Supporting Information

# Hydrogen society: from present to future

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**Supplementary Note #1**

Calculation model:

The supply chain of hydrogen is divided into four stages: production, transmission & storage, distribution and refueling. The total cost of hydrogen ($C_{H_2}$) is shown in equation (S1).

$$C_{H_2} = C_p + C_t + C_d + C_r \tag{S1}$$

where $C_p$ is hydrogen production cost, $C_t$ is the transmission & storage cost, $C_d$ is the distribution cost (from the transportation terminal to the refueling station), and $C_r$ is the refueling cost.

In the four stages of hydrogen production, transmission & storage, distribution and refueling (in the case of sea routine, there are more stages, including production, conditioning, loading, transmission, unloading, reconditioning, distribution and refueling), hydrogen cost at each stage includes initial investment cost and operation and maintenance cost. The initial investment cost is mainly composed of related equipment and infrastructure (hydrogen production plant, hydrogen transport pipeline, etc.). The operation and maintenance cost mainly includes the operation and maintenance cost of the equipment as well as the salary of labors. Specially, for the hydrogen production, it also includes the cost of raw materials (the cost of purchasing electricity, coal, or natural gas) and replacement costs (mainly considering that the life of the electrolytic equipment is shorter than the project life, so the electrolytic equipment will be replaced during the project life cycle). Refueling station is mainly composed of storage system, filling system and control system. The main equipment includes compressor, hydrogen storage tank, hydrogen filling machine, cooler and sequential control valve group. In our calculations, the scale of refueling station is uniformly set as 700 kg per day, and the capacity of high-pressure hydrogen storage tank is set as one day's reserve to reduce the construction cost of refueling station.

In order to estimate the cost of hydrogen more accurately and rationally, the levelized cost of hydrogen (*LCOH*) is calculated as follows (S2):

$$LCOH = \frac{C_{\text{capital}} \times \dfrac{i(1+i)^y}{(1+i)^y - 1} + C_{\text{feedstock}} + C_{\text{OM}} + C_{\text{replacement}}}{P} \quad \text{(S2)}$$

where $C_{\text{capital}}$ is the initial investment cost of hydrogen at each stage (USD, \$). For example, the $C_{\text{capital}}$ of hydrogen production includes the cost of hydrogen production equipment, plant, and the infrastructure construction; $C_{\text{feedstock}}$ is the raw-material cost of hydrogen production (electricity, coal, or natural gas, \$ per year); $C_{\text{OM}}$ and $C_{\text{replacement}}$ are the operation & maintenance cost and replacement cost, respectively; P is the hydrogen flow rate (kg per year); $i$ is the discount rate, and $y$ is the project life (year).

Considering that the life of electrolytic equipment is shorter than that of the project, there will be an additional replacement cost in the process of water electrolysis, which can be calculated by the equation (S3):

$$C_{\text{replacement}} = D_{\text{replacement}} \times N \times \left( \sum_{m=1}^{m=N} \frac{(1 - V_{\text{replacement}})^{m \times A}}{(1+i)^{m \times A}} \right) \times \frac{i(1+i)^y}{(1+i)^y - 1} \quad \text{(S3)}$$

where $D_{\text{replacement}}$ (\$) is the replacement cost of the hydrogen production plant, $N$ is the times of replacement during a project's life cycle, $V_{\text{replacement}}$ is the annual change rate of the replacement cost, and $A$ is the replacement years for the hydrogen-production plants.

For water electrolysis, the feedstock cost is calculated following the equation S4:

$$C_{\text{feedstock}} = B_{\text{elec}} \times d \times \left(\frac{h_{\text{d}}}{\eta}\right) \times \left(\sum_{m=1}^{m=y} \frac{(1+V_{\text{elec}})^m}{(1+i)^m}\right) \times \frac{i(1+i)^y}{(1+i)^y - 1} \quad \text{(S4)}$$

where $h_{\text{d}}$ is the operation hours per day of electrolysis equipment; $d$ is the operation days per year; $\eta$ is the system efficiency; $B_{\text{elec}}$ is the electricity price (\$ kWh$^{-1}$) and $V_{\text{elec}}$ is the annual change rate of $B_{\text{elec}}$.

For coal and natural gas, the feedstock cost is calculated by equation S5:

$$C_{\text{feedstock}} = B_{\text{coal,gas}} \times m_{\text{year}} \times \left(\sum_{m=1}^{m=y} \frac{(1+V_{\text{elec}})^m}{(1+i)^m}\right) \times \frac{i(1+i)^y}{(1+i)^y - 1} \quad \text{(S5)}$$

where $B_{\text{coal,gas}}$ is the price of coal (\$ per ton) or natural gas (\$ per m$^3$), $m_{\text{year}}$ is the raw material demand per year (coal: ton per year, natural gas: m$^3$ per year).

