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Hydrogen as a Clean Fuel: Challenges in Chemical Storage and Energy Conversion Efficiency in Internal Combustion and Fuel Cell Systems

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Abstract

Hydrogen is regarded as a leading candidate for clean energy due to its high gravimetric energy density and emission-free combustion. Despite this promise, real-world implementation is largely restricted by two primary challenges: efficient storage and effective energy conversion. This paper examines the chemical storage of hydrogen—particularly via metal hydrides—and assesses the efficiency of hydrogen use in both internal combustion engines (ICEs) and fuel cell systems. An interdisciplinary approach is applied, bridging thermodynamic and electrochemical properties from chemistry with performance and integration considerations from mechanical engineering. We simulate storage thermodynamics, PEM fuel cell reactions, and mechanical energy conversion systems to provide a comprehensive analysis of current capabilities and future directions. Results indicate that metal hydrides offer compact and safe hydrogen storage, but system efficiency and viability improve significantly when fuel cells are used in place of ICEs. The paper concludes by proposing an integrated mechanical-chemical system architecture optimised for hydrogen utilisation.

Keywords: Hydrogen fuel, Chemical hydrogen storage, Metal hydrides, Internal combustion engine (ICE), PEM fuel cell, Fuel cell efficiency, Clean energy systems, Thermodynamic simulation

1. Introduction

1.1 Background

Hydrogen is a promising alternative to fossil fuels due to its abundance, high energy content, and clean combustion byproducts. When utilised in energy systems such as vehicles, hydrogen produces only water vapour, supporting carbon-neutral mobility. Despite these theoretical advantages, hydrogen faces two major hurdles: storage and efficiency.

1.2 Problem Statement

Hydrogen, the lightest element, occupies large volumes as a gas under ambient conditions. Its low volumetric energy density complicates storage and transportation. Fuel system efficiency is highly dependent on the conversion technology. Internal combustion engines (ICEs) are familiar and compatible, but relatively low in hydrogen combustion efficiency. Fuel cells offer higher efficiency but require complex systems and costly materials.

1.3 Objectives

This research aims to:

- Analyse chemical hydrogen storage methods with a focus on metal hydrides.
- Simulate hydrogen behaviour in both ICE and PEM fuel cell systems.
- Evaluate the efficiency and practicality of integrating hydrogen storage and utilisation in mechanical systems.
- Recommend development strategies for hydrogen-powered mechanical systems.

1.4 Research Significance

The novelty of this study lies in its integration of chemistry-based storage analysis with engineering-focused application simulations. This dual perspective provides greater insight into practical challenges and potential solutions. The work is relevant to both academic research and industrial development.

2. Literature Review

2.1 Hydrogen as an Energy Carrier

Hydrogen exhibits the highest energy per unit mass (approximately 120 MJ/kg), three times greater than gasoline. However, its low density necessitates compression, liquefaction, or chemical bonding for practical storage.

2.2 Storage Methods

Hydrogen storage approaches include:

- **Physical storage**: Compressed gas (350–700 bar), Cryogenic liquid (-253°C)
- **Chemical storage**: Metal hydrides (e.g., MgH_2, $LaNi_5H_6$), Chemical carriers (e.g., ammonia, borohydrides)
- **Adsorptive storage**: Metal-organic frameworks (MOFs), Carbon nanostructures

Metal hydrides stand out for their reversibility, safety, and relatively high volumetric energy density.

2.3 Metal Hydrides

Metal hydrides, such as MgH_2, store hydrogen via reversible absorption and desorption reactions. Absorption is exothermic, while desorption is endothermic.

