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Energy Conversion REPORT

Missing pieces in the hydrogen puzzle

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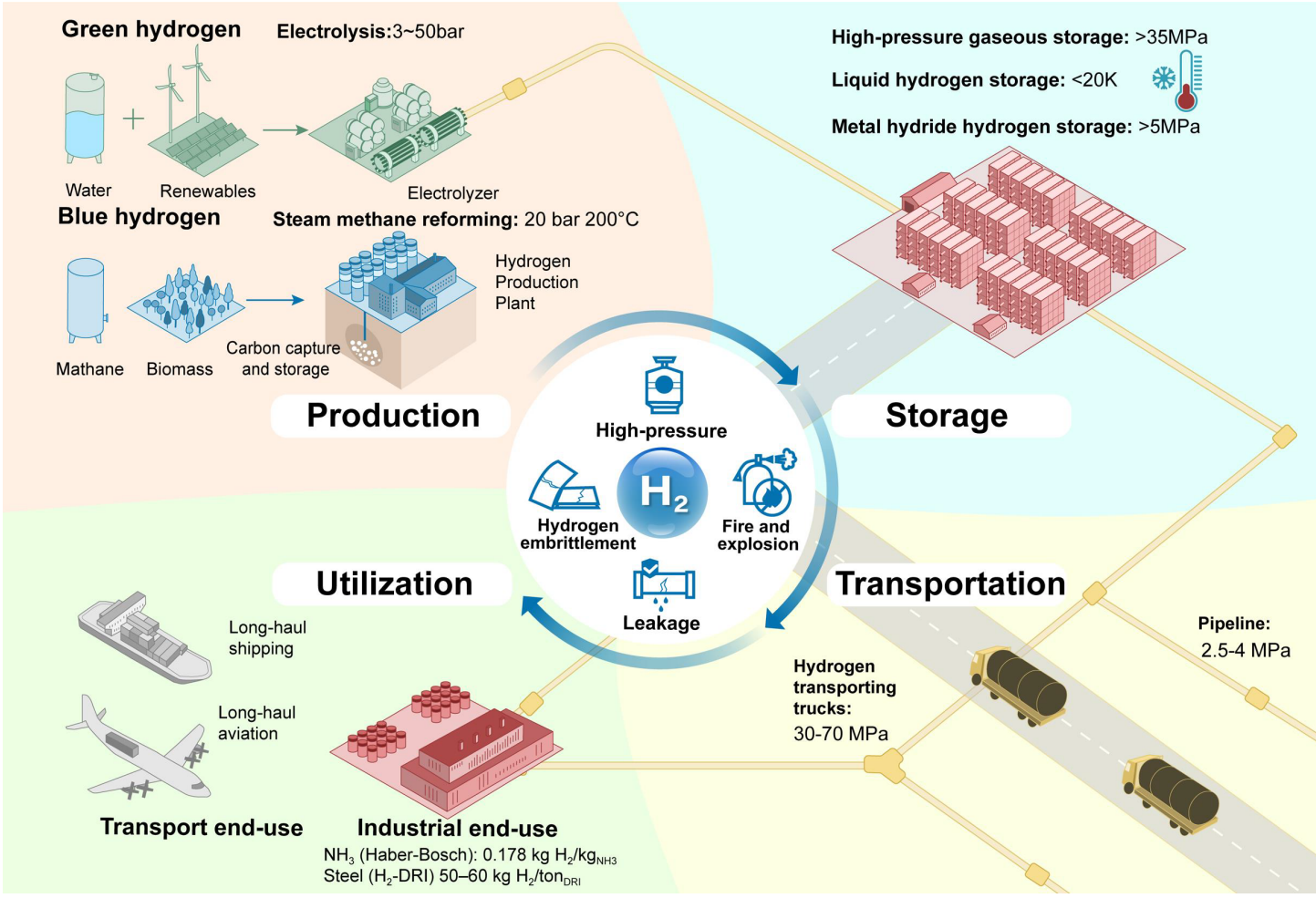
GRAPHICAL ABSTRACT



PUBLIC SUMMARY

- Hydrogen is widely promoted for energy transition, yet its reputation as ultimate clean energy requires systematic re-evaluation via interdisciplinary systems analysis.
- Power-to-hydrogen conversion suffers inherent thermodynamic defects with inevitable exergy loss, while liquefaction and compression induce severe energy penalties.
- Renewable-based green hydrogen still produces measurable carbon footprints, and hydrogen leakage may indirectly exacerbate atmospheric greenhouse effects.
- Hydrogen is irreplaceable for hard-to-abate industries and long-duration energy storage; targeted deployment instead of universal application is rational.

REPORT Energy Conversion

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Missing pieces in the hydrogen puzzle

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Hydrogen has attracted substantial attention and investment as a pathway for climate mitigation and energy transition. However, beneath the grand narrative of the hydrogen economy, its designation as the "ultimate clean energy" requires critical re-examination. Through an interdisciplinary systems analysis framework, this perspective critically evaluates the hydrogen value chain across multiple dimensions. Thermodynamic analysis reveals that power-to-hydrogen conversion inevitably degrades energy quality. Even under ideal oxy-combustion conditions, hydrogen exhibits an exergy coefficient of merely 0.9. This irreversible exergy loss exposes inherent thermodynamic deficiencies in power-to-hydrogen as an energy storage pathway, fundamentally limiting high-quality energy utilization. The energy penalties make electricity-to-hydrogen conversion inherently inefficient. Liquefaction demands a theoretical minimum of 43.2% of hydrogen's energy content, and compression to 70 MPa requires 5.74%. Life-cycle carbon footprint analysis challenges the prevailing "green hydrogen" narrative. Even when produced via renewable electricity, solar photovoltaic pathways yield carbon intensities of 1.98 $kgCO_2/kgH_2$, while wind power pathways generate 0.495 $kgCO_2/kgH_2$. Furthermore, hydrogen's high permeability presents non-negligible leakage risks. Atmospheric hydrogen accumulation indirectly amplifies greenhouse effects through hydroxyl radical interactions. Despite these constraints, hydrogen retains irreplaceable value in hard-to-abate industrial processes, weight-constrained transport, and long-duration energy storage where direct electrification is infeasible. Rational hydrogen deployment requires matching the carrier to its comparative advantages rather than pursuing a universal hydrogen economy.

INTRODUCTION

Hydrogen's combustion in air produces neither greenhouse gases nor harmful pollutants, a characteristic that has long attracted scientific attention. The green hydrogen paradigm has further amplified this enthusiasm, positioning hydrogen as crucial to carbon neutrality and earning it designation as the 21st century's "ultimate energy solution".[1-3]

Driven by the global green economy transition, hydrogen demand is accelerating worldwide. Over 40 countries have established hydrogen-related policies, with projected demands reaching 140 and 660 million tons annually by 2030 and 2050, respectively (Figure S1). The International Hydrogen Council forecasts that hydrogen will constitute 22% of global energy demand by 2050, representing a ten-fold increase to 470 million tonnes.[4]

Investment in the hydrogen sector exhibits explosive growth globally, with 510 hydrogen projects announced worldwide as of 2024 (Figure 1A). Global large-scale hydrogen projects are concentrated in Europe, China, and the United States (Figure 1C). By 2030, 1572 large-scale projects will deliver 375 GW of electrolyzer capacity with total investments reaching $680 billion, where renewable energy sources will power 75% of production capacity and low-carbon sources the remaining 25%.[5] Countries announced only 55 GW of electrolyzer capacity targets for 2030 in 2020, but this figure jumped to 175 GW in 2022 and further soared to 375 GW in 2024, achieving nearly sevenfold growth within four years[5]. Committed investments in global hydrogen pipeline projects similarly grew from $10 billion in 2020 to an estimated $110 billion by 2025, an eleven-fold increase[6]. Academic interest mirrors this industrial enthusiasm (Figure 1B).[7]

Yet amid this fervor, the difficulties facing hydrogen development are now emerging. In the 18 months preceding September 2025, the industry witnessed 52 large-scale hydrogen project cancellations representing 4 million tons of annual production capacity, squandering both resources and capital investments (Figure 1C). High costs and market instability account for the primary reasons for these cancellations. This wave of cancellations reveals critical challenges in the hydrogen sector that have been overlooked in optimistic projections. The literature lacks systematic examination of hydrogen's inherent limitations.

