Electronic Supplementary Information

Feasibility of Electricity Generation Based on Ammonia-to-Hydrogen-to-Power System

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Supplementary Note 1.

Description of process modeling in this study.

Ammonia from a storage tank is preheated by several heat exchangers to the desired reaction temperature. It is assumed that the reaction proceeds isothermally, and the process reaches a steady state that allows the reactor effluent to provide heat to the reactant stream. Because detailed reaction kinetics were not provided in the references for the ammonia decomposition catalysts (Table 1), a reactor model called RStoic, which represents a reactor model with specified conversion values, was used to calculate the reaction heat and compare the impacts of operating temperatures. The produced gases (hydrogen and nitrogen) and unreacted ammonia are compressed to 20 bar and passed through a pressure swing adsorption unit. Using the reported experimental adsorption isotherm in Fig. S2, which shows hydrogen and nitrogen on a 5A zeolite[1] and ammonia on alumina adsorbents[2], the amount of adsorbed hydrogen, nitrogen, and ammonia are determined. Note that the amount of impurities (nitrogen and ammonia) in the hydrogen product stream is restricted by the concentration regulations for a fuel cell, which are 100 ppb and 100 ppm by volume for ammonia and nitrogen, respectively.[3] The product stream is injected into the hydrogen fuel cell with the air stream generating electricity. The impurities are combined with additional fuel (isobutane, ammonia, or a mixture of them) and mixed with the air streams, which react in the fired heater to provide heat requirement for the ammonia decomposition reaction. The outlet stream from the fired heater is 100°C higher than the reaction temperature in each case, and a heating efficiency of 90% was assumed as the base value. The only difference between Cases 1 and 2 is the recycling of unreacted ammonia, and it is the same for Cases 3 and 4. Although Cases 1 and 2 (Cases 3 and 4) used the same type of active material as a catalyst, low conversion is assumed in Cases 1 and 3 due to low operating temperature compared to the high conversion case based on the experimental results. Therefore, 60% of impurities (nitrogen and ammonia) from the PSA unit are recycled to the reactor in Cases 1 and 3. Ammonia conversion, hydrogen recovery in the PSA unit, and hydrogen yield in the overall process are presented in Fig. S5.

Supplementary Note 2.

A detailed explanation of economic analysis.

The costs of equipment in the system are estimated based on the free program of CapCost 2017, which is a Microsoft Excel macro-enabled file.[4] The module costing technique is used in this study for estimating the capital expenditure of the system.[4] This widely used technique is suitable for preliminary cost estimation and calculates the bare module cost considering both direct and indirect costs of a piece of equipment based on equipment type, design temperature, design pressure, and material of construction. The total module cost, the expenses for modifying an existing facility, and fixed capital investment (FCI), which is the grassroots cost, can be calculated using eqn (S1) and (S2).

$$C_{TM} = \int_{i=1}^{n} C_{TM,i} = 1.18 \int_{i=1}^{n} C_{Bm,i} \tag{S1}$$

$$C_{GR} = C_{TM} + 0.50 \int_{i=1}^{n} C_{Bm,i}^{o} \tag{S2}$$

where n is the total number of equipment in the system, C_{TM} is the total module cost, $C_{Bm,i}$ is the bare module cost of the equipment i, C_{GR} is the grassroots cost, and $C_{Bm,i}^{o}$ is the base bare module cost of the equipment i. Results of cost estimation for FCI by case and the impact of economies of scale are shown in Fig. S6.

In addition to estimating the capital costs, it is necessary to calculate the manufacturing costs for electricity generation. These include the cost of raw materials (such as ammonia), utilities (such as electrical power and fuel for heating), and operating labor costs. Economic parameters used in this study are listed in Table S3. It is well known that the raw material cost is the most influential factor among other manufacturing costs, and for this ammonia-based electricity generation system, the price of ammonia becomes even more crucial.