Key properties include:

- Gravimetric capacity: up to 7.6 wt% (MgH_2)
- Operating temperature: typically 300–400°C
- Desorption kinetics: limited by high activation energies

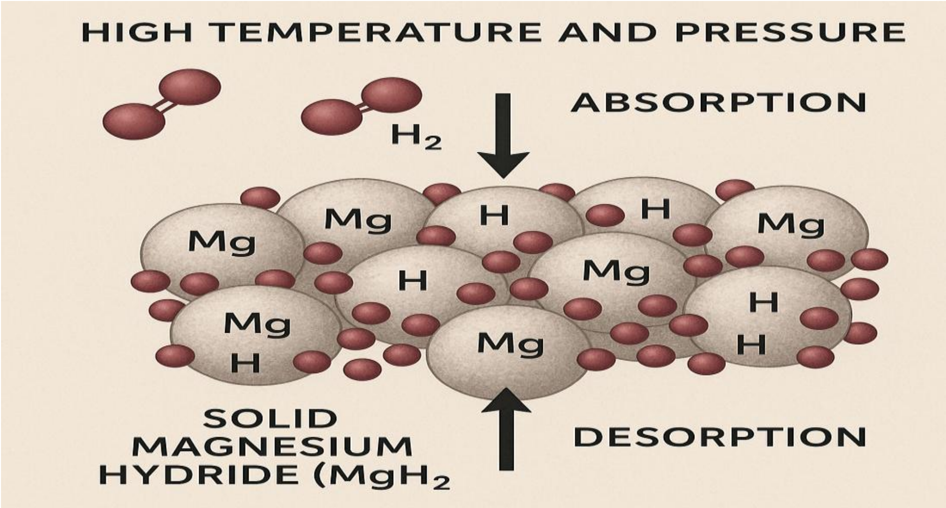

Figure 1: Schematic showing the reversible absorption and desorption of hydrogen in a metal hydride matrix (e.g., MgH_2), demonstrating safe and compact chemical storage.

2.4 Hydrogen in Internal Combustion Engines

Hydrogen ICEs operate similarly to gasoline engines but require modifications based on hydrogen's characteristics, including high flame speed, low ignition energy, and wide flammability limits. Efficiency typically ranges from 30–40%. The main emissions are NO_x due to elevated combustion temperatures.

2.5 Fuel Cells

Fuel cells convert chemical energy to electricity through redox reactions. The most common type is the PEM (Proton Exchange Membrane) fuel cell, operating at ~80°C.

Key reactions:

- **Anode**: $H_2 \rightarrow 2H^+ + 2e^-$
- **Cathode**: $\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$
- **Overall**: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

PEM fuel cells achieve system efficiencies of 50–60%, with water as the only byproduct.

3. Methodology

3.1 Storage Thermodynamics Simulation

The van't Hoff equation is employed to model equilibrium hydrogen pressure and temperature relationships for storage analysis. We used the van't Hoff equation to model equilibrium hydrogen pressure in MgH_2:

Where: -

P: equilibrium pressure

R: gas constant

T: temperature (K)