In this study, we mainly consider two transportation routes, namely land transmission and sea transmission routines. The land transmission routine is designed from Gansu, China to Shanghai, China, in which Gansu and Shanghai are selected as the place of hydrogen production and hydrogen consuming, respectively. The sea transmission is designed from Australia to Japan, where Australia and Japan serve as the place of hydrogen production and hydrogen consuming, respectively. We calculated the levelized cost of hydrogen from production to consuming.

**Table S1.** Detailed parameters of AWE, PEME and SOEC technologies at 2020 and 2050.[1]

| Alkaline water electrolyzer | | | |
|---|---|---|---|
| Parameters | 2020 | 2050 | Focus |
| Voltage (V) | 1.4-3.0 | < 1.7 | Catalysts |
| Current density (A $cm^{-2}$) | 0.2-0.8 | > 2.0 | Diaphragm |
| Cell pressure (bar) | < 30 | > 70 | Diaphragm, frames, cell |
| Cell temperature (°C) | 70-90 | > 90 | Diaphragm, frames, balance of plant components |
| Electrode area ($cm^2$) | 10,000-30,000 | 30,000 | Electrodes |
| Stack unit size (kW) | 1000 | 10,000 | Electrodes |
| Stack lifetime (h) | 60,000 | 100,000 | Electrodes |
| Time of cold start (min) | < 50 | < 30 | Design of insulation |
| $H_2$ purity (%) | 99.9-99.9998 | > 99.9999 | Diaphragm |
| Load range (%) | 15-100 | 5-300 | Diaphragm |
| System capital costs (USD $kW^{-1}$) | 500-1000 | < 200 | Balance of plant |
| Stack capital costs | 270 | < 100 | Electrodes |

| | | | |
|---|---|---|---|
| (USD $kW^{-1}$) | | | |
| System electrical efficiency (kWh $kg^{-1}$ $H_2$) | 50-78 | < 45 | Balance of plant |
| Stack electrical efficiency (kWh $kg^{-1}$ $H_2$) | 47-66 | < 42 | Diaphragm, catalysts |
| Voltage efficiency (%) | 50-68 | > 70 | Catalysts, temperature |
| Proton exchange membrane electrolyzer | | | |
| Parameters | 2020 | 2050 | Focus |
| Voltage (V) | 1.4-2.5 | < 1.7 | Catalysts, membrane |
| Current density (A $cm^{-2}$) | 1-2 | 4-6 | Design, membrane |
| Cell pressure (bar) | < 30 | > 70 | Membrane, reconversion |
| Cell temperature (°C) | 50-80 | 80 | Effect on durability |
| Electrode area ($cm^2$) | 1500 | > 10,000 | Membrane electrode assembly, porous transport layers |
| Stack unit size (kW) | 1000 | 10,000 | Membrane electrode assembly, porous transport layers |

| | | | |
|---|---|---|---|
| Stack lifetime (h) | 50,000-80,000 | 100,000-120,000 | Membrane, catalysts, porous transport layers |
| Time of cold start (min) | < 20 | < 5 | Design of insulation |
| $H_2$ purity (%) | 99.9-99.9999 | 99.9-99.9999 | Membrane |
| Load range (%) | 5-120 | 5-300 | Membrane |
| System capital costs (USD $kW^{-1}$) | 700-1400 | < 200 | Rectifier, water purification |
| Stack capital costs (USD $kW^{-1}$) | 400 | < 100 | Membrane electrode assembly, porous transport layers, bipolar plates |
| System electrical efficiency (kWh $kg^{-1}$ $H_2$) | 50-83 | < 45 | Balance of plant |
| Stack electrical efficiency (kWh $kg^{-1}$ $H_2$) | 47-66 | < 42 | Catalysts, membrane |
| Voltage efficiency (%) | 50-68 | > 80 | Catalysts |
| Solid oxide electrolysis cell | | | |
| Parameters | 2020 | 2050 | Focus |
| Voltage (V) | 1.0-1.5 | < 1.48 | Catalysts |

| | | | |
|---|---|---|---|
| Current density (A $cm^{-2}$) | 0.3-1.0 | > 2.0 | Electrolyte, electrodes |
| Cell pressure (bar) | 1 | > 20 | Electrolyte, electrodes |
| Cell temperature (°C) | 700-850 | < 600 | Electrolyte |
| Electrode area ($cm^2$) | 200 | 500 | All |
| Stack unit size (kW) | 5 | 200 | All |
| Stack lifetime (h) | < 20,000 | 80,000 | All |
| Time of cold start (min) | > 600 | < 300 | Design of insulation |
| $H_2$ purity (%) | 99.9 | > 99.9999 | Electrolyte, electrodes |
| Load range (%) | 30-125 | 0-200 | Electrolyte, electrodes |
| System capital costs (USD $kW^{-1}$) | Unknown | < 300 | All |
| Stack capital costs (USD $kW^{-1}$) | > 2000 | < 200 | Electrolyte, electrodes |
| System electrical efficiency (kWh $kg^{-1}$ $H_2$) | 40-50 | < 40 | Balance of plant |
| Stack electrical efficiency (kWh $kg^{-1}$ $H_2$) | 35-50 | < 35 | Electrolyte, electrodes |
| Voltage efficiency (%) | 75-85 | > 85 | Catalysts |

