

A Review on Magnesium-Based Metal Hydride Reactors for Efficient Solid-State Hydrogen Storage: Materials, Thermal Management and Design Approaches

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Abstract- The global transition toward sustainable energy systems has accelerated interest in hydrogen as a clean and renewable energy carrier. However, the widespread adoption of hydrogen technologies is strongly dependent on the development of efficient, safe, and economically viable hydrogen storage methods. Among the available storage techniques, solid-state hydrogen storage using metal hydrides has emerged as one of the most promising approaches because of its high volumetric hydrogen density, enhanced operational safety, and reversible hydrogen absorption-desorption characteristics. Magnesium-based metal hydrides (MgH_2) have attracted considerable attention owing to their high theoretical hydrogen storage capacity (7.6 wt.%), natural abundance, lightweight nature, and relatively low cost. Despite these advantages, practical implementation remains challenging due to slow hydrogen sorption kinetics, poor thermal conductivity, and high hydrogen desorption temperatures. This review presents a comprehensive overview of recent developments in magnesium-based metal hydride reactor technology. Various hydrogen storage techniques are compared, followed by an in-depth discussion of hydrogen absorption mechanisms, reactor configurations, heat transfer enhancement methods, catalyst-assisted performance improvement, and advanced reactor design strategies. Recent progress in thermal management techniques, including metallic fins, expanded graphite, metal foams, heat exchanger tubes, and nanostructured additives, is critically reviewed. Furthermore, current research gaps and future opportunities in reactor optimization, additive manufacturing, artificial intelligence-based design optimization, and renewable energy integration are discussed. This review aims to provide researchers with a comprehensive understanding of the current state of magnesium-based hydrogen storage technology and its potential contribution to future hydrogen energy systems.

Keywords: Hydrogen Storage, Metal Hydrides, Magnesium Hydride, Solid-State Hydrogen Storage, Thermal Management, Heat Transfer Enhancement, Hydrogen Economy, Reactor Design.

I. INTRODUCTION

The increasing demand for clean energy, combined with growing concerns regarding climate change and depletion of fossil fuel resources, has significantly accelerated research into sustainable energy technologies. Fossil fuels remain the primary source of global energy production; however, their extensive utilization has resulted in severe environmental consequences, including greenhouse gas emissions, air pollution, and global warming.

Consequently, the search for alternative energy carriers capable of supporting carbon-neutral energy systems has become a major scientific and engineering priority.

Among various renewable energy carriers, hydrogen has emerged as one of the most promising candidates because of its exceptionally high gravimetric energy density and environmentally friendly utilization. Unlike conventional fossil fuels, hydrogen produces only water during

electrochemical conversion in fuel cells, making it an attractive option for reducing greenhouse gas emissions across transportation, industrial, and stationary power applications. Furthermore, hydrogen can be generated using renewable electricity through water electrolysis, thereby enabling long-term storage of intermittent renewable energy generated from solar and wind resources.

Despite these advantages, hydrogen storage remains one of the major technological barriers limiting the large-scale implementation of hydrogen-based energy systems. Due to its extremely low density under ambient conditions, hydrogen requires specialized storage techniques capable of achieving high storage capacity while maintaining operational safety and economic feasibility. Conventional storage methods, including compressed gas cylinders and cryogenic liquid hydrogen tanks, involve either extremely high pressures or ultra-low temperatures, both of which increase system complexity, energy consumption, and infrastructure costs.

Solid-state hydrogen storage has emerged as an attractive alternative because hydrogen is stored within solid materials through reversible chemical reactions. Among various solid-state storage materials, metal hydrides have received considerable research attention because they offer high volumetric hydrogen density, reduced leakage risks, and relatively safe operating conditions. Within this category, magnesium hydride (MgH_2) has become one of the most extensively investigated materials due to its exceptional hydrogen storage capacity, natural abundance, low density, and economic viability.

However, practical implementation of magnesium-based hydrogen storage reactors remains challenging. Magnesium hydride exhibits inherently slow hydrogen absorption and desorption kinetics, poor thermal conductivity, and relatively high operating temperatures for hydrogen release. These limitations have motivated extensive research into advanced reactor configurations, thermal management systems, catalytic materials,

nanostructured hydrides, and computational optimization techniques.