This perspective evaluates hydrogen as an energy carrier, not as a chemical feedstock, across four coupled dimensions: second-law limits on energy-quality degradation during conversion, minimum work requirements for storage (compression and liquefaction), life-cycle greenhouse-gas intensities under representative electricity-supply assumptions, and leakage-driven indirect climate impacts. The perspective establishes order-of-magnitude bounds and decision-relevant thresholds that delineate where hydrogen deployment is likely to be climate-beneficial and where direct electrification or alternative carriers offer clear advantages.

MATERIALS AND METHODS

Fundamental barriers for hydrogen development

Thermodynamic constraints. Hydrogen faces fundamental thermodynamic penalties across its entire utilization chain, which are often overlooked in optimistic projections. The following analyses quantify these irreducible losses.

Combustion exergy coefficients. Hydrogen combustion in air achieves a theoretical flame temperature of 1430 °C, rising to 2830 °C in pure oxygen.[8] The exergy fraction of heat released at the adiabatic flame temperature is 0.824 and 0.903, respectively, calculated as $\varepsilon = 1 - T_0/T$, where T is combustion temperature (K) and T_0 is ambient temperature (300 K). Given that electricity has an exergy coefficient of unity, power-to-hydrogen conversion inherently degrades energy quality by approximately 10%. Notably, hydrogen's combustion temperature in air falls below that of methane and ammonia, yielding inferior energy quality. Even in pure oxygen, hydrogen yields a lower exergy fraction for combustion heat than methane/ammonia under the same boundary conditions (Figure 2A).[9]

Solar radiation from the ~5700 K solar surface exhibits an exergy coefficient of 0.933 at Earth's surface, calculated via Petela's formula:[10]

$$\eta_c = 1 - \frac{4}{3}\frac{T_0}{T_{sun}} + \frac{1}{3}\left(\frac{T_0}{T_{sun}}\right)^4 \quad (1)$$

Thus, hydrogen combustion, even in pure oxygen, yields lower exergy coefficient than both electricity (ε=1.0) and terrestrial solar radiation (ε=0.933). While hydrogen fuel cells can achieve ~90% electrical conversion efficiency,[11] this still represents a net exergy loss from the original electrical input. From a thermodynamic perspective, power-to-hydrogen conversion is inefficient except for applications where electrical infrastructure is impractical, notably aviation and aerospace propulsion.

Minimum work for liquefaction. Hydrogen's low molecular weight yields exceptionally poor volumetric energy density at ambient conditions, approximately 0.09 kg/m^3 at 300 K and atmospheric pressure. While liquefaction increases storage density dramatically, hydrogen liquefies only at 20.46 K under atmospheric pressure, presenting severe thermodynamic challenges.

The exergy coefficient for cooling power at T_c= 20 K in a T_0= 300 K environment is:

$$\eta_{ex,C} = \left(\frac{T_0}{T_c} - 1\right) = \frac{300}{20} - 1 = 14 \quad (2)$$

This indicates that the minimum work required is 14 times the cooling

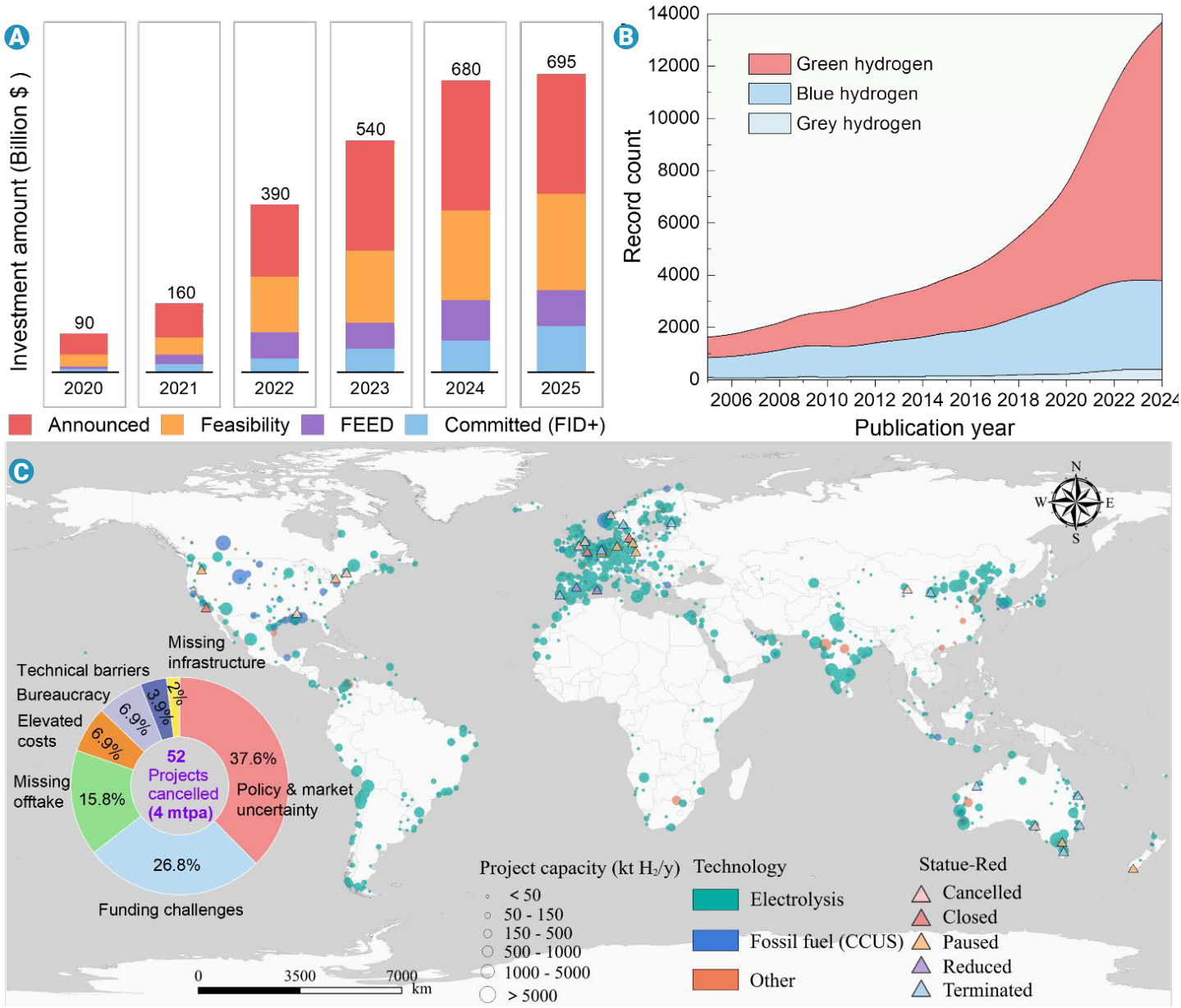

Figure 1. The utilization of hydrogen energy and scientific attention to the development trend (A) The investment situation in hydrogen energy over the past six years. (B) Annual hydrogen-related publications and growth trajectory, 2005-2024. (C) The current distribution of global hydrogen energy projects and the distribution of cancelled projects.

energy Q_c delivered at 20 K. Liquefying 1 kg of hydrogen requires cooling 11.1 m^3 of gas from ambient to 20 K, then providing latent heat for phase transition. Even considering only sensible heat removal (specific heat capacity of 14.05 kJ/kg·K) and latent heat of vaporization (461.4 kJ/kg), the minimum cooling requirement (Q_c) is 4.395 MJ. Then, the theoretical minimum work becomes:

$$P_{min} = \eta_{ex,C} \times Q_c = 14 \times 4.395 = 61.53MJ \quad (3)$$

This represents 43.2% of hydrogen's lower heating value (142.3 MJ/kg), a staggering energy penalty before considering any practical inefficiencies. Real-world liquefaction systems, accounting for equipment inefficiencies and boil-off losses during storage, can consume over 50% of hydrogen's energy content.[12] The additional requirements for sophisticated cryogenic infrastructure render hydrogen liquefaction economically prohibitive for most applications.

