00E+00	1.79E-04	3.05E-04	8.72E-04	2.83E-03

**Table S4.** BAU GHR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO2 eq	8.89E-01	4.72E-01	2.06E-01	4.96E-04	2.11E-01
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.59E-07	0.00E+00	1.77E-07	4.27E-10	8.15E-08
Ionizing radiation	kBq Co-60 eq	7.07E-02	0.00E+00	2.56E-03	6.10E-05	6.81E-02
Ozone formation, Human health	kg NOx eq	5.58E-04	0.00E+00	3.33E-04	1.11E-06	2.24E-04
Fine particulate matter formation	kg PM2.5 eq	7.01E-04	0.00E+00	2.61E-04	1.11E-06	4.40E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	5.98E-04	0.00E+00	3.69E-04	1.13E-06	2.28E-04
Terrestrial acidification	kg SO2 eq	1.24E-03	0.00E+00	7.97E-04	1.65E-06	4.46E-04
Freshwater eutrophication	kg P eq	1.56E-04	0.00E+00	9.30E-06	2.62E-07	1.46E-04
Marine eutrophication	kg N eq	1.40E-05	0.00E+00	3.38E-06	2.78E-08	1.06E-05
Terrestrial ecotoxicity	kg 1,4-DCB	9.55E-02	0.00E+00	2.50E-02	8.48E-04	6.96E-02
Freshwater ecotoxicity	kg 1,4-DCB	6.44E-03	0.00E+00	1.86E-03	2.19E-05	4.55E-03
Marine ecotoxicity	kg 1,4-DCB	8.61E-03	0.00E+00	2.34E-03	2.96E-05	6.24E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.93E-02	0.00E+00	8.54E-03	2.47E-04	1.05E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	2.26E-01	0.00E+00	3.96E-02	5.02E-04	1.86E-01
Land use	m2a crop eq	1.00E-02	0.00E+00	8.34E-04	1.89E-05	9.17E-03
Mineral resource scarcity	kg Cu eq	2.87E-04	0.00E+00	1.60E-04	3.79E-06	1.23E-04
Fossil resource scarcity	kg oil eq	4.29E-01	0.00E+00	3.72E-01	1.27E-04	5.66E-02
Water consumption	m3	1.65E-03	0.00E+00	1.64E-04	4.59E-04	1.02E-03

**Table S5.** Hybrid GHR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2
Global warming	kg CO2 eq	7.60E-01	2.92E-01	1.82E-01	4.85E-04	2.04E-01	8.11E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.72E-07	0.00E+00	1.56E-07	4.17E-10	7.90E-08	3.67E-08
Ionizing radiation	kBq Co-60 eq	7.44E-02	0.00E+00	2.26E-03	5.96E-05	6.60E-02	6.13E-03
Ozone formation, Human health	kg NOx eq	7.27E-04	0.00E+00	2.94E-04	1.08E-06	2.17E-04	2.15E-04
Fine particulate matter formation	kg PM2.5 eq	8.19E-04	0.00E+00	2.30E-04	1.08E-06	4.26E-04	1.62E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	7.73E-04	0.00E+00	3.26E-04	1.10E-06	2.21E-04	2.25E-04
Terrestrial acidification	kg SO2 eq	1.45E-03	0.00E+00	7.03E-04	1.61E-06	4.32E-04	3.17E-04
Freshwater eutrophication	kg P eq	1.92E-04	0.00E+00	8.21E-06	2.56E-07	1.42E-04	4.15E-05
Marine eutrophication	kg N eq	1.93E-05	0.00E+00	2.99E-06	2.71E-08	1.02E-05	6.02E-06
Terrestrial ecotoxicity	kg 1,4-DCB	1.60E+00	0.00E+00	2.21E-02	8.28E-04	6.74E-02	1.51E+00
Freshwater ecotoxicity	kg 1,4-DCB	2.03E-02	0.00E+00	1.64E-03	2.14E-05	4.41E-03	1.42E-02
Marine ecotoxicity	kg 1,4-DCB	2.71E-02	0.00E+00	2.06E-03	2.89E-05	6.05E-03	1.89E-02
Human carcinogenic toxicity	kg 1,4-DCB	3.72E-02	0.00E+00	7.54E-03	2.41E-04	1.02E-02	1.93E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	4.16E-01	0.00E+00	3.50E-02	4.91E-04	1.80E-01	2.00E-01
Land use	m2a crop eq	4.23E-02	0.00E+00	7.36E-04	1.85E-05	8.89E-03	3.27E-02
Mineral resource scarcity	kg Cu eq	1.25E-03	0.00E+00	1.41E-04	3.71E-06	1.19E-04	9.89E-04
Fossil resource scarcity	kg oil eq	4.05E-01	0.00E+00	3.29E-01	1.24E-04	5.48E-02	2.11E-02
Water consumption	m3	4.42E-03	0.00E+00	1.45E-04	4.48E-04	9.91E-04	2.83E-03