This review summarizes recent progress in magnesium-based metal hydride reactor technology by critically examining reactor design methodologies, hydrogen storage mechanisms, heat transfer enhancement approaches, catalyst development, and future research directions. The objective is to provide researchers with a consolidated understanding of current technological advancements while identifying research gaps that must be addressed before large-scale commercialization becomes feasible.

II. HYDROGEN STORAGE TECHNOLOGIES

Hydrogen storage technologies can generally be classified into three major categories:

- Compressed hydrogen storage
- Liquid hydrogen storage
- Solid-state hydrogen storage

Compressed hydrogen storage remains the most widely adopted commercial technology because of its relatively simple system architecture. Hydrogen is stored inside high-pressure cylinders operating between 350 and 700 bar. Although this method provides rapid charging and discharging, the requirement for high-strength pressure vessels significantly increases manufacturing costs while introducing safety concerns associated with high-pressure operation.

Liquid hydrogen storage provides considerably higher volumetric energy density by cooling hydrogen below its boiling temperature of approximately -253°C . Cryogenic storage enables compact storage volumes, making it suitable for aerospace and certain transportation applications. However, continuous refrigeration, boil-off losses, sophisticated insulation systems, and high liquefaction energy consumption considerably reduce its overall efficiency.

Solid-state hydrogen storage offers an alternative approach in which hydrogen atoms are chemically or

physically stored within solid materials. This category includes metal hydrides, complex hydrides, porous carbon materials, metal-organic frameworks (MOFs), and chemical hydrogen carriers. Among these technologies, metal hydrides have attracted extensive research interest because they combine high storage density with improved operational safety under relatively moderate pressures.

Compared with compressed and liquid hydrogen systems, metal hydride reactors significantly reduce hydrogen leakage risks while enabling repeated hydrogen charging and discharging cycles. Nevertheless, reactor performance strongly depends on efficient thermal management due to the exothermic nature of hydrogen absorption and the endothermic characteristics of hydrogen desorption.

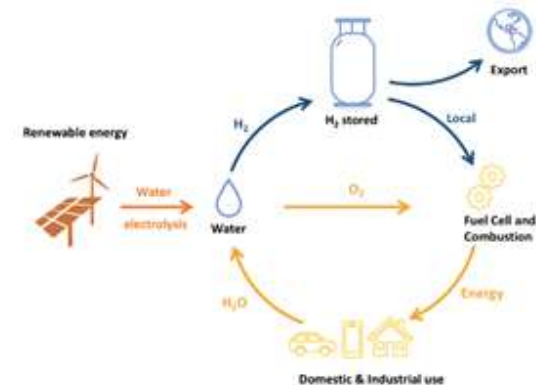


Figure 1: Simplified hydrogen energy cycle illustrating renewable hydrogen production, storage, and utilization

Table 1: Comparison of Hydrogen Storage Technologies

Storage Method	Storage Capacity	Operating Conditions	Advantages	Limitations
Compressed Gas	Low–Moderate	350–700 bar	Mature technology, fast filling	High pressure, safety concerns
Liquid Hydrogen	High	–253°C	High volumetric density	High liquefaction energy
Metal Hydrides	High	Moderate pressure, elevated	High safety,	Thermal management

Storage Method	Storage Capacity	Operating Conditions	Advantages	Limitations
		temperature	compact storage	environmental challenges
Chemical Hydrides	Very High	Controlled reaction	High storage density	Difficult regeneration
Adsorption Materials (MOFs/Carbon)	Moderate	Low temperature	Lightweight	Limited storage capacity

Table 2: Advantages and Limitations of Magnesium Hydride

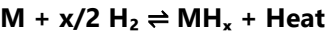
Property	Benefit	Challenge
Hydrogen Capacity	7.6 wt.%	High desorption temperature
Material Cost	Low	Slow reaction kinetics
Density	Lightweight	Powder handling
Availability	Abundant	Thermal conductivity
Reversibility	Excellent cycling	Heat management

III. MAGNESIUM-BASED METAL HYDRIDES

Fundamentals of Metal Hydrides

Metal hydrides are a class of materials capable of reversibly storing hydrogen through chemical absorption within their crystal lattice. Unlike compressed or liquid hydrogen storage systems, metal hydrides store hydrogen in atomic form, resulting in significantly higher volumetric storage density and improved operational safety. During hydrogen charging, hydrogen molecules dissociate into atoms on the metal surface before diffusing into the lattice to form a hydride phase. The reverse process occurs during hydrogen release when thermal energy is supplied.

