Supplementary Information: Techno-economic performances and life cycle greenhouse gas emissions of various ammonia production pathways including conventional, carbon-capturing, nuclear-powered, and renewable production

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S1. Assumptions for techno-economic analysis

The assumptions for techno-economic analysis (TEA) are listed in Table S1. In this work, a plant life and analysis period of 40 years is assumed, which is consistent with existing studies of clean H_2 production.[1,2] The 8% real IRR (internal rate of return) value was employed based on the return-on-equity statistics (adjusted for inflation) from Praxair, Inc., and Air Products and Chemicals, Inc., during the period 2009–2017.[3] The demand for ammonia produced from various pathways is assumed to be significant in the future. Additional details are available in reference.[3]

Table S1 Economic analysis assumptions.

Parameter	Value
Reference year	2016
Length of construction period (years)	3
% of capital spent in 1st year of construction	8
% of capital spent in 2nd year of construction	60
% of capital spent in 3rd year of construction	32
Start-up time (years)	1
Plant life (years)	40
Analysis period (years)	40
Depreciation schedule length (years)	20
Depreciation type	MACRS[a]
% equity financing	40
Interest rate on debt, if applicable (%)	3.7
Debt period (years)	Constant debt
Fixed operating costs during Start-up (%)	75
Revenues during start-up (%)	50
Variable operating costs during start-up (%)	75
Decommissioning costs (% of depreciable capital investment)	10
Salvage value (% of total capital investment)	10
Inflation rate (%)	1.9
After-tax real IRR[b] (%)	8
State taxes (%)	6
Federal taxes (%)	21
Total tax rate (%)	25.74
Working capital (% of yearly change in operating costs)	15

[a] MACRS: Modified accelerated cost recovery system. [b] IRR: Internal rate of return.

S2. Equipment and installation costs

Equipment and installation costs for ammonia production were determined from mass and energy balance results obtained from engineering models using Aspen Process Economic Analyzer. Table S2 shows equipment and installation costs for each process block for NG-based, carbon-capturing, nuclear-powered, and renewable ammonia production.

Table S2 Equipment and installation costs for process blocks for various ammonia production. All the dollar values are based on 2016 U.S. dollars.

Process block	Equipment cost ($)	Installation cost ($)
NG-based ammonia production	50,850,800	80,771,600
Desulfurization	103,800	666,600
Steam methane reforming	5,571,100	6,979,400
Water-gas shift	987,500	2,568,600
CO_2 removal by aMDEA	8,769,800	15,279,900
Methanation	166,500	559,400
Haber-Bosch loop	12,723,100	18,378,300
Boiler and steam turbines	13,365,700	20,972,300
Utility (cooling and water treatment)	9,163,300	15,367,100
Carbon-capturing ammonia production version 1	57,152,700	89,307,000
Desulfurization	103,800	666,600
Steam methane reforming	5,571,100	6,979,400
Water-gas shift	987,500	2,568,600
CO_2 capture by aMDEA	8,769,800	15,279,900
CO_2 compression and cooling	6,227,000	8,397,900
Methanation	166,500	559,400
Haber-Bosch loop	12,723,100	18,378,300
Boiler and steam turbines	13,365,700	20,972,300
Utility (cooling and water treatment)	9,238,200	15,504,600
Carbon-capturing ammonia production version 2	127,939,200	211,236,900
Desulfurization	103,800	666,600
Steam methane reforming	5,571,100	6,979,400
Water-gas shift	987,500	2,568,600
CO_2 capture by aMDEA	8,769,800	15,279,900
CO_2 capture by Cansolv	69,727,500	120,280,000
CO_2 compression and cooling	8,191,100	11,098,600
Methanation	166,500	559,400
Haber-Bosch loop	12,723,100	18,378,300
Boiler and steam turbines	12,446,400	19,895,400
Utility (cooling and water treatment)	9,252,400	15,530,700
Nuclear-powered or renewable ammonia production	38,285,300	53,017,200
Air separation by cryogenic distillation	18,056,200	22,506,100
Haber-Bosch loop	13,061,000	18,642,800
Boiler and steam turbines	4,657,900	7,069,100
Utility (cooling tower)	2,510,200	4,799,200

S3. Costs of utility, byproduct, and catalysts

Table S3 summarizes the costs of feedstock, utility, byproduct, and catalysts used for various ammonia production. The cost of clean hydrogen is described in the main paper. All the dollar values are based on 2016 U.S. dollars.