**Table S2.** Input parameters of water electrolysis.[2-4]

| | AWE | PEME | SOEC | SOEC (waste heat) |
|---|---|---|---|---|
| Plant lifetime (year) | 20 | 20 | 20 | 20 |
| Scale (MW) | 1 | 1 | 1 | 1 |
| Discount rate | 8% | 8% | 8% | 8% |
| Efficiency (%) | 65 | 70 | 61.4 | 87.6 |
| Stack lifetime (h) | 80000 | 40000 | 20000 | 20000 |
| System degradation (%/10000 hour) | 1.30 | 2.70 | 5.90 | 5.9 |
| Electricity cost ($ $kWh^{-1}$) | 0.05 | 0.05 | 0.05 | 0.05 |
| Deionized water ($ $kg^{-1}$) | 0.01 | 0.01 | 0.01 | 0.01 |
| Replacement times | 1 | 2 | 4 | 4 |
| **Capital cost:** | | | | |
| Stock cost ($ $MW^{-1}$) | 340000 | 420000 | 520000 | 520000 |
| Electric heater | -- | -- | 15000 | -- |
| **Balance of plant (BOP) cost:** | | | | |
| Power supply ($ $MW^{-1}$) | 27556 | 27556 | 27556 | 27556 |
| Separator tank of water ($ $MW^{-1}$) | 10000 | 10000 | 10000 | 10000 |
| Circulation pump ($ $MW^{-1}$) | 5500 | 5500 | 5500 | 5500 |
| Piping ($ $MW^{-1}$) | 7600 | 7600 | 7600 | 7600 |
| Valves (control of water, $ $MW^{-1}$) | 7700 | 7700 | 7700 | 7700 |
| Hydrogen dryer ($ $MW^{-1}$) | 13900 | 13900 | 13900 | 13900 |
| Hydrogen separator ($ $MW^{-1}$) | 5300 | 5300 | 5300 | 5300 |
| Tubing ($ $MW^{-1}$) | 3800 | 3800 | 3800 | 3800 |
| **Electric heater:** | | | | |
| Valves (control of hydrogen) | 5200 | 5200 | 5200 | 5200 |
| Heat exchanger | 9000 | 9000 | 9000 | 9000 |
| Cooling pump | 15000 | 15000 | 15000 | 15000 |
| Dry cooler | 4000 | 4000 | 4000 | 4000 |
| Valves control | 3000 | 3000 | 3000 | 3000 |
| Electric resistance heater | 7500 | 7500 | 7500 | 7500 |
| Other BOPs | 6000 | 6000 | 6000 | 6000 |
| **Operation and maintenance cost:** | | | | |
| Operation and maintenance (%capital) | 2 | 2 | 2 | 2 |
| Other operation cost (%capital) | 1 | 1 | 1 | 1 |

**Table S3.** Parameters of natural gas steam reforming.[5]

| Parameters | Values |
|---|---|
| Life | 20 years |
| Discount rate | 8% |
| Annual load (h per year) | 7884 |
| Overall efficiency (%) | 70-80 |
| Feedstock input ($m^3$ (stp) $h^{-1}$) | 65000 |
| Natural gas costs ($ GJ-1) | 5.40 |
| Electricity cost ($ $kWh^{-1}$) | 0.05 |
| Auxiliary electricity input (MW) | 5 |
| Net by-products (MW) | 140 |
| **Capital cost:** | |
| Total capital investment (million $) | 150 |
| Specific total capital investment (million $ $MW^{-1}$)[a] | 0.333 |
| **Operation and maintenance cost:** | |
| Operation & maintenance costs (O&M) (million $ per year) | 7.93 |
| Specific O&M (million $ $MW^{-1}$) | 0.018 |

[a]Based on the annual hydrogen output of 450 MW for large scale and 3 MW for small scale.

**Table S4.** Parameters of coal gasification.[5]

| Parameters | Values |
|---|---|
| Life | 20 years |
| Discount rate | 8% |
| Annual load (h per year) | 7008 |
| Overall efficiency (%) | 53 |
| Feedstock input (unit/h) | 120 t |
| Auxiliary electricity input (MW) | 36 |
| Net by-products (MW) | 43 |
| Feedstock costs ($ $GJ^{-1}$) | 2.10 |
| Electricity cost ($ $kWh^{-1}$) | 0.05 |
| **Capital cost:** | |
| Total capital investment (million $) | 375.500 |
| Specific total capital investment (million $ $MW^{-1}$)[a]. | 0.834 |
| **Operation & maintenance:** | |
| Operation & maintenance costs (O&M) (million $ per $year^{-1}$) | 17.310 |
| Specific O&M (million $ $MW^{-1}$) | 0.038 |

[a]Based on the annual hydrogen output of 450 MW for large scale and 3 MW for small scale.