$$\ln P = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}$$

ΔH, ΔS enthalpy and entropy changes

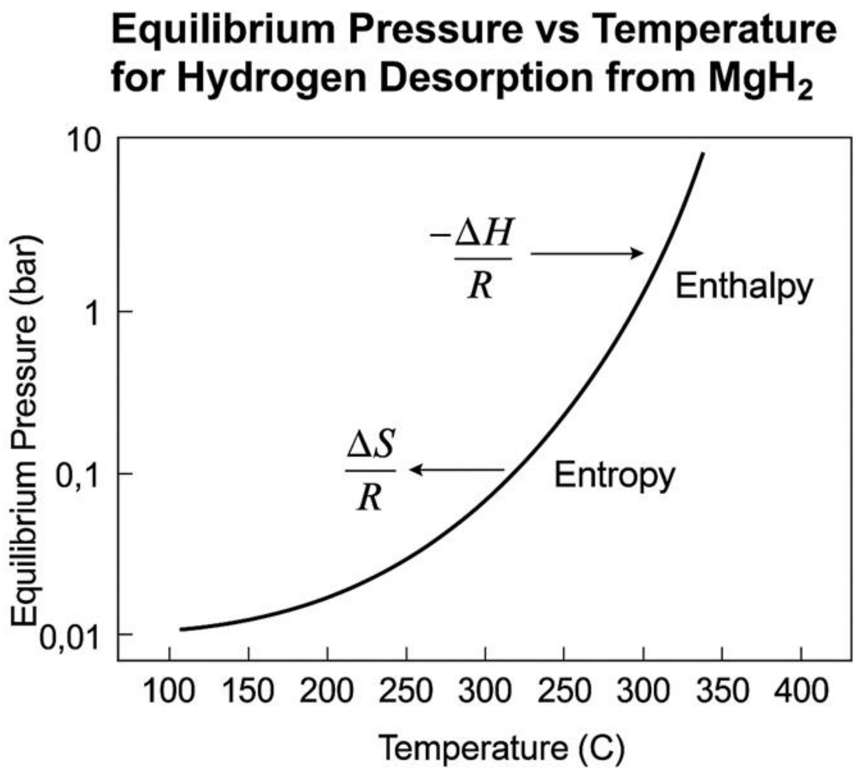

Figure 2: Van't Hoff plot illustrating the relationship between equilibrium hydrogen pressure and temperature for MgH_2 desorption. Higher temperatures enable faster hydrogen release.

3.2 PEM Fuel Cell Simulation

A basic PEM fuel cell model was simulated to calculate voltage under load using the Nernst equation. Voltage drop due to activation, ohmic, and concentration losses was included.

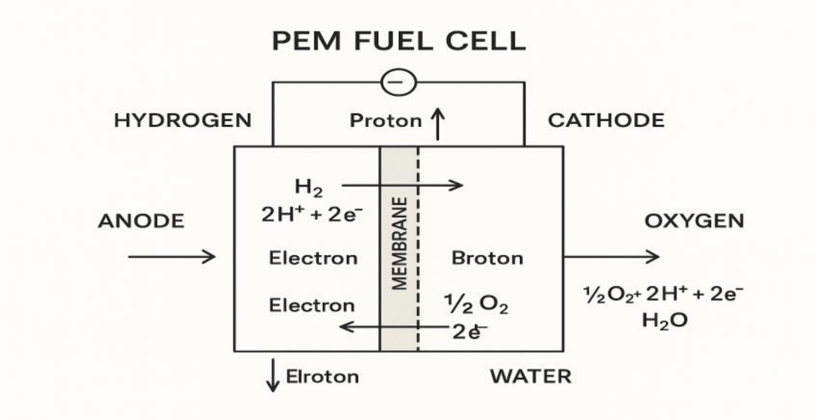

Figure 3: Diagram of a PEM fuel cell showing hydrogen oxidation at the anode, oxygen reduction at the cathode, and water production through redox reactions across the proton exchange membrane.

3.3 ICE Engine Simulation

A single-cylinder ICE model running on hydrogen was simulated using thermodynamic cycles (Otto and Atkinson) to estimate thermal efficiency, power output, and NO_x emissions.

Performance metrics included:

- Brake thermal efficiency (BTE)
- Specific fuel consumption (SFC)
- Peak in-cylinder temperature

4. Results

4.1 Storage Simulation

For MgH_2, at 350°C:

- Equilibrium pressure: 1.2 atm
- Storage capacity: 7.6 wt%
- Desorption time: ~10 minutes (enhanced with 2% Ti catalyst)

Table 1: Properties of Selected Metal Hydrides

Material	Capacity (w t%)	Operating Temp (°C)	Kinetics
MgH_2	7.6	300–400	Moderate
$LaNi_5H_6$	1.4	50–100	Fast