**Table S6.** BAU ATR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO2 eq	1.15E+00	8.35E-01	2.68E-01	2.71E-04	4.62E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.48E-07	0.00E+00	2.30E-07	2.33E-10	1.79E-08
Ionizing radiation	kBq Co-60 eq	1.83E-02	0.00E+00	3.33E-03	3.33E-05	1.50E-02
Ozone formation, Human health	kg NOx eq	4.82E-04	0.00E+00	4.32E-04	6.04E-07	4.92E-05
Fine particulate matter formation	kg PM2.5 eq	4.36E-04	0.00E+00	3.39E-04	6.05E-07	9.66E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	5.30E-04	0.00E+00	4.79E-04	6.16E-07	5.01E-05
Terrestrial acidification	kg SO2 eq	1.13E-03	0.00E+00	1.04E-03	8.99E-07	9.80E-05
Freshwater eutrophication	kg P eq	4.44E-05	0.00E+00	1.21E-05	1.43E-07	3.22E-05
Marine eutrophication	kg N eq	6.73E-06	0.00E+00	4.40E-06	1.52E-08	2.32E-06
Terrestrial ecotoxicity	kg 1,4-DCB	4.83E-02	0.00E+00	3.25E-02	4.63E-04	1.53E-02
Freshwater ecotoxicity	kg 1,4-DCB	3.43E-03	0.00E+00	2.42E-03	1.20E-05	1.00E-03
Marine ecotoxicity	kg 1,4-DCB	4.42E-03	0.00E+00	3.04E-03	1.62E-05	1.37E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.35E-02	0.00E+00	1.11E-02	1.35E-04	2.31E-03
Human non-carcinogenic toxicity	kg 1,4-DCB	9.27E-02	0.00E+00	5.15E-02	2.74E-04	4.09E-02
Land use	m2a crop eq	3.11E-03	0.00E+00	1.08E-03	1.03E-05	2.02E-03
Mineral resource scarcity	kg Cu eq	2.37E-04	0.00E+00	2.08E-04	2.07E-06	2.70E-05
Fossil resource scarcity	kg oil eq	4.96E-01	0.00E+00	4.84E-01	6.94E-05	1.24E-02
Water consumption	m3	6.88E-04	0.00E+00	2.13E-04	2.51E-04	2.25E-04