Compression work requirement. Gaseous hydrogen storage typically requires compression to 35-70 MPa, demanding both specialized pressure vessels and hydrogen-permeation-resistant materials. Beyond these engineering challenges, the thermodynamic work required for compression represents another significant energy penalty.

For isothermal compression, which represents the theoretical minimum, treating hydrogen as an ideal gas, the work required from 1 bar to 350 bar is:

$$w_{t,min} = RT\int_1^2 \frac{1}{p}dp = 7.31\text{MJ/kg} \quad (4)$$

For 70 MPa storage, the minimum isothermal work increases to 8.17 MJ/kg, according to the above equation. Practical compression systems operate far from this theoretical limit. With isothermal efficiencies of only 30-40% for such high compression ratios, actual energy consumption reaches approximately 41 MJ/kg for 70 MPa compression,[13] five times the theoretical minimum.

Hydrogen storage method incurs substantial penalties. Theoretically, liquefaction consumes a minimum of 61.53 MJ/kg (43.2% of hydrogen's energy content), while compression to 70 MPa requires at least 8.17 MJ/kg (5.74%). Practical systems consume a larger amount of energy. These storage penalties significantly reduce hydrogen's effective energy density. Hydrogen barely

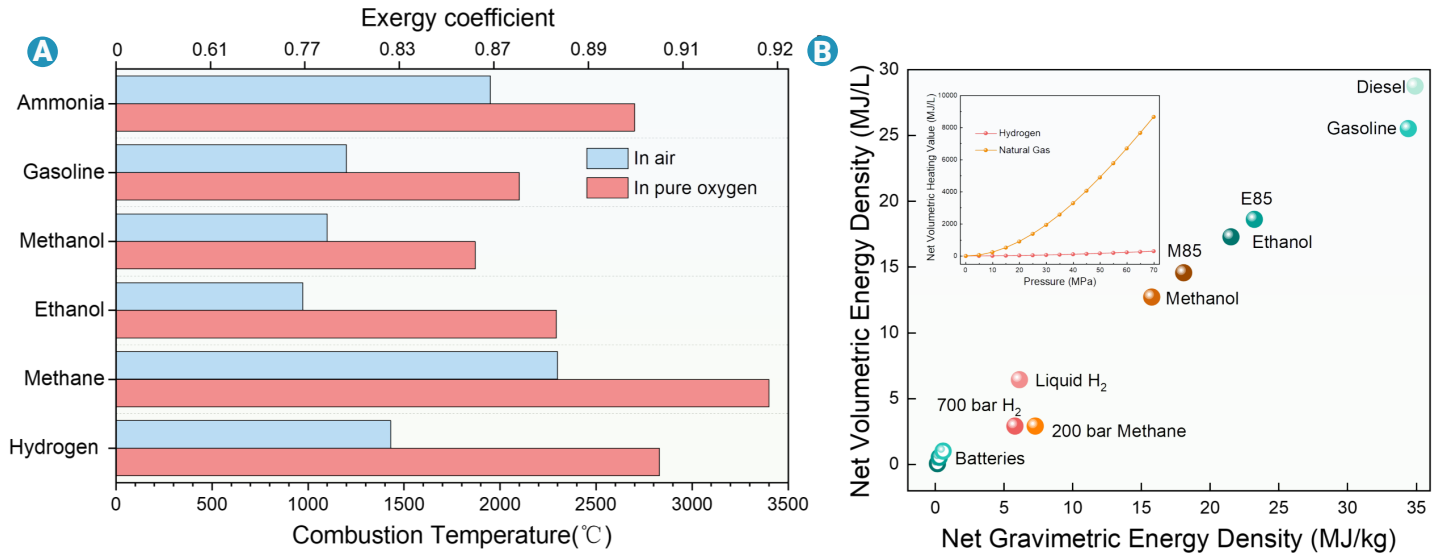

Figure 2. Comparison of combustion temperatures, exergy coefficients and net energy density of several typical fuels (T_0 = 300 K) (A) Combustion temperatures and exergy coefficients of several typical fuels burned in air and pure oxygen. (B) Comparison of volumetric energy density and gravimetric energy density for several typical fuels.

exceeds lithium-ion batteries and falls well below gasoline and diesel in both volumetric and gravimetric terms after reducing storage energy (Figure 2B).[14]

Unless otherwise stated, all exergy and minimum-work calculations use an ambient reference temperature T_0 = 300 K. Combustion exergy fractions follow the Carnot form 1-T_0/T at the adiabatic flame temperature. The storage penalties are theoretical minima (isothermal ideal-gas compression, and Carnot-limited cooling for liquefaction at T_c = 20 K including sensible and latent heat), with practical systems consuming more.

Physical barriers

Hydrogen's central storage paradox, exceptional gravimetric energy density (1.42×10^5 kJ/kg[9]) but poor volumetric performance (Table S1), imposes hard constraints on transportability and end-use economics. Figure 2B compares the volumetric heating values of hydrogen, natural gas, and 92-octane gasoline at various storage pressures. Per unit volume, hydrogen demonstrates the lowest energy density. Even compressed to 70 MPa, its volumetric heating value reaches only 4800 MJ/m^3, approximately 15.4% of 92-octane gasoline's 31,206 MJ/m^3. Hydrogen also underperforms natural gas (mainly methane), delivering only 35.8% of natural gas's energy at atmospheric pressure and 54.6% at 15 MPa.

Volumetric energy density determines fuel transportability. Currently, a dedicated hydrogen transport truck typically carries only ~300 kg of hydrogen, delivering approximately 9% of the total energy transported by a comparable 10-ton gasoline tanker.[15] Consequently, hydrogen incurs the highest transportation costs among conventional fuels.

Three storage routes are in use, and all are limited by the same low volumetric density. High-pressure gas in steel cylinders stores only about 1 wt% hydrogen by system mass; carbon-fiber composite vessels reach about 3 wt%, and 100 MPa designs target about 10 wt%, but thick walls and specialized materials keep costs high.[16,17] Cryogenic liquid storage raises density yet demands cooling below -253 °C, and boil-off drives long-term costs upward.[18] Solid-state hydrides store 5.8 to 19.6 wt% in the laboratory but release hydrogen only at elevated temperatures, consuming additional primary energy[19,20]. No current technology meets the IEA targets of above 5 wt% gravimetric and above 50 kg H_2/m^3 volumetric density for practical storage (Note S1).

Hydrogen transport presents additional challenges due to safety hazards and energy consumption, both rooted in its fundamental physical properties. Current methods rely on compressed gas cylinders and vehicular transport. Pipeline distribution awaits technological maturation to ensure acceptable energy losses and safety standards, particularly given hydrogen's permeation and embrittlement effects on steel infrastructure.

Chemical realities

Producing free H_2 requires breaking thermodynamically stable bonds. The O–H dissociation enthalpy in water is 498.7 kJ/mol. Therefore, the minimum electrolytic energy input (33 kWh/kg H_2) already exceeds the fuel's recoverable heating value by a margin that industrial inefficiencies widen to ~50 kWh/kg.[21] This irreducible chemical penalty propagates through every downstream conversion step and is a principal reason that power-to-H_2-to-X pathways incur larger round-trip losses than direct electrification.