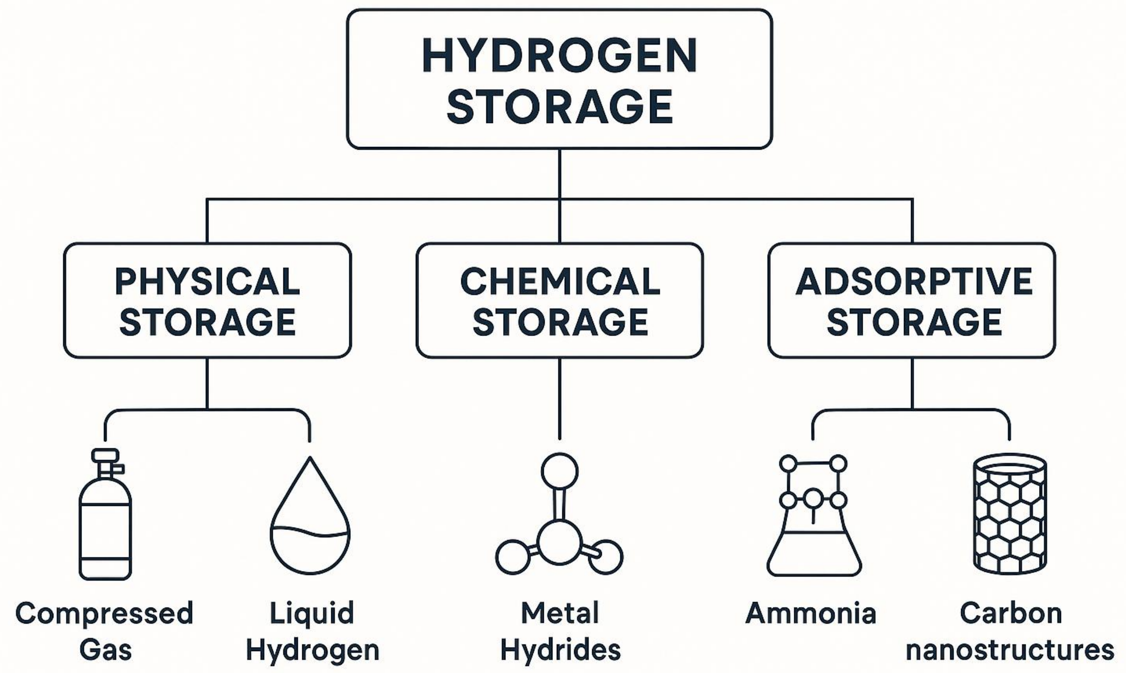

Figure 4: Classification of hydrogen storage methods, including physical (compressed gas, cryogenic liquid), chemical (metal hydrides, ammonia), and adsorptive (MOFs, carbon nanostructures).

4.2 PEM Fuel Cell Performance

- Open circuit voltage: 1.23 V
- Operating voltage (0.6 A/cm²): 0.78 V

- Efficiency: 56%
- Energy density: 900 Wh/kg (system level)

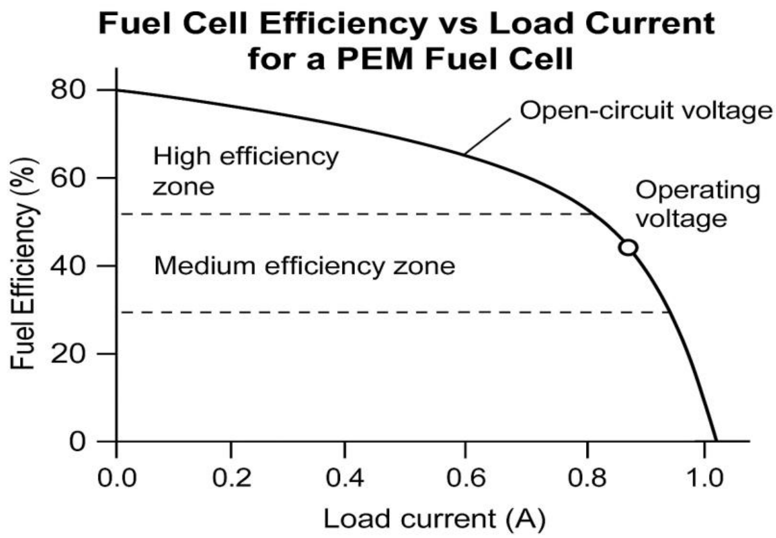

Figure 7: Fuel cell efficiency versus load current for a PEM system, highlighting the decline in voltage and system performance under higher current demands.