**Table S5.** Calculated regional hydrogen production cost (USD $kg^{-1}$ $H_2$) for AWE, PEME and SOEC in representative areas worldwide based on the latest electricity prices.[6]

| Region | Electricity price (USD $kWh^{-1}$) | AWE (USD $kg^{-1}$ $H_2$) | PEME (USD $kg^{-1}$ $H_2$) | SOEC (USD $kg^{-1}$ $H_2$) |
|---|---|---|---|---|
| China | 0.095 | 5.979 | 7.215 | 9.770 |
| India | 0.104 | 6.423 | 7.698 | 10.258 |
| Japan | 0.17 | 9.682 | 11.240 | 13.841 |
| South Korea | 0.095 | 5.979 | 7.215 | 9.770 |
| Thailand | 0.105 | 6.472 | 7.752 | 10.313 |
| Saudi Arabia | 0.068 | 4.645 | 5.766 | 8.304 |
| Russia | 0.132 | 7.805 | 9.201 | 11.778 |
| France | 0.132 | 7.805 | 9.201 | 11.778 |
| Germany | 0.334 | 17.780 | 20.042 | 22.743 |
| United Kingdom | 0.263 | 14.274 | 16.232 | 18.889 |
| Italy | 0.231 | 12.694 | 14.514 | 17.152 |
| USA | 0.115 | 6.966 | 8.288 | 10.855 |
| Canada | 0.098 | 6.127 | 7.376 | 9.933 |
| Brazil | 0.155 | 8.941 | 10.435 | 13.027 |
| Argentina | 0.035 | 3.016 | 3.995 | 6.513 |
| Australia | 0.144 | 8.398 | 9.845 | 12.430 |
| Egypt | 0.061 | 4.300 | 5.390 | 7.924 |

| | | | | |
|---|---|---|---|---|
| DR Congo | 0.097 | 6.077 | 7.322 | 9.878 |
| South Africa | 0.075 | 4.991 | 6.141 | 8.684 |
| Libya | 0.006 | 1.584 | 2.438 | 4.938 |
| Ethiopia | 0.02 | 2.275 | 3.190 | 5.698 |

**Table S6.** Summary of hydrogen storage methods or materials mentioned in Fig. 4.

| Name | Gravimetric capacity (wt.%) | Volumetric capacity (g $H_2$ $L^{-1}$) | Operation temperature ($^oC$) | Type |
|---|---|---|---|---|
| Liq. H (Liquid hydrogen)[7] | 10 | 40 | -253 | Physical method |
| Comp. H (Compressed hydrogen)[8] | 6 | 30 | 25 | Physical method |
| CA (Carbon Aerogel)[9] | 5.3 | 10.6 | -196 | Physical adsorption |
| AC (Activated Carbon)[10] | 3.7 | 26 | -196 | Physical adsorption |
| CNT (Carbon Nanotubes)[11] | 0.5 | 18 | -196 | Physical adsorption |
| MOF-74[12] | 2.8 | / | -196 | Physical adsorption |
| IRMOF-1[13] | 4.3 | / | -196 | Physical adsorption |
| $LaNi_5H_6$[14] | 1.5 | 125.9 | 150 | Interstitial hydride |
| $TiFeH_{1.9}$[15] | 1.8 | 123.6 | 30 | Interstitial hydride |
| $PdH_{0.7}$[16] | 0.7 | 78.1 | 120 | Interstitial hydride |
| $ZrMn_2H_{3.6}$[17] | 1.7 | 130 | 60 | Interstitial hydride |
| Ti-Cr-Mn[18] | 2 | / | -10 | Interstitial hydride |
| NaH[19] | 4.2 | 58 | 440 | Metal |

| | | | | |
|---|---|---|---|---|
| | | | | hydride |
| $BeH_2$[19] | 18.1 | 118 | 260 | Metal hydride |
| LiH[19] | 12.6 | 103 | 740 | Metal hydride |
| $CaH_2$[19] | 4.8 | 82 | 600 | Metal hydride |
| $AlH_3$[20] | 10.1 | 150 | 160 | Metal hydride |
| $MgH_2$[21] | 7.6 | 100 | 290 | Metal hydride |
| $Mg_2NiH_4$[22] | 3.6 | 100 | 240 | Metal hydride |
| $Mg(BH_4)_2$[23] | 14.8 | 77 | 320 | Complex hydride |
| $LiBH_4$[24] | 18.4 | 120 | 380 | Complex hydride |
| $NaBH_4$[24] | 10.7 | 118 | 400 | Complex hydride |
| $NaAlH_4$[25] | 7.5 | 96 | 180 | Complex hydride |
| $NH_3BH_3$[26] | 19.5 | 152 | 500 | Chemical hydride |
| $C_{10}H_{18}$ (Decalin)[27] | 7.2 | 65 | 210 | Chemical hydride |
| $NH_3$[28] | 17.6 | 105 | 700 | Chemical hydride |
| $C_6H_{12}$ (Cyclohexane)[29] | 7.1 | 55 | 300 | Chemical hydride |

| | | | | |
|---|---|---|---|---|
| $C_7H_{14}$ (Cycloheptane)[30] | 6.1 | 47 | 350 | Chemical hydride |