Due to hydrogen's wide flammability range in air (≈4–75 vol% under standard test conditions) and its low minimum ignition energy near stoichiometric compositions (~0.02 mJ), accidental releases can form flammable mixtures, particularly in partially confined spaces[22]. Hydrogen–air mixtures differ from hydrocarbons in combustion characteristics. Under ambient conditions (≈298 K, 1 atm) the laminar burning velocity of hydrogen–air flames is typically on the order of a few m s^{-1}, whereas stoichiometric methane–air flames are ~0.35–0.40 m s^{-1} (Table S2).[23]

Hydrogen containment losses arise from both macroscopic leakage (e.g., joints and seals) and material permeation. For metals, permeation is governed by hydrogen solubility and diffusivity and is strongly material- and temperature-dependent. Annealed austenitic stainless steels exhibit very low diffusion rates at near-ambient temperatures, whereas permeation becomes more relevant at elevated temperatures and in thin membranes.[24] Even without acute incidents, chronic losses reduce delivered energy and can elevate safety and environmental burdens.

Engineering challenges

A complete hydrogen energy value chain encompasses four key stages: production, storage, transportation, and utilization. While hydrogen can be produced from various feedstocks using different technologies, about 96% is currently derived from fossil fuels.[25] However, fossil fuel-based production cannot achieve true carbon neutrality at the source, prompting researchers to focus on green water electrolysis technologies. Engineering challenges persist throughout hydrogen lifecycle .

The high storage cost stems from hydrogen's intrinsic properties, which cannot be eliminated through technological advancement alone.

Current hydrogen transport relies primarily on compressed gas trucks and pipeline delivery. Liquid hydrogen transport employs insulated cryogenic tankers with high energy consumption for temperature maintenance, limiting applications mainly to aerospace and defense sectors. High-pressure gaseous hydrogen transport via tube trailers (20-70 MPa)[26] serves small-scale applications but is limited to approximately 300 kg per trip, resulting in high costs. Long-distance pipeline transport, operating at 2.5-4 MPa,[27] represents the anticipated future for large-scale hydrogen distribution.

Hydrogen's propensity for leakage poses significant challenges (Table S3).[28,29] Hydrogen leaks faster than other fuels: under laminar flow conditions, its leakage rate is approximately 1.26 times that of methane, while under turbulent conditions typical of high-pressure systems, this increases to 2.83 times. Additionally, hydrogen's diffusion rate through membranes is approximately 3.8 times faster than methane.[30]

Hydrogen leakage occurs throughout the value chain, from production through delivery, storage, transport, and end-use applications, with emission rates varying by stage (Table S4).[31]

Hydrogen leakage in pipelines occurs through two mechanisms: permeation through pipe walls and leakage through microcracks. The permeation rate through pipe walls is calculated as:[32]

$$J = A \cdot D \frac{\Delta C}{\delta} \quad (5)$$

where J is the total leakage rate (kg/s), A is the total pipe wall area (m^2), D is the hydrogen diffusion coefficient in the pipe material (m^2/s), ΔC is the hydrogen concentration difference across the pipe wall (kg/m^3), and δ is the wall thickness (m). Notably, hydrogen exhibits high diffusion coefficients in many materials. For a 100-km pipeline constructed from 20-mm-thick steel pipe with 0.2-m diameter, assuming 4 MPa internal hydrogen pressure, Equation (5) yields a daily leakage of approximately 20.6 kg, an alarming 7519 kg annually. Longer pipelines would experience proportionally greater losses.

Leakage through microcracks is set by the critical pressure ratio, which for hydrogen corresponds to a critical pressure of 0.19 MPa.[33] Because commercial storage operates far above this threshold, releases emerge as underexpanded sonic jets governed by the vessel pressure and orifice size. The full mass-flow derivation from the Abel-Nobel equation of state is provided in Note S2.[34]

Safety represents the paramount engineering challenge. In unconfined spaces, leaked hydrogen's buoyancy promotes rapid upward dispersion. However, in confined spaces, hydrogen accumulation combined with its high diffusivity rapidly creates explosive mixtures. Consequently, hydrogen storage facilities and pipelines must avoid densely populated areas to prevent catastrophic losses.

Additionally, hydrogen causes unique embrittlement damage. In high-pressure systems, prolonged exposure of high-strength steels to hydrogen environments promotes embrittlement with increasing pressure. One mechanism involves hydrogen dissociation at steel surfaces into atomic hydrogen, which penetrates the material. Under applied stress, hydrogen accumulates at internal sites, causing stress concentration and localized cracking[35]. Once cracks form, rapid high-pressure hydrogen leakage and dispersion can trigger explosive disasters upon ignition. Mitigation strategies include appropriate material selection for high-pressure components and alloying with elements that reduce hydrogen embrittlement susceptibility, such as chromium and vanadium[36].

Environmental paradoxes

Although hydrogen itself is not a greenhouse gas, its atmospheric oxidation influences methane, ozone, and stratospheric water vapor concentrations, creating indirect climate impacts that remain underappreciated. Hydrogen's environmental impact arises through two pathways: direct atmospheric release via leakage, and emissions from energy-intensive production and storage processes.

Atmospheric Evolution of Hydrogen

While hydrogen molecules exhibit no direct infrared absorption under Earth's atmospheric conditions,[37] hydrogen poses indirect warming effects through atmospheric chemistry that could significantly impact the developing hydrogen economy.[38,39] Hydrogen participates in atmospheric reactions that alter the concentration and tropospheric lifetime of other greenhouse gases, making it an indirect greenhouse gas.

Paulot et al. demonstrated that despite hydrogen's radiative inertness, its chemical reactivity produces indirect radiative effects by perturbing tropospheric concentrations of key species, including ozone.[40] Their analysis of a 10% surface hydrogen increase showed complex hydrogen-ozone interactions. Increased atmospheric hydrogen correlates with elevated tropospheric ozone, which is a greenhouse gas, thereby affecting global temperatures.

Once released, hydrogen is oxidized mainly by the hydroxyl radical. This consumption of hydroxyl slows methane removal and extends its atmospheric lifetime, while the downstream radical chemistry raises tropospheric ozone.[41,42] Both methane and ozone are greenhouse gases, yet the competing pathways of ozone production and depletion make the net sign sensitive to background conditions. Hydrogen therefore acts as an indirect greenhouse gas rather than a radiatively inert one (Note S3; atmospheric lifetimes in Table S5).

Hydrogen leakage throughout the value chain could profoundly affect air quality and climate. Lakshmanan and Bhati.[30] investigated hydrogen's atmospheric oxidation, finding that both OH and O_3 oxidize hydrogen, with the O_3 reaction being thermodynamically favored by approximately 335 kJ/mol over the OH reaction. The O_3-H_2 reaction persists longer in the atmosphere than OH-initiated reactions. Thus, hydrogen not only generates ozone through OH reactions but also depletes stratospheric ozone through direct oxidation (Table S5).[43] Depending on atmospheric hydrogen concentrations, either OH generation is suppressed (extending methane lifetime) or O_3 is consumed.

Chen et al. (2024) quantified hydrogen leakage's global warming potential (GWP).[44] Although hydrogen isn't a direct greenhouse gas, fuel leakage causes indirect warming by effects on methane, tropospheric ozone, and stratospheric water vapor, with methane impacts dominating. Using a comprehensive 66-reaction photochemical box model, they estimated hydrogen's GWP relative to CO_2 as 28^{+18}_{-11} and 10^{+7}_{-4} for 20 and 100-year time frames, respectively. They found hydrogen emissions have approximately three-fold lower climate impact than equivalent fossil CH_4 emissions. However, large-scale hydrogen leakage would contribute to climate change, emphasizing importance of minimizing both hydrogen and methane leakage to achieve net-zero greenhouse gas emissions by 2050.

Emissions from hydrogen production and storage

While hydrogen combustion produces no greenhouse gases at point of use, which is primary rationale for hydrogen economy strategies, lifecycle emissions from hydrogen value chain are substantial.