Discounted cash flow diagrams can be created to verify the profitability of the process, taking into account the capital and manufacturing costs. Since the Ammonia-to-Hydrogen-to-Power (A2H2P) system generates electricity, the Levelized cost of electricity (LCOE) is calculated in each case and compared with other methods of electricity generation. In this study, LCOE is defined as the minimum selling price of electricity required to recover investment and operating costs during the project period of 23 years (3 years for construction and 20 years for operation). In other words, the LCOE can be considered the minimum selling price of electricity that makes the net present value at the end of the project equal to zero.

Supplementary Note 3.

National electricity price and carbon intensity.

To identify the feasibility of the proposed A2H2P system in terms of electricity price and carbon emissions, national household electricity price and carbon intensity data were collected. Household electricity prices in December 2021 were obtained (from ref. 5), with data covering 147 national household electricity prices. Carbon intensity of electricity data from 2000 to 2021 was also collected, which indicates the amount of greenhouse gases emitted for 1 kW h of electrical energy.[6] For each nation, the average values during the period were used, and the number of available countries was 228. Among the countries in the two datasets, common countries that have both household electricity prices and carbon intensity were selected. A total of 134 nations were acquired, and the data was analyzed to obtain statistical trends.

The number of countries in six different continents in descending order is Asia (39), Europe (36), Africa (32), North America (15), South America (10), and Oceania (2), respectively. In terms of the mean value of national household electricity prices, Oceania shows the greatest value of 0.2055 USD per kW h; but the number of countries in this continent is only two, Australia and New Zealand. The order of the mean electricity price in descending order beside Oceania is Europe, North America, South America, Africa, and Asia. On the other hand, a different trend in the order is observed in carbon intensity for electricity. North America indicates the greatest carbon intensity followed by Asia, Oceania, Europe, Africa, and South America. The results are presented in Fig. S7, and detailed statistical values of household electricity price and carbon intensity are tabulated in Tables S4 and S5.