The general reversible reaction governing metal hydride formation can be expressed as:



where M represents the metal or alloy and MH_x denotes the corresponding metal hydride.

This reversible reaction enables repeated hydrogen charging and discharging over many operating cycles, making metal hydrides attractive for stationary energy storage, portable power systems, and fuel-cell-based applications.

Metal hydrides are generally classified into:

- Intermetallic hydrides ($LaNi_5$, TiFe)
- Lightweight hydrides (MgH_2)
- Complex hydrides ($NaAlH_4$, $LiBH_4$)
- Reactive hydride composites

Among these materials, magnesium hydride has attracted exceptional research interest because of its high gravimetric hydrogen storage capacity and economic feasibility.

Magnesium Hydride as a Hydrogen Storage Material

Magnesium hydride (MgH_2) is considered one of the most promising solid-state hydrogen storage materials because it combines high hydrogen storage capacity, low density, natural abundance, and relatively low production cost. Magnesium is the eighth most abundant element in the Earth's crust and can also be extracted from seawater, making it economically attractive for large-scale hydrogen storage applications.

The most significant advantage of magnesium hydride is its theoretical hydrogen storage capacity of approximately 7.6 wt.%, which is considerably higher than many commercially available intermetallic hydrides. This high gravimetric capacity makes magnesium particularly suitable for applications where weight reduction is essential, including transportation, aerospace, and portable energy systems.

Furthermore, magnesium exhibits excellent cycling stability under appropriate operating conditions, enabling repeated hydrogen absorption and desorption without severe degradation of storage performance.

However, several technical limitations continue to hinder its widespread commercialization. Magnesium hydride possesses relatively low thermal conductivity, leading to non-uniform temperature distribution inside the reactor. In addition, hydrogen desorption generally requires temperatures exceeding 300°C because of the high thermodynamic stability of MgH_2 . Slow hydrogen diffusion within the hydride layer further limits charging and discharging rates.

Consequently, recent research has focused on improving magnesium hydride performance through catalyst addition, particle size refinement, nano structuring, composite materials, and advanced thermal management systems.

Table 3: Comparison of Common Metal Hydrides

Material	Hydrogen Capacity (wt.%)	Operating Temperature	Advantages	Major Limitation
$LaNi_5$	1.4	Low	Fast kinetics	Low storage capacity
TiFe	1.9	Moderate	Good reversibility	Activation required
MgH_2	7.6	High	High capacity, low cost	Slow kinetics, poor thermal conductivity
$NaAlH_4$	5.6	Moderate	Good storage density	Catalyst dependent
$LiBH_4$	18.5	Very High	Extremely high capacity	High operating temperature

IV. HYDROGEN ABSORPTION AND DESORPTION MECHANISMS

Hydrogen storage in magnesium hydride involves two reversible processes: hydrogen absorption

(hydrogenation) and hydrogen desorption (dehydrogenation).

During hydrogen absorption, molecular hydrogen first adsorbs onto the magnesium surface and dissociates into atomic hydrogen. These hydrogen atoms diffuse into the magnesium crystal lattice, forming magnesium hydride while releasing heat.

Hydrogen Absorption Reaction



Since this reaction is exothermic, the generated heat must be rapidly removed to maintain favorable reaction kinetics. Insufficient heat removal causes localized temperature increases, slowing further hydrogen absorption.

Conversely, hydrogen desorption is an endothermic reaction requiring continuous heat input.

Hydrogen Desorption Reaction



Efficient reactor performance therefore depends heavily on optimized thermal management systems capable of both removing heat during absorption and supplying heat during desorption.

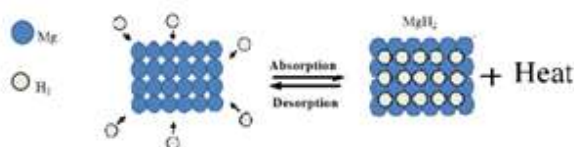


Figure 2: Absorption and Desorption of MgH₂

V. THERMODYNAMICS AND REACTION KINETICS

The thermodynamic properties of magnesium hydride determine the equilibrium conditions for hydrogen absorption and release. MgH₂ exhibits a relatively high enthalpy of formation, making it thermodynamically stable. While this stability enhances storage safety, it also necessitates elevated temperatures for hydrogen desorption.