By production route, the cost and carbon footprint of hydrogen move inversely (Figure 3A):[45] grey hydrogen is the cheapest but emits 10 to 25 kg CO_2 per kg, green hydrogen falls below 0.3 kg CO_2 per kg but costs $2.5 to 6.5 per kg, and natural geologic hydrogen is the rare option that is low on both. Even renewable-powered electrolysis carries a footprint of at least 0.3 kg CO_2 per kg H_2 under optimistic lifetime assumptions, and actual emissions are higher. Liquefying hydrogen to 20 K requires a theoretical minimum of 17.092 kWh/kg; using China's grid emission factor of 0.5703 kg CO_2/kWh,[46,47] this step alone generates 9.75 kg CO_2. On a delivered-energy basis (Figure 3B), gaseous and liquefied hydrogen emit 3.2 and 4.2 times the CO_2 of gasoline per MJ, with liquefaction the dominant penalty.[46]

Hydrogen exhibits the highest total carbon emissions among fuels under current conditions, challenging its environmental credentials. While green hydrogen concepts assume carbon-free renewable electricity, all energy systems have embedded carbon from manufacturing and lifecycle considerations. No truly zero-carbon electricity exists today without adopting additional carbon capture and storage.

After accounting for system lifecycles and manufacturing, the carbon footprint of green hydrogen varies more than thirtyfold with the electricity source (Figure 3C),[48-50] from 396 g CO_2 per kg for nuclear to 11,550 g CO_2 per kg for biomass, the latter comparable to fossil grey hydrogen.

Currently, most hydrogen derives from natural gas (i.e., grey hydrogen), with minimal green hydrogen production. Despite hydrogen's clean combustion, production emissions undermine its role as an ideal decarbonization solution. For 100 km of vehicle travel (Figure 3D),[49] only green hydrogen, in a fuel cell or an engine, falls below the gasoline carbon level, and at a cost premium. Grey and blue hydrogen engines provide no carbon benefit over gasoline, while a lithium battery delivers comparable carbon at the lowest cost under the current grid. Transport costs from production to point of use remain unaccounted, and actual electrolysis efficiencies would raise both emissions and costs further.

Carbon emissions and costs for vehicles traveling 100 km with calculation assumptions as followed. Electrolysis at 33 kWh/kg H_2 (theoretical); grid

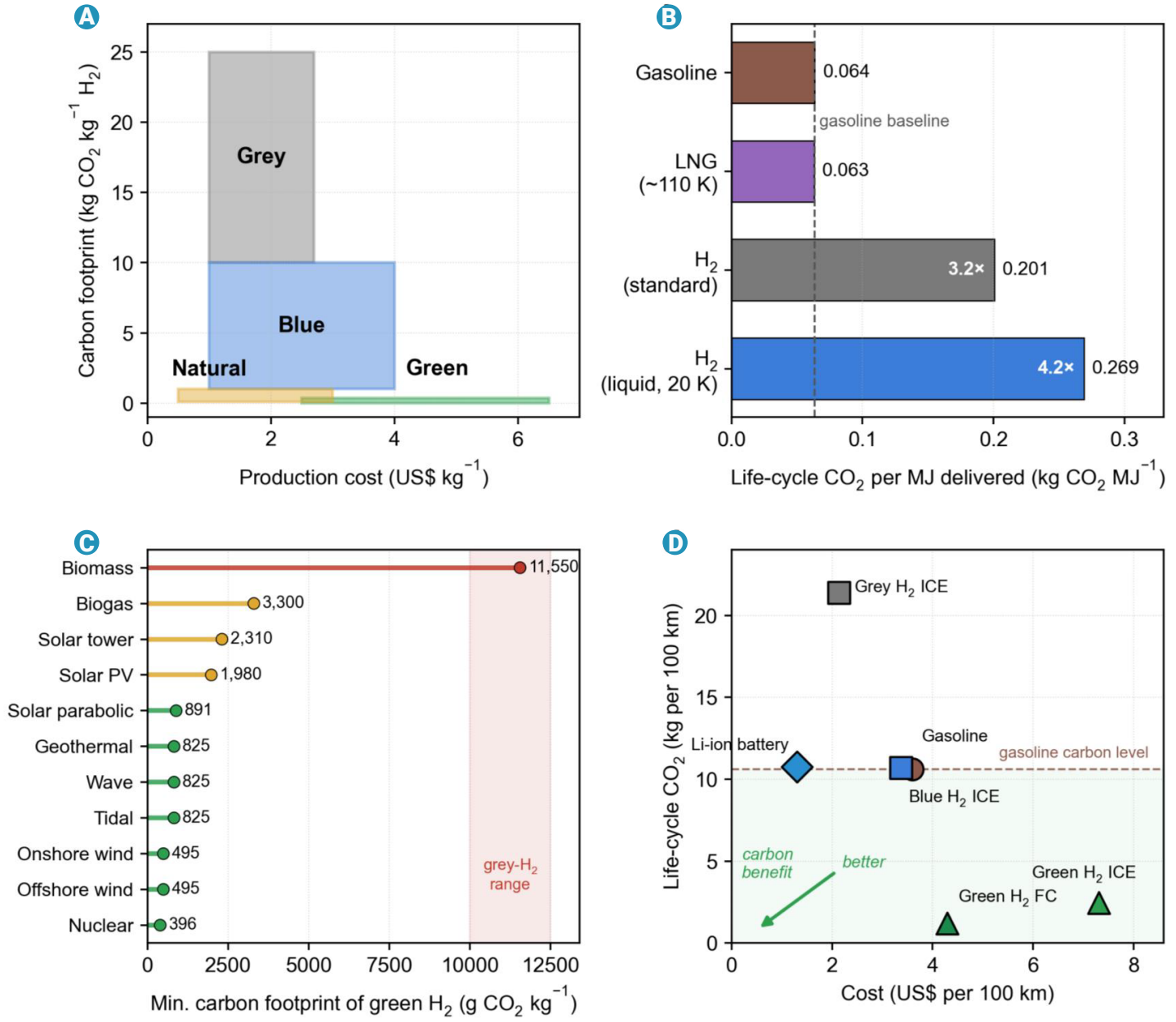

Figure 3. Carbon and cost of hydrogen across production, energy basis, electricity source, and end use (A) Production cost versus carbon footprint for grey, blue, green, and natural hydrogen; (B) life-cycle CO_2 per MJ of delivered energy for gasoline, LNG, and hydrogen; (C) minimum carbon footprint of green hydrogen by electricity source; (D) cost versus life-cycle CO_2 for 100 km of travel by different fuels and powertrains.

emissions 0.5703 kg CO_2/kWh;[46] solar thermal electricity at 0.07 kg CO_2/kWh;[44] gasoline heating value 46 MJ/kg, density 0.725 kg/L; hydrogen heating value 140 MJ/kg; ICE efficiencies 45% (gasoline) and 50% (hydrogen); fuel cell efficiency 85%; battery efficiency 90%. Hydrogen compression to 35 MPa requires 7.31 MJ/kg (theoretical minimum). Manufacturing emissions for fuel cells and batteries excluded. Prices reflect current Chinese markets.

Resource competition

From a resource competition perspective, hydrogen faces challenges on two fronts: production-stage competition for resources such as freshwater, and end-use competition from alternatives including ammonia, methane, methanol, and ethanol.