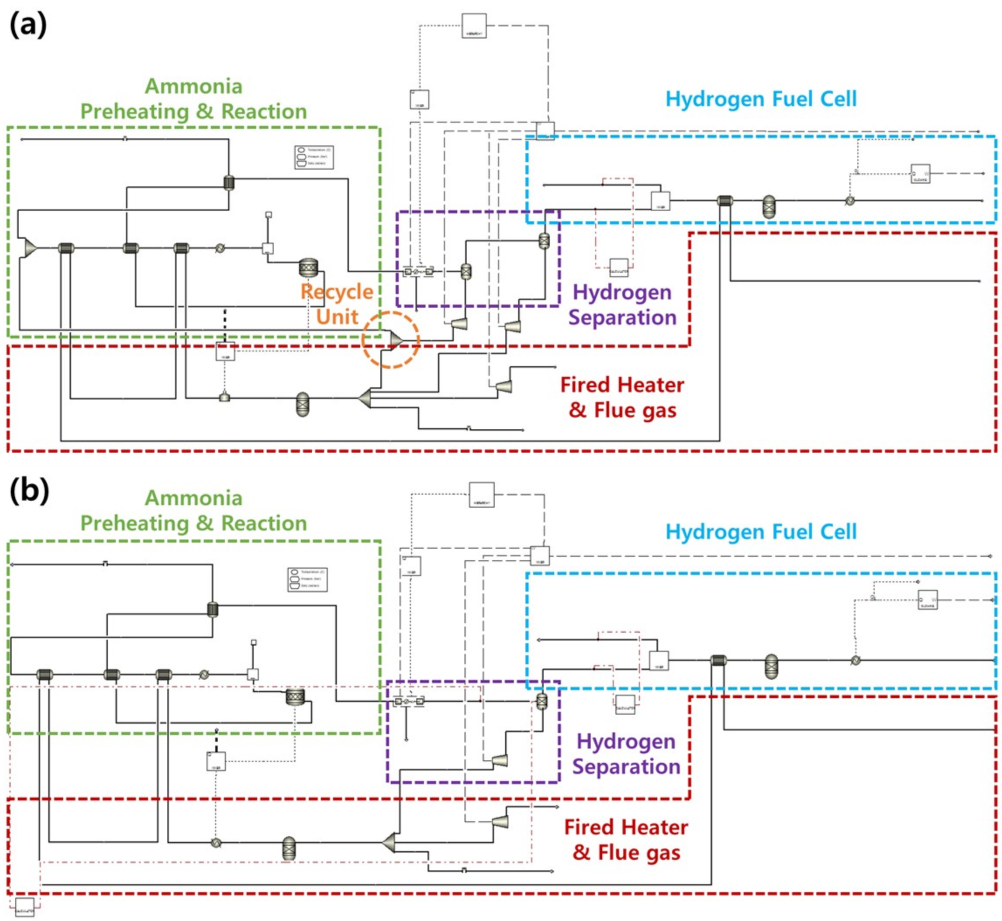

Fig. S1 Aspen flow sheet of the proposed power generation system based on ammonia decomposition and hydrogen fuel cell (a) Cases 1 and 3, which have a recycle stream due to low conversion of ammonia and (b) Cases 2 and 4, which present sufficiently high conversion of ammonia.