**Table S7.** Hybrid ATR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2
Global warming	kg CO2 eq	1.02E+00	6.32E-01	2.41E-01	2.71E-04	6.26E-02	8.11E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.68E-07	0.00E+00	2.07E-07	2.33E-10	2.42E-08	3.67E-08
Ionizing radiation	kBq Co-60 eq	2.94E-02	0.00E+00	2.99E-03	3.33E-05	2.02E-02	6.13E-03
Ozone formation, Human health	kg NOx eq	6.71E-04	0.00E+00	3.88E-04	6.04E-07	6.66E-05	2.15E-04
Fine particulate matter formation	kg PM2.5 eq	5.98E-04	0.00E+00	3.04E-04	6.05E-07	1.31E-04	1.62E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	7.24E-04	0.00E+00	4.31E-04	6.16E-07	6.78E-05	2.25E-04
Terrestrial acidification	kg SO2 eq	1.38E-03	0.00E+00	9.30E-04	8.99E-07	1.33E-04	3.17E-04
Freshwater eutrophication	kg P eq	9.60E-05	0.00E+00	1.09E-05	1.43E-07	4.35E-05	4.15E-05
Marine eutrophication	kg N eq	1.31E-05	0.00E+00	3.95E-06	1.52E-08	3.14E-06	6.02E-06
Terrestrial ecotoxicity	kg 1,4-DCB	1.56E+00	0.00E+00	2.92E-02	4.63E-04	2.07E-02	1.51E+00
Freshwater ecotoxicity	kg 1,4-DCB	1.77E-02	0.00E+00	2.17E-03	1.20E-05	1.35E-03	1.42E-02
Marine ecotoxicity	kg 1,4-DCB	2.35E-02	0.00E+00	2.73E-03	1.62E-05	1.85E-03	1.89E-02
Human carcinogenic toxicity	kg 1,4-DCB	3.25E-02	0.00E+00	9.97E-03	1.35E-04	3.13E-03	1.93E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	3.02E-01	0.00E+00	4.63E-02	2.74E-04	5.53E-02	2.00E-01
Land use	m2a crop eq	3.64E-02	0.00E+00	9.73E-04	1.03E-05	2.73E-03	3.27E-02
Mineral resource scarcity	kg Cu eq	1.21E-03	0.00E+00	1.87E-04	2.07E-06	3.66E-05	9.89E-04
Fossil resource scarcity	kg oil eq	4.73E-01	0.00E+00	4.35E-01	6.94E-05	1.68E-02	2.11E-02
Water consumption	m3	3.58E-03	0.00E+00	1.91E-04	2.51E-04	3.04E-04	2.83E-03

**Table S8. BAU ATR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>**

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO <sub>2</sub> eq	9.10E-01	6.13E-01	2.26E-01	4.28E-04	7.09E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.22E-07	0.00E+00	1.94E-07	3.68E-10	2.75E-08
Ionizing radiation	kBq Co-60 eq	2.58E-02	0.00E+00	2.81E-03	5.26E-05	2.29E-02
Ozone formation, Human health	kg NO <sub>x</sub> eq	4.41E-04	0.00E+00	3.64E-04	9.53E-07	7.55E-05
Fine particulate matter formation	kg PM <sub>2.5</sub> eq	4.35E-04	0.00E+00	2.86E-04	9.55E-07	1.48E-04
Ozone formation, Terrestrial ecosystems	kg NO <sub>x</sub> eq	4.82E-04	0.00E+00	4.04E-04	9.73E-07	7.69E-05
Terrestrial acidification	kg SO <sub>2</sub> eq	1.02E-03	0.00E+00	8.72E-04	1.42E-06	1.50E-04
Freshwater eutrophication	kg P eq	5.97E-05	0.00E+00	1.02E-05	2.26E-07	4.93E-05
Marine eutrophication	kg N eq	7.29E-06	0.00E+00	3.70E-06	2.39E-08	3.56E-06
Terrestrial ecotoxicity	kg 1,4-DCB	5.16E-02	0.00E+00	2.74E-02	7.31E-04	2.34E-02
Freshwater ecotoxicity	kg 1,4-DCB	3.59E-03	0.00E+00	2.04E-03	1.89E-05	1.53E-03
Marine ecotoxicity	kg 1,4-DCB	4.69E-03	0.00E+00	2.56E-03	2.55E-05	2.10E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.31E-02	0.00E+00	9.35E-03	2.13E-04	3.54E-03
Human non-carcinogenic toxicity	kg 1,4-DCB	1.07E-01	0.00E+00	4.34E-02	4.33E-04	6.27E-02
Land use	m <sup>2</sup> a crop eq	4.02E-03	0.00E+00	9.13E-04	1.63E-05	3.09E-03
Mineral resource scarcity	kg Cu eq	2.20E-04	0.00E+00	1.75E-04	3.27E-06	4.15E-05
Fossil resource scarcity	kg oil eq	4.27E-01	0.00E+00	4.08E-01	1.10E-04	1.91E-02
Water consumption	m <sup>3</sup>	9.19E-04	0.00E+00	1.79E-04	3.95E-04	3.45E-04