**Table S7.** Parameters of pipeline transmission.[31-33]

| Parameters | Values |
|---|---|
| Life | 30 years |
| Pipeline length | 2000 km |
| Discount rate | 8% |
| Electricity price | 0.015 \$ $kWh^{-1}$ |
| Mass flow rate | 151893 kg $H_2$ per day |
| Capital recovery period | 15 years |
| Hydrogen loss rate | 486.25 kg per km per year |
| **Capital cost:** | |
| Material cost | 74649 \$ $km^{-1}$ |
| Miscellaneous | 264245 \$ |
| Reconstruction of natural gas pipeline | 12% of new pipeline |
| **Operation and maintenance:** | |
| Labor cost | 240015 \$ $km^{-1}$ |
| Labor hours | 9019 hours per year |
| Salary | 33.54 \$ per hour |
| Operation and maintenance cost | 5% of capital investment cost |

**Table S8.** Parameters of pipeline distribution [a].[31]

| Parameters | Values |
|---|---|
| Life | 30 years |
| Pipeline length | 830.4 km |
| Discount rate | 8% |
| Capital recovery period | 15 years |
| Hydrogen loss rate | 97.5 kg per km per year |
| Mass flow rate | 151893 kg per day |
| **Capital cost:** | |
| Material cost | 119380 $ $km^{-1}$ |
| Miscellaneous | 149315 $ |
| **Operation and maintenance:** | |
| Labor cost | 88805 $ $km^{-1}$ |
| Electricity price | 0.05 $ $kWh^{-1}$ |
| Labor hours | 9019 hours per year |
| Salary | 33.54 $ $hour^{-1}$ |
| Operation and maintenance cost | 5% of capital cost |

[a]In the sea-transmission scenario, pipeline distribution methods are used for all routes. The transmission cost from port to receiving station is included in the receiving cost.

**Table S9.** Parameters of compressor.[31,34]

| Parameter | Value |
|---|---|
| Z (Compress factor) | 1.28216 |
| m (Mass flow rate, kg/s) | 700/ (12×3600)[a] |
| R (Universal gas constant) | 8.3144 kJ $(kg.mole.K)^{-1}$ |
| T (Inlet temperature) | 300 K |
| n (Compressor stage) | 2 |
| K (k is the ratio of specific heats) | 1.4 |
| $\eta$ (The isentropic efficiency) | 0.75 |
| $P_{outlet}$ | 20 MPa (Trailer)<br>45 MPa (High-pressure tank) |
| $P_{inlet}$ | 2 MPa (Trailer)<br>10.3 MPa (Operation pressure of pipeline) |

[a]Work 12 hours per day.

**Table S10.** Parameters of refueling station.[31,34]

| Parameters | Values |
|---|---|
| Scale | 700 kg per day |
| Life year | 20 |
| Discount rate | 8% |
| Inlet pressure | 20 MPa (Tank trailer), 10 MPa (Pipeline) |
| Output pressure | 45 MPa |
| Capacity of hydrogen tank (45 MPa) | $700\times1.5$ |
| **Capital cost:** | |
| Compressor cost | 7500*$P_{compressor}$ (power of compressor) |
| Filling machine cost | 100000×2 $ |
| Tank cost | 1495 $ per kg hydrogen |
| **Operation and maintenance:** | |
| Operation and maintenance cost of compressor | 5% of compressor cost |
| Operation and maintenance cost of tank | 3.5% of tank cost |
| Worker | 2 |
| Salary | 1500 ($/month)×2 (worker)×12 (month)×20 (year) |

**Table S11.** Input parameters of methanol synthesis.[35]

| Parameters | Values |
|---|---|
| Project life (year) | 20 |
| Discount rate | 8% |
| Electricity ($ $kWh^{-1}$) | 0.05 |
| Scale (ton methanol per year) | 10000 |
| Operation hours | 8400 |
| Exchange rate of RMB to $ | 6.8 |
| Exchange rate of RMB to € | 7.73 |
| Methanol purity | 99.92 wt.% |
| $CO_2$ usage (ton per ton methanol) | 1.59 |
| $H_2$ usage (ton per ton methanol) | 0.22 |
| $H_2$ compressor power (kW) | 77.2 |
| Recycle compressor power (kW) | 115.17 |
| Electricity usage (kWh per ton-MeOH) | 161.75 |
| Steam usage (ton/ton-MeOH) | 0.43 |
| Colling water usage (ton per ton methanol) | 618.77 |
| Heat duty of reboiler1 (kW) | 281.22 |
| Heat duty of reboiler2 (kW) | 204.3 |
| **Capital cost:** | |
| Methanol reactor ($) | $1.6\times10^{7}\times((\text{Mass in kg h}^{-1})/54000)^{0.65}$ |
| Compressor ($) | $4.0\times10^{4}\times P(\text{kW})^{0.6038}$ |
| Boiler ($) | $4.6397\times10^{6}\times((\text{Heat duty MW})/55.6)^{0.6}$ |
| $CO_2$ ($ $ton^{-1}$) | 58.1618 |
| Fresh water ($ $ton^{-1}$) | 0.22 |
| Cooling water ($ $ton^{-1}$) | 0.05 |
| Steam ($ $ton^{-1}$) | 14.71 |
| Cooler (million $) | 0.028 |
| Heat exchanger (million $) | 0.038 |
| Recycle pump (million $) | 0.703 |
| Compressor (million $) | 0.553 |
| Reactor (million $) | 4.385 |
| Heat duty of reboiler (million $) | 0.393 |
| Separator (million $) | 0.046 |
| Boiler (million $) | 0.276 |
| **Indirect capital cost:** | |
| General facilities (% capital cost) | 10% |
| Engineering permitting and start up | 10% |
| Contingencies (% capital cost) | 5% |
| Working capital, land, and miscellaneous (% capital cost) | 3% |
| **Operation and maintenance cost:** | |
| Water (million $ per year) | 1.856 |