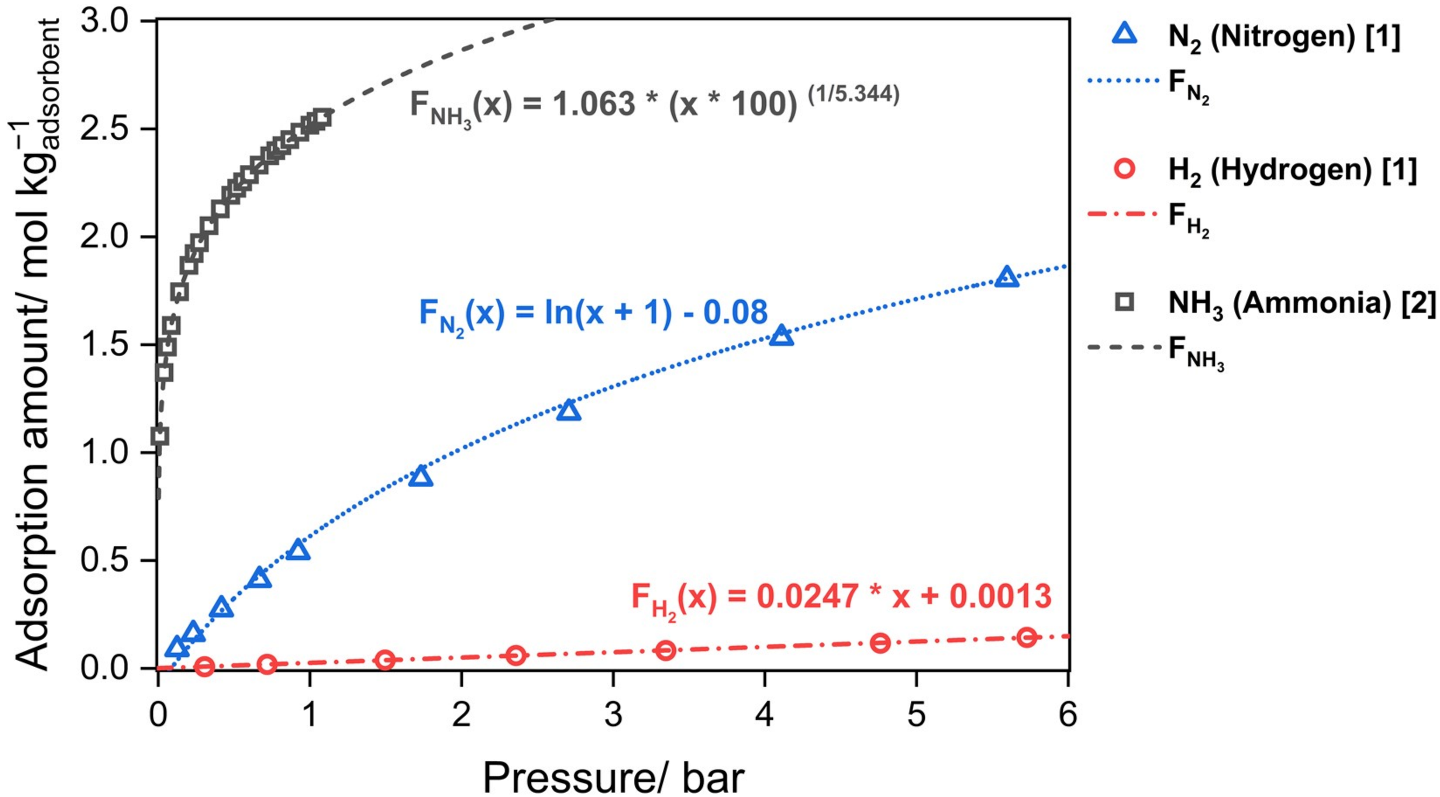

Fig. S2 Adsorption isotherms of nitrogen and hydrogen on 5A zeolite and ammonia on alumina.[1, 2]

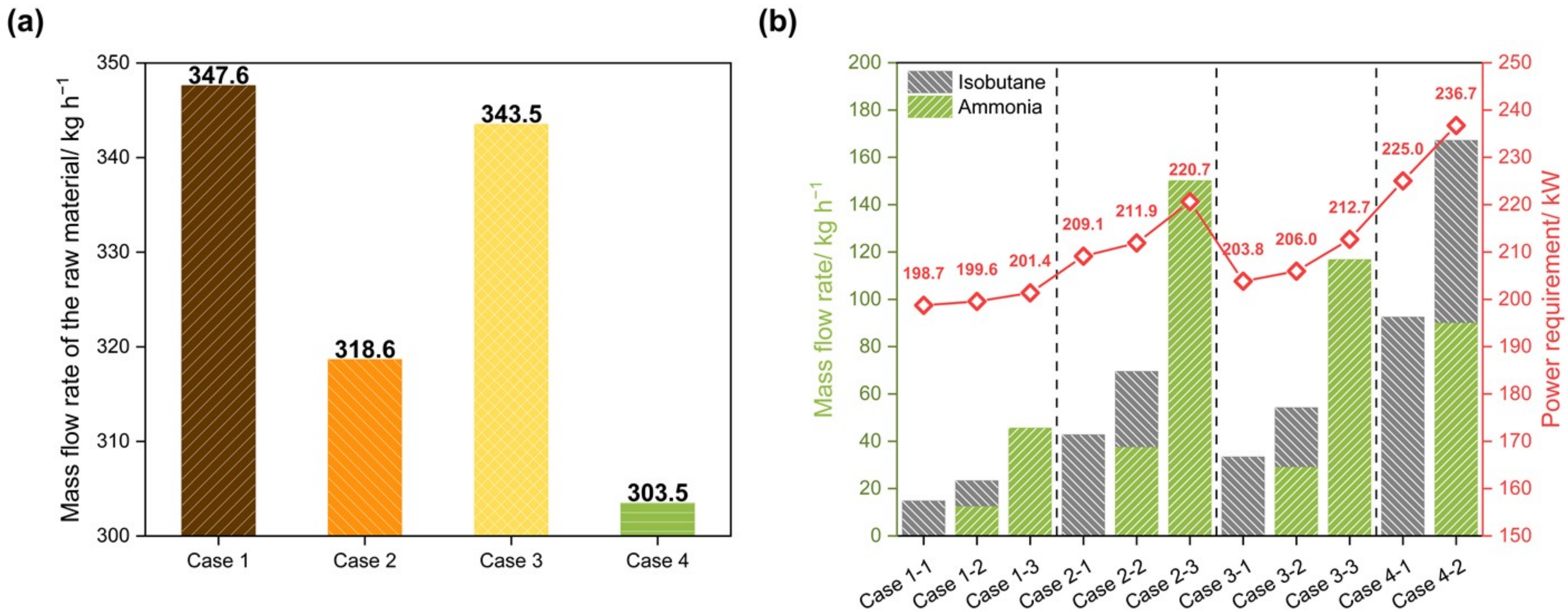

Fig. S3 Results of (a) required raw material of ammonia and (b) fuel consumption and power requirement in each case.