Hydrogen production presents significant freshwater challenges. Current green hydrogen electrolysis consumes 30-70 L of freshwater per kilogram, with even theoretical minimum requirements reaching 9 kg of water per kilogram of hydrogen.[51] Achieving the 2050 global annual target of 660 Mt hydrogen (Figure S1) would require 19.8-46.2 Gt of freshwater, and even with substantial water usage efficiency improvements, the minimum consumption would still reach 5940 Mt annually. This enormous demand will intensify global water stress, particularly given the geographical mismatch between renewable energy resources and water availability. Most solar PV installations occupy arid regions with abundant sunlight but scarce rainfall, while wind farms typically locate in mountainous or offshore areas where freshwater access remains limited, creating fundamental conflicts for water electrolysis.[52] Although researchers have proposed various solutions including seawater desalination, enhanced industrial water recycling, and atmospheric water harvesting in arid regions, these approaches introduce system complexity and increase costs, further undermining green hydrogen economics. Reverse osmosis desalination, for instance, not only requires substantial additional investment but also relies heavily on membranes composed of crosslinked aromatic polyamides, polysulfones, and polyester nonwovens. These materials exhibit bioaccumulate toxicity and resist natural degradation, creating environmental risks when deployed at the scale required for hydrogen production.[53]

Hydrogen also faces strong competition from alternative energy carriers. Methane can be extracted from natural gas and coal, while methanol and

ethanol derive from abundant biomass resources with established handling infrastructure. Recent research identifies ammonia as hydrogen's most formidable competitor.[54] Ammonia surpasses hydrogen in three critical dimensions: storage and transport efficiency, energy density, and industrial maturity, while maintaining environmental compatibility and commercial viability (Table S6).

Ammonia's liquefaction temperature permits conventional refrigeration, yielding an energy density 2.8 times higher than 70 MPa compressed hydrogen and 1.3 times higher than liquid hydrogen. Liquid ammonia transport efficiency exceeds liquid hydrogen by 50%, with 100 km transport costs only 1.7% of liquid hydrogen, utilizing modified LNG infrastructure.[55] Ammonia's narrower explosive limits and distinctive odor provide inherent safety advantages.

As a zero-carbon fuel, ammonia combustion produces only nitrogen and water:

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \quad (6)$$

Ammonia's high-octane rating and anti-knock properties suit various power systems, including blending with conventional fuels for emissions reduction in internal combustion engines.

Critically, ammonia benefits from mature industrial infrastructure. The global ammonia industry, primarily serving fertilizer production, provides existing synthesis plants, storage facilities, transport systems, and end-use applications. Repurposing this infrastructure for "energy ammonia" requires substantially less investment than building hydrogen infrastructure from scratch.

Finally, ammonia synthesis requires hydrogen feedstock, creating synergy with renewable energy intermittency. Excess renewable electricity can produce green ammonia for storage. During periods without wind or solar generation, ammonia can fuel dedicated power plants or co-firing systems, providing dispatchable clean electricity and long-duration energy storage (Figure 4).

Grid-scale storage limitations

The intermittent nature of renewable energy sources, particularly wind and solar power, necessitates the integration of energy storage systems. Hydrogen-based power generation systems are frequently employed for energy storage due to hydrogen's high gravimetric energy density and facile conversion to electricity via fuel cells or hydrogen internal combustion engines. The process involves water electrolysis to produce hydrogen, high-pressure storage, and subsequent reconversion to electricity through fuel cells or hydrogen engines when power is required, thereby ensuring stable electricity supply to end users.

In fuel cells, hydrogen's chemical energy is directly converted to electrical energy. However, thermodynamic constraints limit the theoretical efficiency to the ratio of Gibbs free energy to enthalpy change. For the hydrogen-oxygen reaction, with ΔG = 237 kJ/mol and higher heating value Q = 286 kJ/mol, the theoretical efficiency reaches $\Delta G/Q \approx 83\%$.[56] Total system efficiency could theoretically approach 90% if waste heat were fully utilized, though this proves challenging in practice. In reality, polarization losses including activation polarization (electrochemical kinetic resistance), ohmic polarization (proton conduction resistance), and concentration polarization (reactant diffusion limitations) reduce the electrical conversion efficiency to 40-60%, typical values for current proton exchange membrane fuel cells (PEMFCs)[57].

Alternative hydrogen utilization through combustion-based heat engines (e.g., Rankine cycle, gas turbines) faces Carnot efficiency limitations, with theoretical efficiency of 82% when burning in air. Current gas turbine efficiencies remain at 30-40%, reaching approximately 50% with combined-cycle configurations and waste heat recovery, still substantially below fuel cell performance.[58]

The complete renewable energy-to-hydrogen pathway, encompassing power generation, water electrolysis, hydrogen storage, and utilization, is illustrated with both theoretical and current practical efficiencies at each stage (Figure 5). The analysis reveals that hydrogen-based energy storage systems exhibit maximum theoretical round-trip efficiencies below 75%. In contrast, lithium-ion battery storage currently achieves 90-95% round-trip efficiency,[59] significantly exceeding hydrogen storage systems. While lithium-ion batteries face challenges, primarily cost-related, these are amenable to technological solutions without fundamental thermodynamic constraints, suggesting superior development potential for battery-based energy storage.

Comparing hydrogen and lithium-based energy systems is essential for evaluating hydrogen's future prospects. Reference[60] provides a comprehensive comparison between hydrogen fuel cells and lithium-ion batteries (Table S7). Reversible hydrogen fuel cells (RHFCs) offer advantages only in resource abundance, energy density, and recyclability, while underperforming lithium batteries in virtually all other metrics.

RESULTS

Hydrogen's irreplaceable value within defined boundaries

The preceding analysis should not be interpreted as a rejection of hydrogen, but as a boundary-setting exercise. Hydrogen is most defensible where at least one of three conditions is met: electrification cannot provide the same service, mass rather than volume constrains the system, or storage duration and spatial mismatch make batteries and grid expansion less suitable. Under these conditions, hydrogen functions less as a universal energy carrier than as a strategic molecule. The market within these boundaries remains substantial. IEA net-zero scenarios project 530 Mt of annual hydrogen demand by 2050, concentrated in sectors where direct electrification is technically infeasible[6].

Thermochemical irreplaceability in hard-to-abate industry

Steel, cement, and primary chemicals collectively account for roughly 17% of global CO_2 emissions.[61] In primary steelmaking, carbon serves a dual role as fuel and chemical reductant, making simple fuel switching insufficient for decarbonization. Hydrogen-based direct reduction of iron (H-DRI) replaces carbon as the reductant and produces water rather than CO_2:

$$Fe_2O_3 + 3H_2 \rightarrow 2Fe + 3H_2O$$

This pathway achieves 90–95% CO_2 reduction compared with conventional blast furnace routes.[62] The HYBRIT project (SSAB/LKAB/Vattenfall) delivered the first fossil-free steel in August 2021 and is scaling toward 1.3 Mt yr^{-1} production capacity.[62] The European green steel market, driven partly by the Carbon Border Adjustment Mechanism entering compliance in January 2026, is projected to grow from ?1.15 billion in 2025 to ?59.7 billion by 2034. Glass furnace combustion and cement calcination present analogous challenges: process temperatures exceed 1400 °C and carbon-based chemistry is integral to the production pathway, positioning hydrogen as the primary zero-carbon substitute.[61]

Gravimetric advantage in weight-constrained transport

Hydrogen's gravimetric energy density (142 MJ kg^{-1}) exceeds jet fuel by a factor of three and lithium-ion battery packs by a factor of 100. This disparity becomes decisive in transport modes where payload capacity or range is weight-limited.