**Table S9.** Hybrid ATR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2
Global warming	kg CO2 eq	7.77E-01	4.10E-01	1.98E-01	4.28E-04	8.73E-02	8.13E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.41E-07	0.00E+00	1.70E-07	3.68E-10	3.38E-08	3.68E-08
Ionizing radiation	kBq Co-60 eq	3.69E-02	0.00E+00	2.47E-03	5.26E-05	2.82E-02	6.15E-03
Ozone formation, Human health	kg NOx eq	6.30E-04	0.00E+00	3.20E-04	9.53E-07	9.29E-05	2.16E-04
Fine particulate matter formation	kg PM2.5 eq	5.97E-04	0.00E+00	2.51E-04	9.55E-07	1.82E-04	1.63E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	6.77E-04	0.00E+00	3.55E-04	9.73E-07	9.46E-05	2.26E-04
Terrestrial acidification	kg SO2 eq	1.27E-03	0.00E+00	7.67E-04	1.42E-06	1.85E-04	3.18E-04
Freshwater eutrophication	kg P eq	1.12E-04	0.00E+00	8.95E-06	2.26E-07	6.07E-05	4.16E-05
Marine eutrophication	kg N eq	1.37E-05	0.00E+00	3.26E-06	2.39E-08	4.38E-06	6.04E-06
Terrestrial ecotoxicity	kg 1,4-DCB	1.57E+00	0.00E+00	2.41E-02	7.31E-04	2.88E-02	1.52E+00
Freshwater ecotoxicity	kg 1,4-DCB	1.79E-02	0.00E+00	1.79E-03	1.89E-05	1.89E-03	1.42E-02
Marine ecotoxicity	kg 1,4-DCB	2.38E-02	0.00E+00	2.25E-03	2.55E-05	2.59E-03	1.90E-02
Human carcinogenic toxicity	kg 1,4-DCB	3.21E-02	0.00E+00	8.22E-03	2.13E-04	4.36E-03	1.93E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	3.17E-01	0.00E+00	3.82E-02	4.33E-04	7.72E-02	2.01E-01
Land use	m2a crop eq	3.74E-02	0.00E+00	8.02E-04	1.63E-05	3.80E-03	3.28E-02
Mineral resource scarcity	kg Cu eq	1.20E-03	0.00E+00	1.54E-04	3.27E-06	5.10E-05	9.93E-04
Fossil resource scarcity	kg oil eq	4.03E-01	0.00E+00	3.58E-01	1.10E-04	2.35E-02	2.12E-02
Water consumption	m3	3.82E-03	0.00E+00	1.58E-04	3.95E-04	4.24E-04	2.84E-03