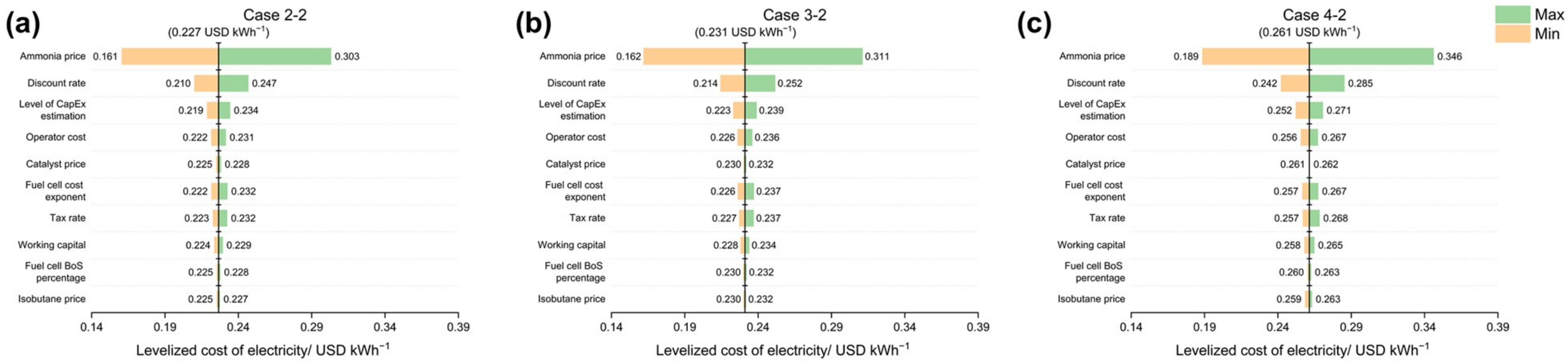

Fig. S4 Levelized cost of electricity in the proposed system in terms of economic parameters ((a), (b), and (c) for Cases 2, 3, and 4, respectively).

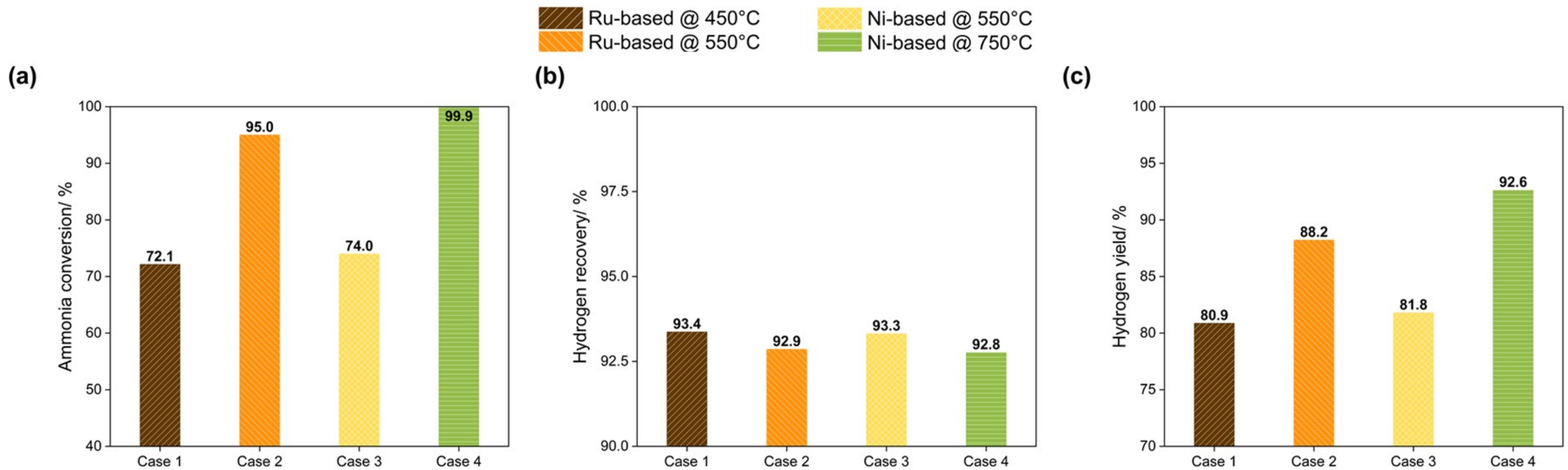

Fig. S5 Technical performance of the cases in this study in terms of (a) ammonia conversion in a reformer, (b) hydrogen recovery in pressure swing adsorption, and (c) hydrogen yield in the overall system.