| | |
|---|---|
| $CO_2$ (million $ per year) | 6.29 |
| Electricity (million $ per year) | 0.57 |
| Others (million $ per year) | 4% of capital cost |

**Table S12.** Input parameters of methanol cracking.[36]

| Parameters | Values |
|---|---|
| Scale | 532 kg $H_2$ per day |
| Project life (year) | 20 |
| Electricity ($ kWh$^{-1}$) | 0.05 |
| Discount rate | 8% |
| **Capital cost:** | |
| Methanol storage (million $) | 0.004 |
| Methanol reformer (million $) | 0.455 |
| Hydrogen compressor (million $) | 0.09 |
| Hydrogen storage (million $) | 0.115 |
| Hydrogen dispenser (million $) | 0.021 |
| Total process unit (million $) | 0.685 |
| **Indirect capital cost:** | |
| General facilities (million $) | 0.137 |
| Engineering permitting and start up (million $) | 0.069 |
| Contingencies (million $) | 0.069 |
| Working capital, land and miscellaneous (million $) | 0.034 |
| **Operation and maintenance:** | |
| Variable non-fuel O&M ($ per kg $H_2$) | 0.028 |
| Labor ($ per kg $H_2$) | 0.069 |
| Electricity ($ per kg $H_2$) | 0.142 |
| Variable operating cost ($ per kg $H_2$) | 0.239 |
| Fixed operating cost ($ per kg $H_2$) | 0.171 |

**Table S13.** Capital Cost parameters of ammonia synthesis.[36]

| Parameters | Values |
|---|---|
| Scale | 300 tons ammonia per day |
| Project life (year) | 20 |
| Electricity ($ $kWh^{-1}$) | 0.05 |
| Discount rate | 8% |
| Natural gas costs ($ $GJ^{-1}$) | 5.40 |
| Water Electrolysis +Haber-Bosch | 12000 (kWh per ton $NH_3$) |
| **Capital Cost of installing cryogenic air distillation:** | |
| Heat exchangers (million $) | 2.63 |
| Compressors (million $) | 8.21 |
| Columns (million $) | 6.04 |
| Pump (million $) | 0.02 |
| Indirect capital Cost: | |
| Contingency and fees (%capital cost) | 18% |
| Auxiliary facility, land, infrastructure (%capital cost) | 27% |
| **Capital cost Haber Bosch Process:** | |
| Heat exchangers (million $) | 11.31 |
| Compressors (million $) | 21.06 |
| Reactors (million $) | 2.46 |
| Separator (million $) | 2.55 |
| Furnace (million $) | 2.39 |
| Indirect capital Cost: | |
| Contingency and fees (%capital cost) | 18% |
| Auxiliary facility, land, infrastructure (%capital cost) | 18.70% |
| **Capital cost of Electric Haber Bosch Process:** | |
| Heat exchangers (million $) | 11.31 |
| Compressors (million $) | 21.06 |
| Reactors (million $) | 2.46 |
| Separator (million $) | 2.55 |
| Indirect capital Cost: | |
| Contingency and fees (%capital cost) | 18% |
| auxiliary facility, land, infrastructure (%capital cost) | 21.40% |
| **Capital cost of installing ammonia storage system:** | |
| Heat exchanger (million $) | 0.16 |
| Compressors (million $) | 0.09 |
| Tank (Inner and Outer) (million $) | 5.33 |
| Separator (million $) | 0.07 |
| Indirect capital Cost: | |
| Contingency and fees (%module cost) (million $) | 18% |

| | |
|---|---|
| Others (million $) | 31% |

**Table S14.** Operation and maintenance cost parameters of ammonia synthesis.[36]

| Operation and maintenance cost | Haber Bosch Process | Storage system | Air separation unit |
|---|---|---|---|
| Water Consumption ($m^3$ per year) | 1371018 | 6669 | 185157 |
| Cost of Water (million $ per year) | 3.06 | 0.01 | 0.41 |
| Electric Consumption (MWh per year) | 71655 | 185 | 25829 |
| Natural Gas Consumption (tons per year) | 1860 | | |
| Total number of operators | 16 | 12 | 14 |
| Labor cost (million $ $year^{-1}$) | 0.87 | 0.65 | 0.76 |
| Salvage value (million $ $year^{-1}$) | 5.58 | 0.84 | 2.45 |
| Depreciation (million $ $year^{-1}$) | 2.51 | 0.38 | 1 |
| Miscellaneous cost (million $ $year^{-1}$) | 9.2 | 2.02 | 4.5 |
| Manufacture cost | 31.55 | 3.06 | 6.77 |