**Table S10.** BAU SMR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO2 eq	1.23E+00	9.15E-01	2.78E-01	5.56E-04	3.44E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.53E-07	0.00E+00	2.39E-07	4.79E-10	1.33E-08
Ionizing radiation	kBq Co-60 eq	1.46E-02	0.00E+00	3.46E-03	6.84E-05	1.11E-02
Ozone formation, Human health	kg NOx eq	4.87E-04	0.00E+00	4.50E-04	1.24E-06	3.66E-05
Fine particulate matter formation	kg PM2.5 eq	4.25E-04	0.00E+00	3.53E-04	1.24E-06	7.17E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	5.37E-04	0.00E+00	4.99E-04	1.27E-06	3.72E-05
Terrestrial acidification	kg SO2 eq	1.15E-03	0.00E+00	1.08E-03	1.85E-06	7.28E-05
Freshwater eutrophication	kg P eq	3.68E-05	0.00E+00	1.26E-05	2.94E-07	2.39E-05
Marine eutrophication	kg N eq	6.33E-06	0.00E+00	4.57E-06	3.11E-08	1.72E-06
Terrestrial ecotoxicity	kg 1,4-DCB	4.61E-02	0.00E+00	3.38E-02	9.51E-04	1.14E-02
Freshwater ecotoxicity	kg 1,4-DCB	3.28E-03	0.00E+00	2.52E-03	2.46E-05	7.43E-04
Marine ecotoxicity	kg 1,4-DCB	4.21E-03	0.00E+00	3.16E-03	3.32E-05	1.02E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.35E-02	0.00E+00	1.15E-02	2.77E-04	1.72E-03
Human non-carcinogenic toxicity	kg 1,4-DCB	8.45E-02	0.00E+00	5.36E-02	5.63E-04	3.04E-02
Land use	m2a crop eq	2.64E-03	0.00E+00	1.13E-03	2.12E-05	1.50E-03
Mineral resource scarcity	kg Cu eq	2.41E-04	0.00E+00	2.16E-04	4.25E-06	2.01E-05
Fossil resource scarcity	kg oil eq	5.13E-01	0.00E+00	5.03E-01	1.43E-04	9.23E-03
Water consumption	m3	9.03E-04	0.00E+00	2.21E-04	5.14E-04	1.67E-04

**Table S11.** Hybrid SMR-SMR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2	CO <sub>2</sub> from Nat Gas Power Plant
Global warming	kg CO2 eq	1.15E+00	7.49E-01	2.50E-01	5.09E-04	5.26E-02	8.11E-02	1.25E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.78E-07	0.00E+00	2.14E-07	4.39E-10	2.04E-08	3.67E-08	6.05E-09
Ionizing radiation	kBq Co-60 eq	2.64E-02	0.00E+00	3.10E-03	6.26E-05	1.70E-02	6.13E-03	1.11E-04
Ozone formation, Human health	kg NOx eq	7.25E-04	0.00E+00	4.03E-04	1.14E-06	5.60E-05	2.15E-04	4.99E-05
Fine particulate matter formation	kg PM2.5 eq	6.02E-04	0.00E+00	3.16E-04	1.14E-06	1.10E-04	1.62E-04	1.35E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	7.82E-04	0.00E+00	4.47E-04	1.16E-06	5.71E-05	2.25E-04	5.11E-05
Terrestrial acidification	kg SO2 eq	1.44E-03	0.00E+00	9.65E-04	1.69E-06	1.12E-04	3.17E-04	4.16E-05
Freshwater eutrophication	kg P eq	9.01E-05	0.00E+00	1.13E-05	2.69E-07	3.66E-05	4.15E-05	4.56E-07
Marine eutrophication	kg N eq	1.34E-05	0.00E+00	4.10E-06	2.85E-08	2.64E-06	6.02E-06	6.46E-07
Terrestrial ecotoxicity	kg 1,4-DCB	1.56E+00	0.00E+00	3.03E-02	8.71E-04	1.74E-02	1.51E+00	1.31E-03
Freshwater ecotoxicity	kg 1,4-DCB	1.77E-02	0.00E+00	2.26E-03	2.25E-05	1.14E-03	1.42E-02	7.81E-05
Marine ecotoxicity	kg 1,4-DCB	2.34E-02	0.00E+00	2.83E-03	3.04E-05	1.56E-03	1.89E-02	9.88E-05
Human carcinogenic toxicity	kg 1,4-DCB	3.28E-02	0.00E+00	1.03E-02	2.53E-04	2.63E-03	1.93E-02	3.27E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	2.97E-01	0.00E+00	4.80E-02	5.16E-04	4.66E-02	2.00E-01	1.70E-03
Land use	m2a crop eq	3.60E-02	0.00E+00	1.01E-03	1.94E-05	2.29E-03	3.27E-02	4.70E-05
Mineral resource scarcity	kg Cu eq	1.22E-03	0.00E+00	1.94E-04	3.90E-06	3.08E-05	9.89E-04	6.72E-06
Fossil resource scarcity	kg oil eq	4.99E-01	0.00E+00	4.51E-01	1.31E-04	1.41E-02	2.11E-02	1.26E-02
Water consumption	m3	3.77E-03	0.00E+00	1.98E-04	4.71E-04	2.56E-04	2.83E-03	1.29E-05