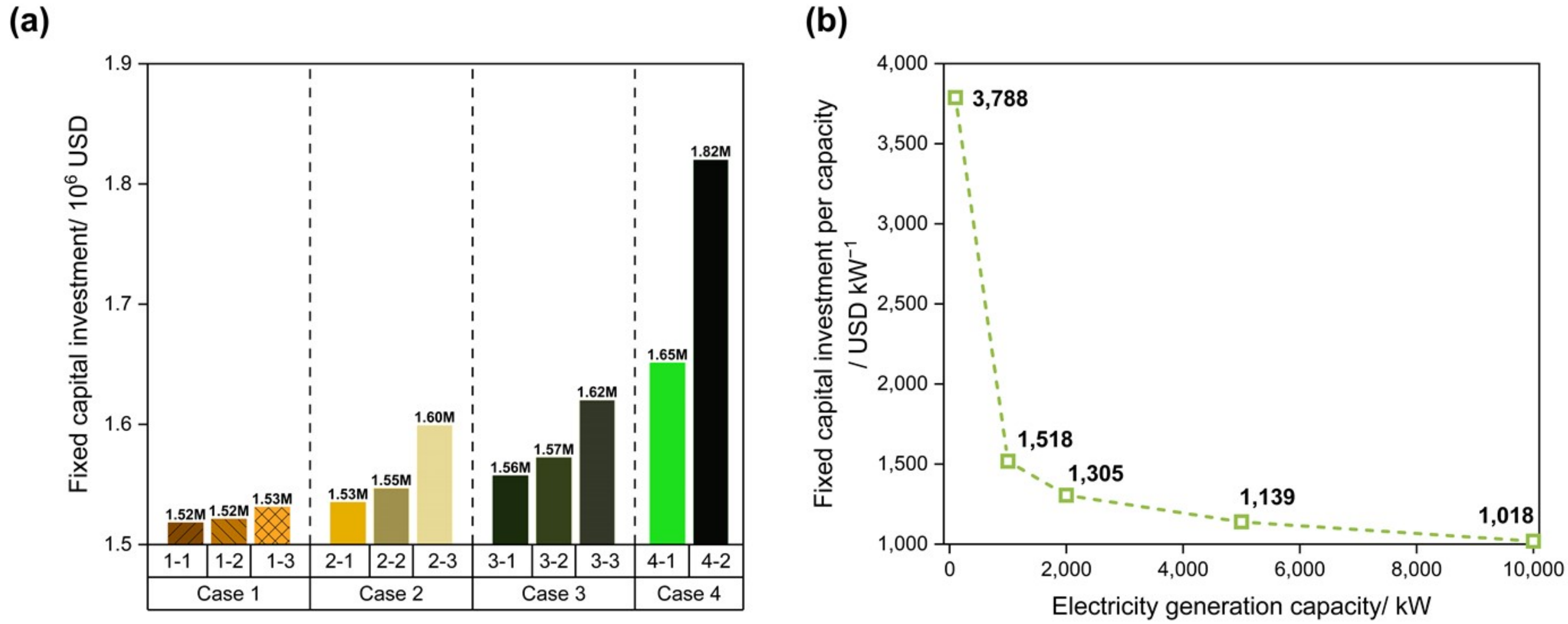

Fig. S6 Results of (a) fixed capital investment (FCI) in each case and (b) reduction of FCI as electricity generation capacity increases (Case 1-1 at 1MW-scale).