Table S3 Costs of utility, byproduct, and catalysts used in this work. All the dollar values are based on 2016 U.S. dollars.

Feedstock, utility, byproduct, or catalyst	Cost	Reference
Industrial electricity ($/kWh)	0.07	[4]
Industrial NG ($/MMBtu–LHV[a])	4.24	[4]
Cooling water ($/gal)	0.0001	[3]
Oxygen byproduct ($/kg)	0.03	[3]
ZnO adsorbent ($/kg)	2.88	[5]
Catalyst (primary reformer)	16.5	[6]
Catalyst (secondary reformer)	16.5	[6]
Catalyst (high temperature water-gas shift)	20.2	[6]
Catalyst (low temperature water-gas shift)	22.6	[6]
Catalyst (methanation)	16.5	[6]
Catalyst (Haber-Bosch ammonia synthesis)	23.2	[6]

[a] LHV: Low heating value.

S4. CO_2 pipeline transportation costs

CO_2 pipeline transportation costs are estimated using the National Energy Technology Laboratory (NETL)'s CO_2 transport cost model.[7] Table S4 shows the financial inputs used in the cost model to estimate the CO_2 pipeline transportation costs.

Table S4 Financial inputs used in the CO_2 transport cost model.

Parameter	Value
Capitalization	50%
Cost of equity	12%
Cost of debt	4.5%
Tax rate	25.7%
Escalation rate	3%
Project contingency factor	15%
Depreciation method	DB150[a] – 15 years
Duration of construction in years	3
Duration of operation in years	40
Capacity factor	90%
Commercial electricity cost (2011$/MWh)	102.3

[a] DB150: 150% declining balance.

S5. Physical values for major streams

Table S5 shows physical values for major streams in the NG-based and nuclear-powered/renewable ammonia production systems.

Table S5 Physical values for major streams in the NG-based and nuclear-powered/renewable ammonia production systems.

Pathway	ID	Major Stream[b]	T (°C)	P (bar)	Mole Fraction[a]									Mass Flow ($kg/kg\ NH_3$)
					CO_2	CO	H_2	N_2	CH_4	Ar	NH_3	H_2O	O_2	
NG-based NH_3	1	Process NG	45.0	38.3	0.00	0.00	0.00	0.01	0.80	0.00	0.00	0.00	0.00	0.52
	2	NG Fuel	47.0	1.3	0.00	0.00	0.00	0.01	0.80	0.00	0.00	0.00	0.00	0.17
	3	Process Steam	360.0	35.3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.93
	4	SMR Outlet	976.1	28.7	0.05	0.08	0.35	0.15	0.00	0.00	0.00	0.35	0.00	3.76
	5	WGS Outlet	232.7	26.5	0.13	0.00	0.44	0.15	0.00	0.00	0.00	0.27	0.00	3.76
	6	Steam from WGS	407.7	111.8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	4.32
	7	aMDEA Outlet	41.6	26.5	0.00	0.00	0.75	0.24	0.00	0.00	0.00	0.00	0.00	1.16
	8	CO_2 from aMDEA	15	2.9	0.97	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.00	1.32
	9	Make-up Feed Gas	280.0	26.5	0.00	0.00	0.75	0.25	0.00	0.00	0.00	0.00	0.00	1.13
	10	Recycle Feed	14.7	275.0	0.00	0.00	0.64	0.20	0.04	0.00	0.12	0.00	0.00	2.47
	11	Liquid Condensate 1	12.2	274.5	0.00	0.00	0.01	0.00	0.00	0.00	0.98	0.00	0.00	0.23
	12	Reactor Inlet Gas	180.0	292.0	0.00	0.00	0.70	0.23	0.03	0.00	0.05	0.00	0.00	3.37
	13	Reactor Outlet Gas	467.1	284.0	0.00	0.00	0.54	0.17	0.03	0.00	0.25	0.00	0.00	3.37
	14	Steam from HB	346.7	45.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.98
	15	Liquid Condensate 2	45.3	275.0	0.00	0.00	0.02	0.01	0.00	0.00	0.97	0.00	0.00	0.84
	16	Liquid NH_3 Product	37.4	20.0	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00
	17	Purge Gas	14.7	275.0	0.00	0.00	0.69	0.22	0.04	0.00	0.05	0.00	0.00	0.07
	18	Boiler Flue Gas	43.0	1.0	0.09	0.00	0.00	0.81	0.00	0.01	0.00	0.07	0.02	3.73
Nuclear-powered or renewable NH_3	19	N_2 Feed from ASU	30.0	20.0	0.00	0.00	0.00	0.99	0.00	0.01	0.00	0.00	0.00	0.93
	20	O_2 Byproduct from ASU	28.8	4.7	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.97	0.29
	9	Make-up Feed Gas	25.8	20.0	0.00	0.00	0.75	0.25	0.00	0.00	0.00	0.00	0.00	1.13
	10	Recycle Feed	7.5	275.0	0.00	0.00	0.63	0.24	0.00	0.02	0.11	0.00	0.00	2.60
	11	Liquid Condensate 1	7.2	274.5	0.00	0.00	0.01	0.00	0.00	0.00	0.99	0.00	0.00	0.23
	12	Reactor Inlet Gas	180.0	292.0	0.00	0.00	0.69	0.25	0.00	0.01	0.04	0.00	0.00	3.50
	13	Reactor Outlet Gas	482.4	284.0	0.00	0.00	0.53	0.20	0.00	0.01	0.25	0.00	0.00	3.50
	14	Liquid Condensate 2	43.2	275.0	0.00	0.00	0.02	0.01	0.00	0.00	0.97	0.00	0.00	0.83
	15	Steam from HB	347.4	45.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.98
	16	Liquid NH_3 Product	35.9	20.0	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	1.00
	17	Purge Gas	7.5	275.0	0.00	0.00	0.68	0.26	0.00	0.02	0.04	0.00	0.00	0.07
	18	Boiler Flue Gas	43.0	1.0	0.00	0.00	0.00	0.88	0.00	0.02	0.00	0.07	0.03	0.49