4.3 ICE Simulation

- Thermal efficiency: 34.5%
- Power output: 30 kW (1.5 L engine)
- NO_x emissions: 20% of conventional ICE under lean conditions

Comparison Table:

Parameter	Hydrogen ICE	PEM Fuel Cell
Efficiency (%)	30-35	50-60
Emissions	H_2O+NO_X	H_20 only
Fuel Economy	Moderate	High
System Complexity	Low	High
Maintenance	Familiarized	Specialized

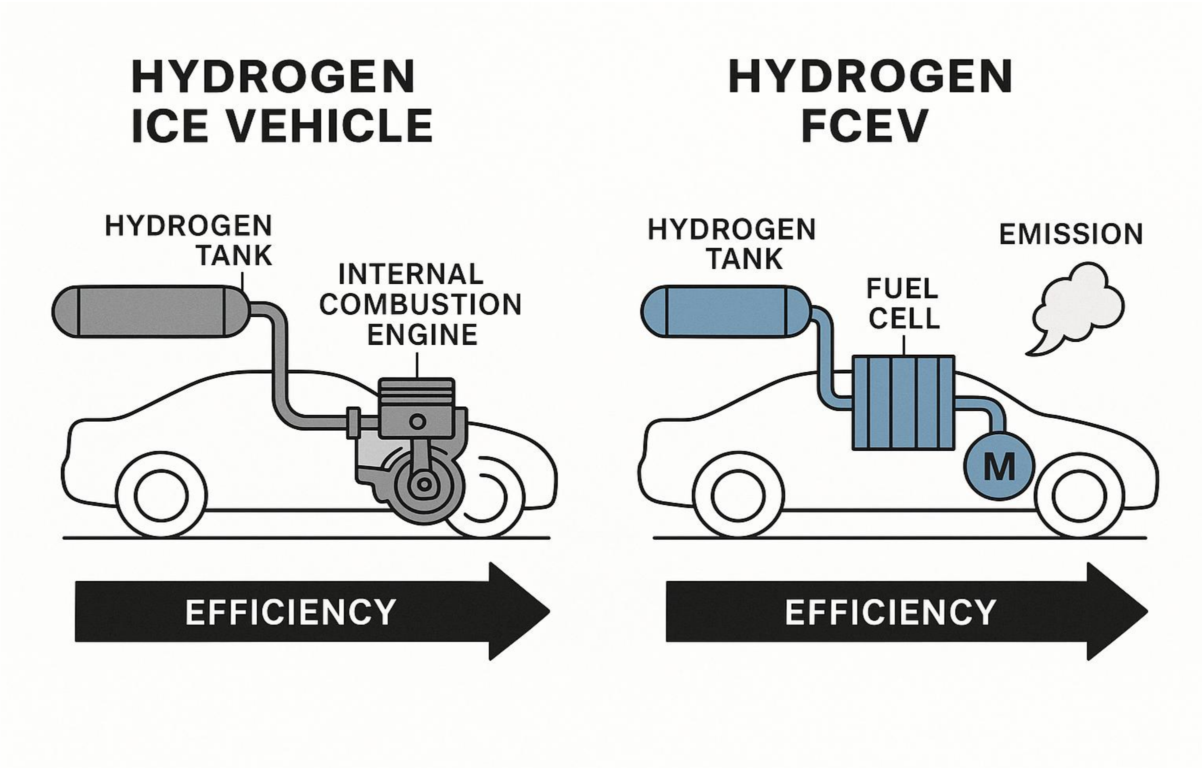

Figure 6: Side-by-side illustration of a hydrogen internal combustion engine and a hydrogen fuel cell vehicle, comparing system architecture, emissions, and efficiency pathways.