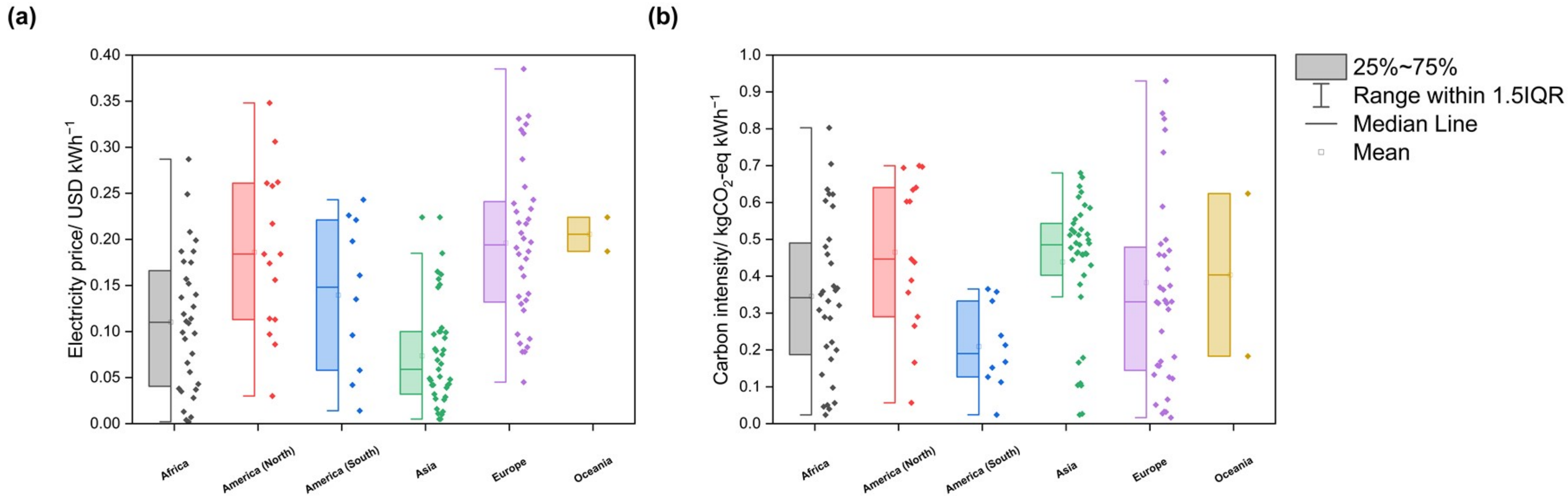

Fig. S7 Data of (a) national electricity price and (b) carbon intensity used in this study.[5, 6]

Table S1 Parameters and assumptions used in unit operations (base case process design).

Process unit	Parameters	Values/ Assumptions	Unit	Reference
Ammonia storage tank	Operating pressure	10	bar	7
	Operating temperature	25.1	°C	Calculated value
Reactor	Operating temperature	Isothermal at an inlet temperature	-	8
[a]PSA	Hydrogen recovery	80	%	9
	Adsorption pressure	20	bar	10
	Desorption pressure	0.5	bar	11
Fired heater	Heat transfer efficiency	90	%	12
[b]PEMFC	Capacity	1	MW	13
	Efficiency	60	%	14
	Operating temperature	80	°C	15

[a]PSA: Pressure swing adsorption

[b]PEMFC: Proton exchange membrane fuel cell

Table S2 Description of unit operations in the Aspen flow sheet.