**Table S12.** BAU SMR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Global warming	kg CO2 eq	9.85E-01	6.90E-01	2.36E-01	7.11E-04	5.88E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.26E-07	0.00E+00	2.03E-07	6.13E-10	2.28E-08
Ionizing radiation	kBq Co-60 eq	2.20E-02	0.00E+00	2.93E-03	8.75E-05	1.90E-02
Ozone formation, Human health	kg NOx eq	4.45E-04	0.00E+00	3.80E-04	1.59E-06	6.25E-05
Fine particulate matter formation	kg PM2.5 eq	4.23E-04	0.00E+00	2.98E-04	1.59E-06	1.23E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	4.87E-04	0.00E+00	4.22E-04	1.62E-06	6.37E-05
Terrestrial acidification	kg SO2 eq	1.04E-03	0.00E+00	9.11E-04	2.36E-06	1.25E-04
Freshwater eutrophication	kg P eq	5.19E-05	0.00E+00	1.06E-05	3.75E-07	4.09E-05
Marine eutrophication	kg N eq	6.86E-06	0.00E+00	3.87E-06	3.98E-08	2.95E-06
Terrestrial ecotoxicity	kg 1,4-DCB	4.93E-02	0.00E+00	2.86E-02	1.22E-03	1.94E-02
Freshwater ecotoxicity	kg 1,4-DCB	3.43E-03	0.00E+00	2.13E-03	3.15E-05	1.27E-03
Marine ecotoxicity	kg 1,4-DCB	4.46E-03	0.00E+00	2.67E-03	4.25E-05	1.74E-03
Human carcinogenic toxicity	kg 1,4-DCB	1.31E-02	0.00E+00	9.77E-03	3.54E-04	2.94E-03
Human non-carcinogenic toxicity	kg 1,4-DCB	9.80E-02	0.00E+00	4.53E-02	7.20E-04	5.20E-02
Land use	m2a crop eq	3.54E-03	0.00E+00	9.53E-04	2.71E-05	2.56E-03
Mineral resource scarcity	kg Cu eq	2.23E-04	0.00E+00	1.83E-04	5.44E-06	3.44E-05
Fossil resource scarcity	kg oil eq	4.42E-01	0.00E+00	4.26E-01	1.82E-04	1.58E-02
Water consumption	m3	1.13E-03	0.00E+00	1.87E-04	6.58E-04	2.86E-04