Long-haul heavy-duty trucking. Battery-electric trucks have reached commercial viability for routes below 300 km but face structural constraints at longer ranges. The battery pack required for 500+ km range in a Class 8 truck imposes a multi-ton weight penalty that directly reduces revenue-generating payload.[63] Fuel cell trucks match diesel refueling times at 10–15 min versus multi-hour battery charging. Hyundai's XCIENT fuel cell fleet, with over 250 units deployed across 13 countries and 20 million cumulative kilometers by early 2026, demonstrates operational viability for long-haul logistics.[64] For continuous-operation applications (mining haul trucks exceeding 16 h of daily runtime, 24-hour port machinery, and time-sensitive freight corridors), hydrogen's rapid refueling preserves the operational tempo of conventional diesel systems.[65]

Short-to-medium-range aviation. Aviation ranks among the most challenging sectors to decarbonize. Sustainable aviation fuels remain constrained by feedstock availability and cannot achieve zero-carbon combustion. Liquid hydrogen's gravimetric energy density (120 MJ kg^{-1}, roughly three times kerosene) makes it technically viable for regional aircraft.[66] The Airbus ZEROe program targets a 100-seat fuel-cell-powered aircraft with 1850 km range, reaching Technology Readiness Level 3 in 2026. Hydrogen remains the only

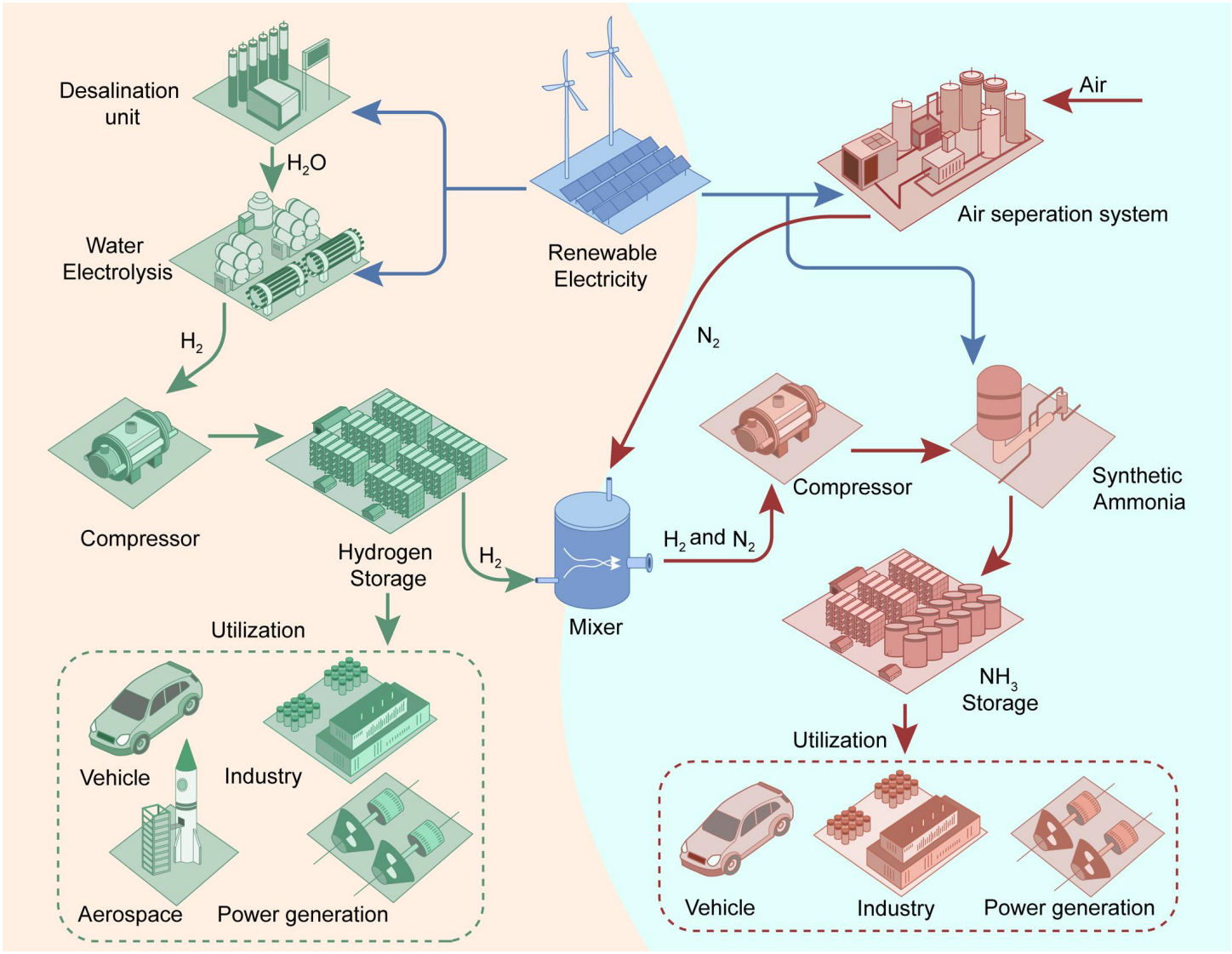

Figure 4. Vision pathway from renewable electricity generation by ammonia storage to utilization

credible pathway to zero-emission powered flight beyond the size and range addressable by batteries.[66]

Cold-climate resilience

In regions where ambient temperatures routinely fall below -20 °C, lithium-ion batteries suffer capacity losses of 20–40%, reduced charge acceptance, and substantial auxiliary heating demands. PEM fuel cells operate at 60–80 °C and start unassisted from -30 °C, with laboratory tests achieving startup from -40 °C within 30–100 s.[67] Waste heat from fuel cell operation provides cabin and system heating without additional energy input, enabling combined heat and power operation that raises system-level energy utilization from 40–60% (electricity only) to above 80%. This thermal synergy is particularly valuable for heavy-duty vehicles and remote power systems in subarctic environments.

Long-duration energy storage

Lithium-ion batteries dominate short-duration storage (2–8 h) at round-trip efficiencies of 90–95%, but their cost scales linearly with duration, making seasonal storage economically prohibitive. Where suitable geology is available, underground salt caverns offer a low-cost route for multi-day to seasonal hydrogen storage. Reported estimates include levelized storage costs of approximately \$0.8 kg-H_2^{-1},[68] and cavern capacity costs on the order of \$2–10 kWh-H_2,[69] while the very low self-discharge of stored hydrogen makes it more suitable than lithium-ion batteries for long-duration balancing, despite lower round-trip efficiency. Modeling studies indicate that hydrogen-based long-duration storage (>100 h) integrated into wind- and solar-dominated grids reduces total system costs by 10–40% compared with battery-only configurations, by absorbing multi-week generation surpluses and supplying dispatchable power during extended low-generation periods[70].

Synergistic integration with complementary carriers

Hydrogen's value is maximized through integration with complementary carriers that offset its storage and transport limitations, not as a standalone energy system.

Fuel cell–battery hybrid powertrains combine lithium-ion batteries' high-power density and rapid transient response with fuel cells' sustained range and environmental tolerance. The battery handles peak demands during acceleration and regenerative braking. The fuel cell provides steady-state baseload power. This architecture outperforms either technology alone in duty cycles requiring both high instantaneous power and extended operating hours, conditions typical of mining haul trucks, port container handlers, and long-distance buses.[63]

Ammonia and methanol serve as hydrogen-derived carriers that resolve hydrogen's transport cost penalties. Producing hydrogen at renewable energy sites, converting it to ammonia or methanol for shipment, and reconverting at the point of use reduces long-distance transport costs by one to two orders of magnitude.[71] Ammonia's volumetric energy density (12.7 MJ L^{-1}) exceeds compressed hydrogen at 700 bar (4.5 MJ L^{-1}) by a factor of 2.8, and its lique-

