

## Supplementary material

**Table S1.** Life cycle inventory (LCI) of ammonia production, FU 1 t of liquid NH<sub>3</sub>.

Product/Element Flow	Unit	Ammonia via SMR		Ammonia via elect.		Comments / Process used from Ecoinvent
		20000 t/annum	100000 t/annum	20000 t/annum	100000 t /annum	
Inputs						
Natural gas	Nm³	888	1036	-	-	market for natural gas, high pressure   natural gas, high pressure   APOS, U - GB
Demineralized water	T	1.30	2.70	1.90	1.90	market for water, deionised   water, deionised   APOS, U *
Electricity	MWh	0.78	-	11	9.0 – 10.0	market for electricity, medium voltage   electricity, medium voltage   APOS, U *
Reformer catalyst¹	Kg	0.13	0.13	-	-	Composition (wt%): 18% NiO, 0.1% SiO₂, 0.05% SO₃, 81.85% Al₂O₃
WGS catalyst¹	kg	0.17	0.17	-	-	Composition (wt%): 88% FeO3, 9% Cr₂O₃, 2.6% CuO, 0.4% Al₂O₃
Ammonia synthesis catalyst¹	kg	0.2	0.2	0.2	0.2	Composition (wt%): 96% Fe, 1% KOH, 3% Al₂O₃
Methanation catalyst¹	kg	1.89	1.89	-	-	Composition (wt%): 32% NiO, 42% Al₂O₃, 26% ZrO2
With Carbon Capture and Storage						
Chilled ammonia¹	kg	-	0.33	-	-	ammonia solution 10%
Electricity¹	kWh	-	100.94	-	-	For compression: 50 kWh/t CO₂, for injection: 7 kWh/t CO₂
Heat³	MJ	-	2.6	-	-	steam production, as energy carrier, in chemical industry   heat, from steam, in chemical industry   APOS, U - RER
Outputs						
NH₃ (product)	t	1	1	1	1	-
NH₃ (emissions)	kg	0.11	0.13	0.08	0.07	-
CH₄ (emissions)²	kg	15.68	18.29	-	-	Methane slip 2.5% (average for North America)
NOx (emissions)	kg	1	0.6 – 1.3	-	-	-
Wastewater²	kg	78	162	-	-	treatment of wastewater, average, capacity 1E9l/year   wastewater, average   APOS, U *
CO₂	t	1.80	2.13	-	-	-
Oxygen	Nm3	-	-	1040	1020	-
With Carbon Capture and Storage						
CO₂ emitted	t	-	0.35	-	-	CCS efficiency aprox. 85%
CO₂ losses¹	kg	-	10.45	-	-	losses 0.59% of CO₂ stored

<sup>1</sup> Reference: [1]

<sup>2</sup> Reference: [2]

<sup>3</sup> Reference: [3]

\* The selected process depends on the location.

**Table S2.** Life cycle inventory of ammonia storage and transport, FU 1 t of liquid NH<sub>3</sub>.

Product/Element Flow	Unit	Value	Comments / Process used from Ecoinvent
<i>Storage</i>			
Electricity input for refrigeration	kWh	60 – 75	market for electricity, medium voltage   electricity, medium voltage   APOS, U *
Ammonia (NH <sub>3</sub> ) emissions <sup>1</sup>			
Leakage (0.02%)	kg	0.2	-
BOG (0.03%, 5 d in manufacturing location)	kg	1.5	-
BOG (0.03%, 3 d in destination port)	kg	0.9	-
<i>Transport</i>			
Marine transport work			
From Morocco to UK	tkm	2.0798	market for transport, freight, sea, tanker for liquid goods other than petroleum and liquefied natural gas   transport, freight, sea, tanker for liquid goods other than petroleum and liquefied natural gas   APOS, U - GLO
From Australia to UK	tkm	17.327	
From Chile to UK	tkm	12.340	
From Brazil to UK	tkm	7.004	
From Iceland to UK	tkm	1.795	
Land transport work	tkm	0.199	market for transport, freight, lorry, unspecified   transport, freight, lorry, unspecified   APOS, U - RER
Ammonia (NH <sub>3</sub> ) emissions <sup>1</sup>			
BOG From Morocco to UK	kg	1.167	-
BOG From Australia to UK	kg	9.750	-
BOG From Chile to UK	kg	6.938	-
BOG From Brazil to UK	kg	3.938	-
BOG From Iceland to UK	kg	1.011	-
BOG during loading and unloading	kg	0.00031	-

<sup>1</sup> Reference: [4,5] \* The selected process depends on the location.

**Table S3.** Life cycle inventory of ammonia-based power generation, FU 1 kWh of electricity.

Product/Element Flow	Unit	Value	Comments / Process used from Ecoinvent
<i>Inputs</i>			
Ammonia, anhydrous, liquid	kg	0.77	-
Gas turbine	p	7.84 x 10 <sup>-10</sup>	micro gas turbine production, 100kW electrical   micro gas turbine, 100kW electrical   APOS, U - RoW
Water, completely softened	kg	0.31	water production, completely softened   water, completely softened   APOS, U - RER
<i>Outputs</i>			
Electricity production	kWh	1	-
Heat, district or industrial	kWh	2.58	heat production, natural gas, at boiler modulating >100kW   heat, district or industrial, natural gas   APOS, U - Europe without Switzerland
Ammonia, NH <sub>3</sub>	kg	3.33 x 10 <sup>-6</sup>	-
Dinitrogen monoxide, N <sub>2</sub> O	kg	2.31 x 10 <sup>-6</sup>	-
Nitric oxide, NO	Kg	6.69 x 10 <sup>-6</sup>	-
Nitrogen oxides, NO <sub>2</sub>	Kg	9.66 x 10 <sup>-4</sup>	-
Water vapour, H <sub>2</sub> O	m <sup>3</sup>	1.21	-

## References

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2. European Commission Reference Document on Best Available Techniques for the Manufacture of Large Volume Inorganic Chemicals - Ammonia, Acids and Fertilisers. *Best Available Tech. Ref. Doc.* **2007**, *1*, 513–527.
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