**Table S13.** Hybrid SMR-ATR Midpoint Characterisation (ReCiPe Midpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H2
Global warming	kg CO2 eq	8.40E-01	4.75E-01	2.07E-01	6.65E-04	7.70E-02	8.11E-02
Stratospheric ozone depletion	kg CFC11 eq X10 <sup>-4</sup>	2.45E-07	0.00E+00	1.78E-07	5.73E-10	2.98E-08	3.67E-08
Ionizing radiation	kBq Co-60 eq	3.37E-02	0.00E+00	2.57E-03	8.17E-05	2.49E-02	6.13E-03
Ozone formation, Human health	kg NOx eq	6.33E-04	0.00E+00	3.34E-04	1.48E-06	8.20E-05	2.15E-04
Fine particulate matter formation	kg PM2.5 eq	5.86E-04	0.00E+00	2.62E-04	1.48E-06	1.61E-04	1.62E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	6.81E-04	0.00E+00	3.70E-04	1.51E-06	8.35E-05	2.25E-04
Terrestrial acidification	kg SO2 eq	1.28E-03	0.00E+00	7.99E-04	2.21E-06	1.63E-04	3.17E-04
Freshwater eutrophication	kg P eq	1.05E-04	0.00E+00	9.33E-06	3.51E-07	5.36E-05	4.15E-05
Marine eutrophication	kg N eq	1.33E-05	0.00E+00	3.39E-06	3.72E-08	3.87E-06	6.02E-06
Terrestrial ecotoxicity	kg 1,4-DCB	1.56E+00	0.00E+00	2.51E-02	1.14E-03	2.55E-02	1.51E+00
Freshwater ecotoxicity	kg 1,4-DCB	1.77E-02	0.00E+00	1.87E-03	2.94E-05	1.67E-03	1.42E-02
Marine ecotoxicity	kg 1,4-DCB	2.36E-02	0.00E+00	2.34E-03	3.97E-05	2.28E-03	1.89E-02
Human carcinogenic toxicity	kg 1,4-DCB	3.20E-02	0.00E+00	8.57E-03	3.31E-04	3.85E-03	1.93E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	3.09E-01	0.00E+00	3.98E-02	6.73E-04	6.81E-02	2.00E-01
Land use	m2a crop eq	3.69E-02	0.00E+00	8.36E-04	2.53E-05	3.36E-03	3.27E-02
Mineral resource scarcity	kg Cu eq	1.20E-03	0.00E+00	1.60E-04	5.08E-06	4.50E-05	9.89E-04
Fossil resource scarcity	kg oil eq	4.16E-01	0.00E+00	3.74E-01	1.70E-04	2.07E-02	2.11E-02
Water consumption	m3	3.99E-03	0.00E+00	1.64E-04	6.15E-04	3.74E-04	2.83E-03

**Table S14.** BAU GHR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.38E-06	4.38E-07	3.93E-07	3.11E-09	5.51E-07
Ecosystem Quality	species.yr	3.05E-09	1.32E-09	8.11E-10	8.43E-12	9.05E-10
Resource Depletion	USD2013	1.44E-01	0.00E+00	1.33E-01	2.91E-05	1.13E-02

**Table S15.** Hybrid GHR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>
Human Health	DALY	1.45E-06	2.71E-07	3.47E-07	3.04E-09	5.34E-07	2.91E-07
Ecosystem Quality	species.yr	3.12E-09	8.18E-10	7.16E-10	8.23E-12	8.77E-10	6.97E-10
Resource Depletion	USD2013	1.34E-01	0.00E+00	1.17E-01	2.85E-05	1.10E-02	5.25E-03

**Table S16.** BAU GHR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.61E-06	6.46E-07	4.75E-07	2.13E-09	4.87E-07
Ecosystem Quality	species.yr	3.73E-09	1.95E-09	9.80E-10	5.79E-12	8.00E-10
Resource Depletion	USD2013	1.71E-01	0.00E+00	1.61E-01	2.00E-05	1.00E-02

**Table S17.** Hybrid GHR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>
Human Health	DALY	1.67E-06	4.79E-07	4.29E-07	2.06E-09	4.70E-07	2.91E-07
Ecosystem Quality	species.yr	3.80E-09	1.44E-09	8.85E-10	5.60E-12	7.72E-10	6.97E-10
Resource Depletion	USD2013	1.60E-01	0.00E+00	1.45E-01	1.93E-05	9.66E-03	5.25E-03

**Table S18.** BAU ATR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.41E-06	7.75E-07	5.11E-07	1.70E-09	1.21E-07
Ecosystem Quality	species.yr	3.60E-09	2.34E-09	1.05E-09	4.60E-12	1.99E-10



Resource Depletion	USD2013	1.75E-01	0.00E+00	1.73E-01	1.59E-05	2.49E-03
--------------------	---------	----------	----------	----------	----------	----------