System	Process unit	Block in Aspen Plus	Set up conditions	Value
Ammonia preheating & reaction	Pre-heater 1	HeatX	Hot stream outlet temperature	30°C
	Pre-heater 2		Cold stream outlet temperature	350°C
	Pre-heater 3		Hot stream outlet temperature	380°C (Case 1) 390°C (Case 2 & 3) 410°C (Case 4)
	Pre-heater 4		Cold stream outlet temperature	400°C (Case 1) 550°C (Case 2 & 3) 750°C (Case 4)
	Decomposing reactor	RStoic	Temperature	400°C (Case 1) 550°C (Case 2 & 3) 750°C (Case 4)
			Pressure drop	−0.1 bar
Hydrogen separation	[a]PSA compressor	MCompr	Number of stages	3
			Discharge pressure	20 bar
	PSA	Sep	Amount of adsorption	Based on experimental data (Fig. S2)
[b]PEMFC	Fuel cell pre-heater	HeatX	Cold stream outlet temperature	80°C
	Fuel cell	RGibbs	Pressure	1 bar
			Heat duty	0 MW (Adiabatic)

Fired heater & flue gas	Compressor 1	Compr	Discharge pressure	1.5 bar (Case 1 & 3)
	Compressor 2	Compr	Discharge pressure	1.5 bar
	Air compressor	Compr	Discharge pressure	1.5 bar
	Fired heater	RGibbs	Pressure drop	-0.5 bar
			Heat duty	0 MW (Adiabatic)
		HeatX	Temperature	The reaction temperature in each case+100°C

[a]PSA: Pressure swing adsorption

[b]PEMFC: Proton exchange membrane fuel cell

Table S3 Major parameters in economic and environmental analyses.

	Parameters	Value	Unit	Reference
Economic analysis	[1]Project period	23 (3 years construction/20 years operation)	y	16
	Annual operating hours	8,000	h	17
	Discount rate	10	%	18
	Tax rate	30	%	19
	Salvage value	0	-	4
	Depreciation method	5-year [a]MACRS	-	4
	[2]Raw material price (ammonia)	390.0	USD per t	20
	[3]Fuel price (isobutane)	234.7	USD per t	21
Carbon footprint analysis	[b, 4]GWP of nitrogen oxide	298.0	-	22
	[5]Global average carbon intensity	0.475	kgCO_2-eq per kW h	23

[a]MACRS: Modified accelerated cost recovery system

[b]GWP: Global warming potential

[1]Project period includes a 3-year construction period.

[2]Mean value of production cost in Illinois and Iowa in the United States (2020)

[3]Mean value in the United States (2020)

[4]In this study, the total amount of nitrogen oxide is the sum of nitric oxide, nitrogen dioxide, and nitrous oxide.

[5]Global average value of carbon intensity during electricity generation

Table S4 Statistical results of national electricity price by continent.

Continent	Number of countries	Minimum	Q1 (1st quartile)	Q2 (Median)	Mean	Q3 (3rd quartile)	Maximum
Africa	32	0.002	0.0405	0.11	0.11025	0.166	0.287
America (North)	15	0.03	0.113	0.184	0.186	0.261	0.348
America (South)	10	0.014	0.058	0.148	0.1394	0.221	0.243
Asia	39	0.005	0.032	0.059	0.07359	0.1	0.224
Europe	36	0.045	0.132	0.194	0.196	0.241	0.385
Oceania	2	0.187	0.187	0.2055	0.2055	0.224	0.224

Table S5 Statistical results of national carbon intensity by continent.

Continent	Number of countries	Minimum	Q1 (1st quartile)	Q2 (Median)	Mean	Q3 (3rd quartile)	Maximum
Africa	32	0.02371	0.1873	0.34183	0.34558	0.49001	0.80271
America (North)	15	0.05646	0.29007	0.44655	0.46524	0.64071	0.69983
America (South)	10	0.02404	0.12671	0.19023	0.20908	0.33283	0.36518
Asia	39	0.02407	0.40268	0.48542	0.43867	0.54323	0.68013
Europe	36	0.01642	0.14466	0.33045	0.38272	0.47879	1.67695
Oceania	2	0.18299	0.18299	0.40354	0.40354	0.6241	0.6241

Nomenclature and abbreviation

A2H2P	Ammonia-to-Hydrogen-to-Power
FCI	Fixed capital investment
LCOE	Levelized cost of electricity
n	Total number of equipment in a system
$C_{Bm,\,i}^{o}$	Base bare module cost of the equipment i
$C_{Bm,\,i}$	Bare module cost of the equipment i
C_{GR}	Grassroots cost
C_{TM}	Total module cost

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