**Table S15.** Input parameters of Ammonia cracking.[36]

| Parameters | Values |
|---|---|
| Life | 30 years |
| Scale | 100 tons $H_2$ per day |
| Electricity ($ $kWh^{-1}$) | 0.05 |
| Discount rate | 8% |
| **Capital cost:** | |
| Equipment purchase ($) | 77417838.39 |
| Installation ($) | 36386383.66 |
| Piping ($) | 52644129.81 |
| Electrical System ($) | 8515962.423 |
| Instrumentation & controls ($) | 27870421.23 |
| Buildings ($) | 13935211.14 |
| Yard improvement ($) | 7741783.734 |
| Service facilities ($) | 54192487.19 |
| Indirect cost: | |
| Engineering & supervision ($) | 25547886.22 |
| Construction expenses ($) | 31741313.63 |
| Legal expenses ($) | 3096713.704 |
| Contractor's fee ($) | 17031924.85 |
| Contingency ($) | 34063848.64 |
| Working capital ($) | 58527885.96 |
| **Operation and maintenance (O & M) cost:** | |
| O & M fixed cost: | |
| Operating labor ($) | 467821.0685 |
| Supervision labor ($) | 116955.2671 |
| Direct salary overhead ($) | 233910.5343 |
| Maintenance cost ($) | 19509294.97 |
| Insurance cost ($) | 7803717.987 |
| General plant overhead ($) | 12196789.1 |
| O & M variable cost: | |
| Water ($) | 48723.00 |
| Heating utilities ($) | 3953070.00 |
| Colling Utilities ($) | 3922179.00 |
| Cracker catalyst ($) | 4320953.00 |
| Electricity ($) | 18986406.00 |

**Table S16.** Parameters of methanol shipment.[37]

| Parameters | Values |
|---|---|
| Transport distance | 7500 km (Japan-Australia) |
| Load of ship | 110000 tons |
| Discount rate | 8% |
| Average speed | 32 km $h^{-1}$ |
| Fuel consumption | 99 ton per day |
| Material loss rate | 0.01% per day |
| Loading period | 2 days |
| Life of ship | 15 years |
| **Capital cost:** | |
| Capital investment of ship | 76000000 $ |
| Indirect capital cost | 45% of capital cost |
| **Operation and maintenance (O & M) cost:** | |
| Diesel cost | 358.3 $ $ton^{-1}$ |
| Operation cost of ship | 5550 $ per day |
| Labor cost | $20\times15\times100000$ [a] |
| Load cost | 37.5 $ per ton methanol |
| Receiving cost | 37.5 $ per ton methanol |

[a]20 crews of one ship and the salary each crew is 10000 $ per year.

**Table S17.** Parameters of ammonia shipment.[37]

| Parameters | Values |
|---|---|
| Transport distance | 7500 km (Japan-Australia) |
| Load of ship | 53000 ton |
| Discount rate | 8% |
| Average speed | 32 km $h^{-1}$ |
| Fuel consumption | 61tons per day |
| Material loss rate | 0.04% per day |
| Loading period | 2 days |
| Life of ship | 15 years |
| **Capital cost:** | |
| Capital investment of ship | 85000000 $ |
| Indirect capital cost | 45% of capital cost |
| **Operation and maintenance (O & M) cost:** | |
| Operation cost of ship | 5550 $ $day^{-1}$ |
| Diesel cost | 358.3 $ $ton^{-1}$ |
| Labor cost | $20 \times 15 \times 100000$ |
| Load cost | 33.5 $ per ton methanol |
| Receiving cost | 35.3 $ per ton methanol |

## References


1 Green hydrogen cost reduction: scaling up electrolysers to meet the 1.5 °C climate goal, International Renewable Energy Agency, 2020.

2 D. Jang, J. Kim, D. Kim, W.-B. Han and S. Kang, *Energy Convers. Manag.*, 2022, **258**, 115499.

3 M. D. Rashid, M. K. Al Mesfer, H. Naseem and M. Danish, *Int. J. Eng. Adv. Tech.*, 2015, **4**, 80-93.

4 F. M. Sapountzi, J. M. Gracia, C. J. Weststrate, H. O. A. Fredriksson and J. W. Niemantsverdriet, *Prog. Energy Combust. Sci.*, 2017, **58**, 1-35.