[a] For the mole fraction of NG, hydrocarbons higher than CH_4 are not shown.

[b] SMR = steam methane reforming. WGS = water-gas shift. aMDEA = activated methyl diethanolamine. HB = Haber-Bosch. ASU = air separation units.

S6. Carbon balance for NG-based and carbon-capturing ammonia production

Table S6 shows the carbon balance for NG-based and carbon-capturing ammonia production.

Table S6 Carbon balance for NG-based and carbon-capturing ammonia production. The unit of all values is kmol-C/hr.

Major Stream[a]	NG-based NH_3				Carbon-capturing NH_3 v1				Carbon-capturing NH_3 v2			
	CO_2	CO	CH_4	C_nH_m (n≥2)	CO_2	CO	CH_4	C_nH_m (n≥2)	CO_2	CO	CH_4	C_nH_m (n≥2)
Process NG	0	0	1143.5	567.9	0	0	1143.5	567.9	0	0	1143.5	567.9
NG fuel	0	0	384.7	191.2	0	0	384.7	191.2	0	0	384.7	191.2
Process and combustion air	2.8	0	0	0	2.8	0	0	0	2.8	0	0	0
Pre-SMR outlet	1.4	99.1	1610.9	0	1.4	99.1	1610.9	0	1.4	99.1	1610.9	0
Primary SMR outlet	598.3	524.0	589.0	0	598.3	524.0	589.0	0	598.3	524.0	589.0	0
Secondary SMR outlet	628.6	1036.9	46.6	0	628.6	1036.9	46.6	0	628.6	1036.9	46.6	0
HT WGS outlet	1393.9	271.6	46.6	0	1393.9	271.6	46.6	0	1393.9	271.6	46.6	0
LT WGS outlet	1638.5	27.1	46.6	0	1638.5	27.1	46.6	0	1638.5	27.1	46.6	0
aMDEA outlet	0	27.1	0	0	0	27.1	0	0	0	27.1	0	0
Methanation outlet	0	0	26.7	0	0	0	26.7	0	0	0	26.7	0
Process gas emissions	1638.1	0.1	47.2	0	78.6	0.1	26.1	0	78.6	0.1	26.1	0
Flue gas emissions	604.6	0	0	0	604.6	0	0	0	60.5	0	0	0
NH_3 product	0	0	1.5	0	0	0	1.5	0	0	0	1.5	0
Captured CO_2	0	0	0	0	1559.6	<0.1	21.1	0	2103.7	<0.1	21.1	0

[a] SMR = steam methane reforming. HT WGS = high-temperature water-gas shift. LT WGS = low-temperature water-gas shift. aMDEA = activated methyl diethanolamine.

References

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