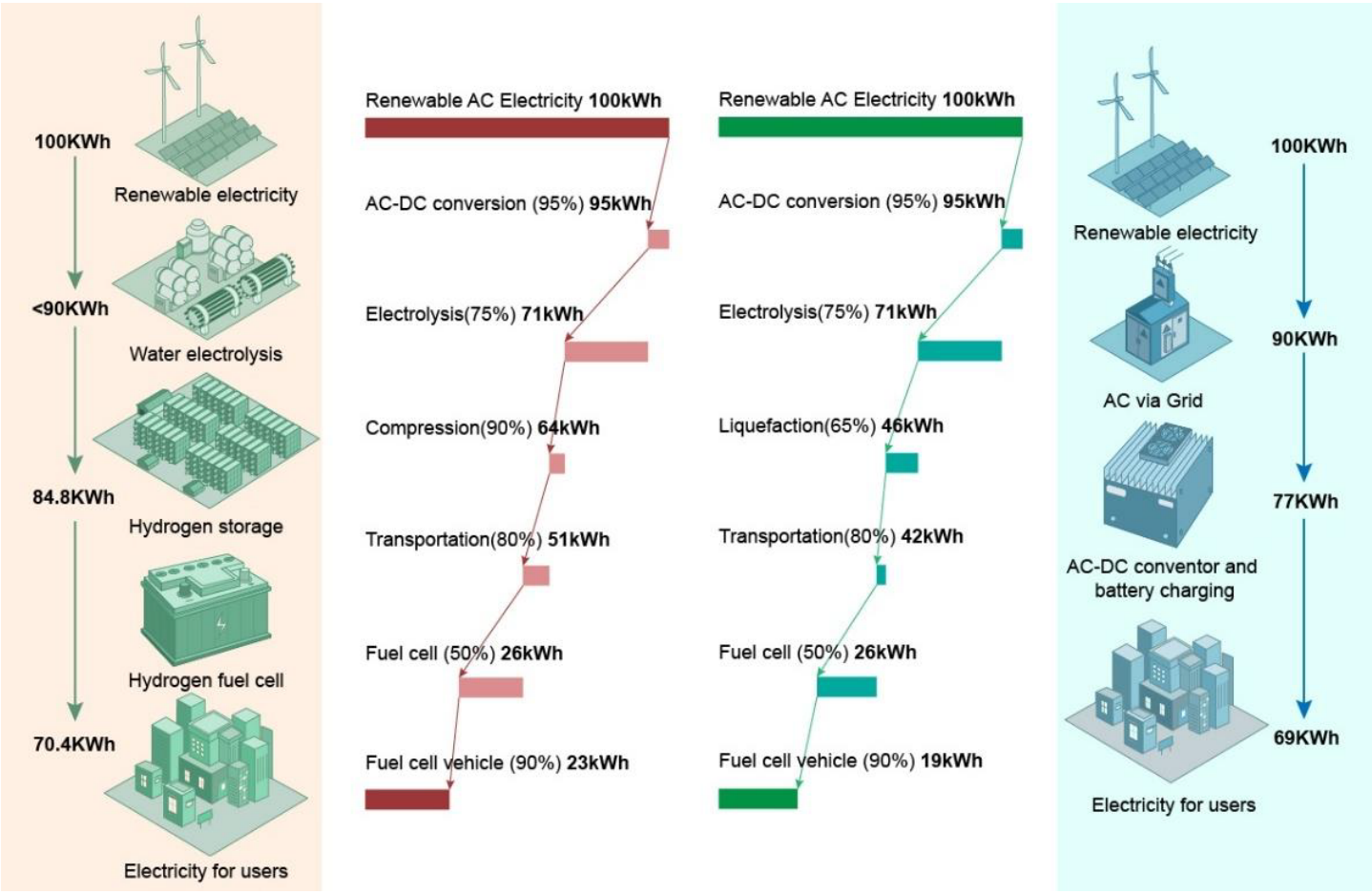

Figure 5. Energy flow and conversion efficiencies across the hydrogen energy storage pathway.

faction at −33 °C permits conventional refrigeration infrastructure. This hydrogen–ammonia–methanol nexus leverages existing chemical logistics while enabling intercontinental renewable energy trade.[71]

These roles require strict boundary conditions: geographically coupled production and use when possible, high asset utilization to amortize infrastructure, verified low-carbon electricity supply, and leakage control across the value chain. Outside these boundaries, particularly in light-duty vehicles, building heat, and short-duration grid storage, direct electrification generally remains the higher-efficiency and lower-risk option.

CONCLUSION AND FUTURE PERSPECTIVES

The trajectory of human energy utilization reveals a clear decarbonization trend: from wood (C:H=10:1) to coal (C:H=2:1), petroleum (C:H=1:2), and natural gas (C:H=1:4),[72] with steadily increasing hydrogen-to-carbon ratios. This progression seemingly heralds an era of pure hydrogen. However, such linear extrapolation overlooks the critical reality that electricity, as a secondary energy carrier, has demonstrated decisive advantages in efficiency, controllability, and infrastructure maturity. Given the energy demand characteristics of digital transformation and artificial intelligence development, electrification rather than hydrogen will dominate the future energy landscape.

This report identifies both the systemic constraints and the irreplaceable contributions of hydrogen within well-defined boundaries. In primary steelmaking, long-duration energy storage exceeding 100 h, and chemical feedstock roles for ammonia and methanol synthesis, no electron-based substitute currently exists. These applications exploit hydrogen's unique thermochemical properties rather than treating it as a generic energy carrier. Outside these domains, hydrogen's physicochemical constraints reassert themselves. As the lightest element, its volumetric energy density is merely one-third that of natural gas, with compression to 700 bar or liquefaction at −253 °C consuming 20–40% of its energy content. These thermodynamic penalties cannot be eliminated through engineering refinement alone. Liquid hydrogen shipping costs remain 4–6 times those of liquefied natural gas,[73] and only 25% of Europe's existing gas infrastructure is technically feasible for hydrogen conversion.[74]

Environmental and economic realities impose additional boundaries. While hydrogen combustion produces no CO_2, atmospheric leakage induces indirect warming through effects on methane oxidation, tropospheric ozone, and stratospheric water vapor, creating radiative forcing that scales with deployment volume. Green hydrogen production costs of $6–13/kg in Europe (2023) remain far above the US Hydrogen Shot target of $1/kg.[75] Even with the Inflation Reduction Act's maximum $3/kg subsidy, green hydrogen costs exceed fossil-derived grey hydrogen by approximately 50%.[76] Cost-competitive green hydrogen is a prerequisite for, not a consequence of, large-scale deployment.

From an energy quality perspective, electricity surpasses hydrogen in convertibility, transmissibility, and safety, making electricity-to-hydrogen conversion warranted only when necessary. In resource competition, hydrogen faces challenges from alternative energy carriers including ammonia, methanol, and ethanol. Notably, ammonia, with 1.5 times liquid hydrogen's energy density, superior storage, transport, safety profiles, and industrial maturity, shows potential to supersede hydrogen. Compared to rapidly advancing lithium battery technology, hydrogen fuel cells' disadvantages in convenience, energy density, and safety appear insurmountable in the foreseeable future.

Hydrogen's contribution to decarbonization is determined by precision of deployment, not breadth. Concentrating investment in sectors where thermochemical irreplaceability is established (heavy industry, long-haul transport, seasonal storage, and chemical feedstock) while pursuing direct electrification wherever grid infrastructure can serve represents the rational path forward. Matching each energy carrier to its comparative advantage, rather

than pursuing a universal hydrogen economy, is essential for directing R&D resources and infrastructure investment toward the pathways that yield the largest emission reductions per unit of capital and primary energy committed. Priorities for future work include fuel-cell and battery hybrid powertrains for high-utilization transport, hydrogen-derived carriers such as ammonia and methanol for long-distance trade, low-leakage and embrittlement-resistant materials and higher-efficiency electrolysis to cut storage and production losses, and data-driven optimization of integrated hydrogen systems.[77]

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AUTHOR CONTRIBUTIONS

Yanjie Zheng: Writing-Original draft, Validation, Investigation, Software, Formal analysis; **Ziye Zhu**: Data Curation, Software, Investigation; **Zhiwei Ouyang**: Data Curation, Software; **Shen Liang**: Resources, Conceptualization, Writing-Review & Editing; **Xinglong Ma**: Project administration, Writing-Review & Editing.

DECLARATION OF INTERESTS

We declare that we do not have any commercial or associative interest that represents a conflict of interest in connection with the work submitted.

DATA AND CODE AVAILABILITY

Data are available from the corresponding author upon reasonable request.

SUPPLEMENTAL INFORMATION

It can be found online at: https://doi.org/10.59717/j.xinn-energy.2026.100173