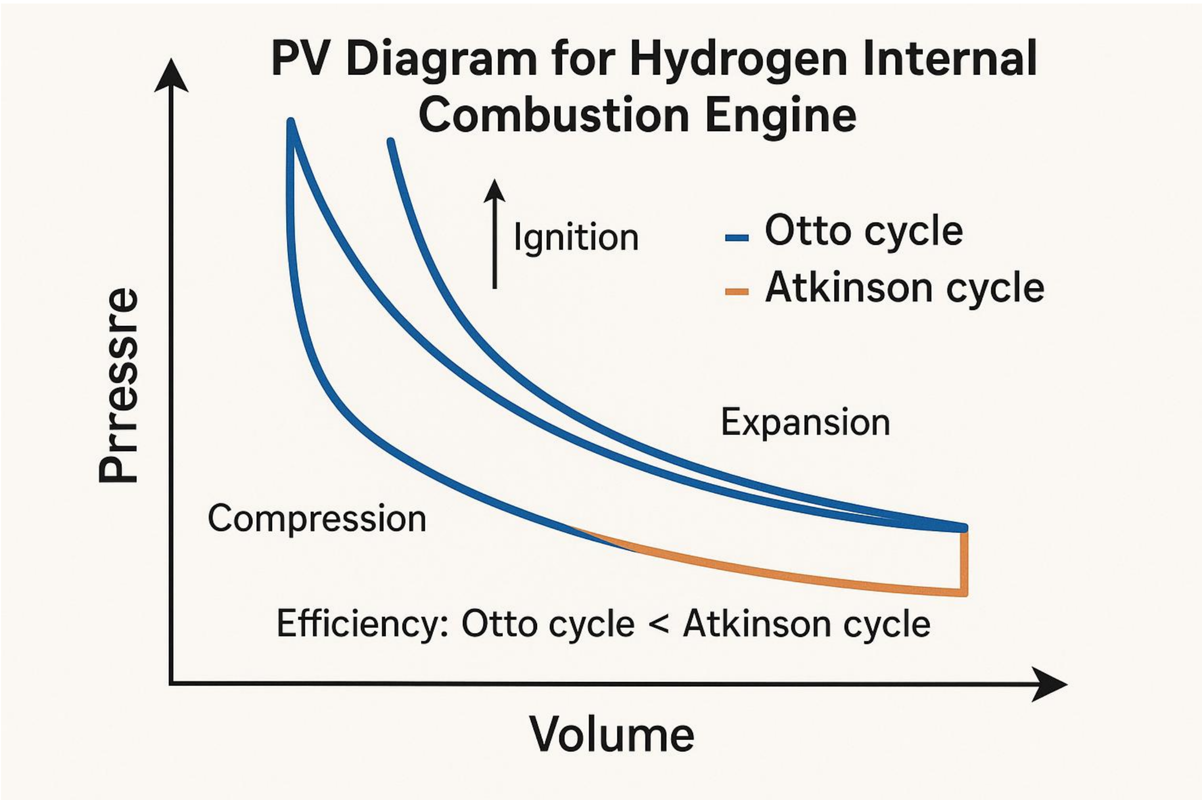

Figure 5: Thermodynamic pressure-volume diagram comparing the Otto and Atkinson cycles in a hydrogen-powered ICE, showing the differences in expansion and efficiency.

5. Discussion

Metal Hydrides as Hydrogen Storage

Metal hydrides provide a mid-density and comparatively safe alternative to compressed hydrogen storage. Magnesium hydride (MgH_2) is particularly promising, though it presents challenges related to heat management and kinetics. Catalysts such as titanium (Ti) and niobium (Nb) have been shown to improve reaction rates, enhancing practicality for vehicular applications.

Fuel Cells and System Integration

Fuel cells offer significantly higher efficiency and lower emissions than internal combustion engines (ICEs). Despite their advantages, fuel cells require complex systems for water and heat management. Platinum catalyst costs also present a barrier. Integration with electric drive systems is advancing rapidly, as demonstrated by the increasing number of commercial fuel cell electric vehicles (FCEVs).

Hydrogen Internal Combustion Engines (ICEs)

Hydrogen ICEs are less efficient than fuel cells but provide a transitional pathway using existing engine platforms. These engines are particularly beneficial for heavy-duty applications where battery weight is a limiting factor.

6. Conclusion

Hydrogen possesses the potential to transform clean energy transport, but widespread adoption depends on solving core issues of storage and efficiency. Metal hydrides offer safe, reversible, and compact hydrogen storage, though they require further thermal and catalytic advancements. Fuel cells demonstrate superior efficiency but are limited by economic and engineering hurdles. The future of hydrogen-powered mobility depends on integrating chemical innovations in storage with advancements in system design. Research should focus on hybrid solutions, such as low-temperature hydrides supplying high-efficiency fuel cells within robust mechanical architectures.

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