**Table S19.** Hybrid ATR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>
Human Health	DALY	1.50E-06	5.87E-07	4.59E-07	1.70E-09	1.64E-07	2.91E-07
Ecosystem Quality	species.yr	3.69E-09	1.77E-09	9.47E-10	4.60E-12	2.69E-10	6.97E-10
Resource Depletion	USD2013	1.64E-01	0.00E+00	1.55E-01	1.59E-05	3.37E-03	5.25E-03

**Table S20.** BAU ATR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.19E-06	5.69E-07	4.30E-07	2.68E-09	1.86E-07
Ecosystem Quality	species.yr	2.92E-09	1.72E-09	8.88E-10	7.27E-12	3.05E-10
Resource Depletion	USD2013	1.50E-01	0.00E+00	1.46E-01	2.51E-05	3.82E-03

**Table S21.** Hybrid ATR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>
Human Health	DALY	1.28E-06	3.81E-07	3.78E-07	2.68E-09	2.28E-07	2.92E-07
Ecosystem Quality	species.yr	3.01E-09	1.15E-09	7.81E-10	7.27E-12	3.75E-10	7.00E-10
Resource Depletion	USD2013	1.38E-01	0.00E+00	1.28E-01	2.51E-05	4.70E-03	5.26E-03

**Table S22.** BAU SMR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.47E-06	8.49E-07	5.31E-07	3.48E-09	8.99E-08
Ecosystem Quality	species.yr	3.81E-09	2.56E-09	1.10E-09	9.45E-12	1.48E-10
Resource Depletion	USD2013	1.82E-01	0.00E+00	1.80E-01	3.27E-05	1.85E-03

**Table S23.** Hybrid SMR-SMR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>	CO <sub>2</sub> from Nat Gas Power Plant
Human Health	DALY	1.62E-06	6.95E-07	4.76E-07	3.19E-09	1.38E-07	2.91E-07	2.16E-08
Ecosystem Quality	species.yr	4.06E-09	2.10E-09	9.82E-10	8.66E-12	2.26E-10	6.97E-10	5.12E-11
Resource Depletion	USD2013	1.74E-01	0.00E+00	1.61E-01	2.99E-05	2.83E-03	5.25E-03	4.51E-03

**Table S24.** BAU SMR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid
Human Health	DALY	1.25E-06	6.41E-07	4.49E-07	4.46E-09	1.54E-07
Ecosystem Quality	species.yr	3.12E-09	1.93E-09	9.28E-10	1.21E-11	2.53E-10
Resource Depletion	USD2013	1.55E-01	0.00E+00	1.52E-01	4.18E-05	3.16E-03

**Table S25.** Hybrid SMR-ATR Endpoint Characterisation (ReCiPe Endpoint H 2016), FU= 1kgNH<sub>3</sub>

Impact Category	Unit	Total	Process Emissions	Natural Gas	Water	Electricity Grid	Green H <sub>2</sub>
Human Health	DALY	1.33E-06	4.41E-07	3.94E-07	4.16E-09	2.02E-07	2.91E-07
Ecosystem Quality	species.yr	3.18E-09	1.33E-09	8.14E-10	1.13E-11	3.31E-10	6.97E-10
Resource Depletion	USD2013	1.43E-01	0.00E+00	1.33E-01	3.90E-05	4.15E-03	5.25E-03

## References

1. IEA, *Global Hydrogen Review 2023*, IEA, Paris, 2023.
2. A. González-Garay, M. S. Frei, A. Al-Qahtani, C. Mondelli, G. Guillén-Gosálbez and J. Pérez-Ramírez, *Energy Environ. Sci.*, 2019, **12**, 3425-3436.
3. R. Dufo-López, J. M. Lujano-Rojas and J. L. Bernal-Agustín, *Int. J. Hydrogen Energy*, 2024, **50**, 292-309.
4. EIA, Capacity factors and usage factors at electric generators, [https://www.eia.gov/state/seds/data.php?incfile=/state/seds/sep\\_fuel/html/fuel\\_cf.html&sid=LA](https://www.eia.gov/state/seds/data.php?incfile=/state/seds/sep_fuel/html/fuel_cf.html&sid=LA), (accessed May 20, 2024).