5 F. Mueller-Langer, E. Tzimas, M. Kaltschmitt and S. Peteves, *Int. J. Hydrogen Energy*, 2007, **32**, 3797-3810.

6 Electricity market report, International Energy Agency, 2022.

7 E. Rivard, M. Trudeau and K. Zaghib, *Materials*, 2019, **12**, 1973.

8 H. Barthelemy, M. Weber and F. Barbier, *Int. J. Hydrogen Energy*, 2017, **42**, 7254-7262.

9 H. Kabbour, T. F. Baumann, J. H. Satcher, A. Saulnier and C. C. Ahn, *Chem. Mater.*, 2006, **18**, 6085-6087.

10 R. J. Anderson, T. P. McNicholas, A. Kleinhammes, A. Wang, J. Liu and Y. Wu, *J. Am. Chem. Soc.*, 2010, **132**, 8618-8626.

11 Y. Ye, C. C. Ahn, C. Witham, B. Fultz, J. Liu, A. G. Rinzler, D. Colbert, K. A. Smith and R. E. Smalley, *Appl. Phys. Lett.*, 1999, **74**, 2307-2309.

12 Y. Liu, C. M. Brown, D. A. Neumann, H. Kabbour and C. C. Ahn, *Mater. Res.*

*Soc. Symp. Proc.*, 2007, 1041.

13 A. Dailly, J. J. Vajo and C. C. Ahn, *J. Phys. Chem. B*, 2006, **110**, 1099-1101.

14 P. D. Goodell and P. S. Rudman, *J. Less-common Met.*, 1983, **89**, 117-125.

15 J. J. Reilly and R. H. Wiswall, *Inorg. Chem.*, 1974, **13**, 218-222.

16 F. D. Manchester, A. San-Martin and J. M. Pitre, *J. Phase Equilibria*, 1994, **15**, 62-83.

17 J. M. Park and J. Y. Lee, *J. Alloys Comp.*, 1992, **182**, 43-54.

18 Y. Komazaki, M. Uchida, S. Suda, A. Suzuki, S. Ono and N. Nishimiya, *J. Less-common Met.*, 1983, **89**, 269-274.

19 Q. Lai, Y. Sun, T. Wang, P. Modi, C. Cazorla, U. B. Demirci, J. R. Ares Fernandez, F. Leardini and K. F. Aguey‐Zinsou, *Adv. Sustainable Syst.*, 2019, **3**, 1900043.

20 J. Graetz and J. J. Reilly, *J. Phys. Chem. B*, 2005, **109**, 22181-22185.

21 L. Schlapbach and A. Züttel, *Nature*, 2002, **414**, 353-358.

22 L. Li, T. Akiyama and J. Yagi, *J. Alloys Comp.*, 2000, **308**, 98-103.

23 I. Saldan, *Int. J. Hydrogen Energy*, 2016, **41**, 11201-11224.

24 H. I. Schlesinger, H. C. Brown, H. R. Hoekstra and L. R. Rapp, *J. Am. Chem. Soc.*, 1953, **75**, 199-204.

25 B. Bogdanović and M. Schwickardi, *J. Alloys Comp.*, 1997, **253**, 1-9.

26 R. P. Shrestha, H. V. K. Diyabalanage, T. A. Semelsberger, K. C. Ott and A. K. Burrell, *Int. J. Hydrogen Energy*, 2009, **34**, 2616-2621.

27 A. N. Kalenchuk and L. M. Kustov, *Molecules*, 2022, **27**, 2236.

28 S. Mukherjee, S. V. Devaguptapu, A. Sviripa, C. R. F. Lund and G. Wu, *Appl. Catal. B Environ.*, 2018, **226**, 162-181.

29 G. Cacciola, N. Giordano and G. Restuccia, *Int. J. Hydrogen Energy*, 1984, **9**, 411-419.

30 F. Alhumaidan, D. Cresswell and A. Garforth, *Energy Fuels*, 2011, **25**, 4217-4234.

31 DOE $H_2$: a delivery analysis, https://www.hydrogen.energy.gov/h2a_delivery.html.

32 B. Miao, L. Giordano and S. H. Chan, *Int. J. Hydrogen Energy*, 2021, **46**, 18699-18718.

33 Transporting pure hydrogen by repurposing existing gas infrastructure: overview of existing studies and reflections on the conditions for repurposing, European Union Agency for the Cooperation of Energy Regulators, 2021.

34 Y. Gu, Q. Chen, J. Xue, Z. Tang, Y. Sun and Q. Wu, *Energy Convers. Manag.*, 2020, **223**, 113240.

35 Y. Gu, D. Wang, Q. Chen and Z. Tang, *Int. J. Hydrogen Energy*, 2022, **47**, 5085-5100.

36 S. A. Nosherwani and R. C. Neto, *J. Energy Storage*, 2021, **34**, 102201.

37 J.-S. Lee, A. Cherif, H.-J. Yoon, S.-K. Seo, J.-E. Bae, H.-J. Shin, C. Lee, H. Kwon and C.-J. Lee, *Renew. Sust. Energy Rev.*, 2022, **165**, 112556.