Hydrogen reaction kinetics are equally important because they determine charging and discharging speed. Magnesium hydride generally exhibits slow hydrogen diffusion through the hydride layer, leading to prolonged storage times.

Several approaches have been proposed to overcome kinetic limitations:

- High-energy ball milling
- Nanostructured magnesium particles
- Transition metal catalysts (Ni, Ti, Fe, Nb)
- Carbon nanotube reinforcement
- Expanded graphite composites
- Metal foam structures
- Severe plastic deformation techniques

These methods increase surface area, reduce diffusion distances, introduce lattice defects, and improve thermal conductivity, thereby accelerating hydrogen sorption.

Table 4: Factors Affecting Hydrogen Storage Performance

Parameter	Effect on Reactor Performance
Operating Temperature	Controls hydrogen equilibrium pressure
Hydrogen Pressure	Influences absorption rate
Particle Size	Smaller particles improve kinetics
Thermal Conductivity	Higher conductivity accelerates heat transfer
Catalyst Addition	Enhances hydrogen diffusion
Reactor Geometry	Affects temperature distribution
Heat Exchanger Design	Improves charging/discharging efficiency

VI. PERFORMANCE ENHANCEMENT USING CATALYSTS

One of the most active research areas in magnesium-based hydrogen storage involves catalyst-assisted enhancement of hydrogen sorption kinetics.

Transition metals such as titanium, nickel, niobium, vanadium, iron, and cobalt have demonstrated

significant improvements in hydrogen absorption rates. Similarly, carbon-based nanomaterials—including graphene, carbon nanotubes, and expanded natural graphite—improve thermal conductivity and facilitate hydrogen diffusion.

Recent studies have also explored advanced catalyst systems based on metal oxides, MXenes, and high-entropy alloys. These materials create additional diffusion pathways, reduce activation energy, and improve long-term cycling stability.

Although catalyst addition significantly enhances reactor performance, optimization of catalyst concentration, particle morphology, and dispersion techniques remains an active area of investigation.

VII. ADVANCED METAL HYDRIDE REACTOR DESIGNS AND THERMAL MANAGEMENT STRATEGIES

Introduction

The performance of a metal hydride hydrogen storage system depends not only on the hydrogen storage material but also on the reactor design. During hydrogen absorption, a considerable amount of heat is released due to the exothermic nature of the reaction. If this heat is not removed efficiently, the reactor temperature increases, slowing hydrogen absorption and reducing storage efficiency. Conversely, hydrogen desorption requires continuous heat input because the decomposition of magnesium hydride is an endothermic process. Therefore, the development of advanced reactor designs with efficient thermal management systems has become one of the primary research areas in solid-state hydrogen storage.

Modern reactor designs aim to maximize heat transfer while maintaining high hydrogen storage density, structural integrity, operational safety, and compact dimensions. Recent studies have proposed various reactor configurations that significantly improve reactor performance through enhanced thermal management.

Conventional Cylindrical Reactor

The cylindrical reactor remains the most commonly used configuration because of its structural

simplicity and ability to withstand high internal pressures. It consists of a cylindrical pressure vessel filled with magnesium hydride powder, together with hydrogen inlet and outlet ports, pressure monitoring devices, and temperature sensors.

Advantages include:

- Uniform pressure distribution
- Simple fabrication
- High mechanical strength
- Easy maintenance
- Low manufacturing cost

However, due to the poor thermal conductivity of magnesium hydride, conventional cylindrical reactors often develop large temperature gradients during hydrogen absorption and desorption, reducing overall reactor efficiency.

Finned Metal Hydride Reactors

One of the simplest approaches to improve heat transfer is the incorporation of metallic fins inside the hydride bed. Fins increase the heat transfer surface area and reduce thermal resistance between the hydride material and cooling medium.

Longitudinal fins, radial fins, pin fins, and spiral fins have all been investigated. Among these, spiral fin configurations generally provide more uniform temperature distribution throughout the reactor.

Benefits include:

- Improved thermal conductivity
- Reduced charging time
- Faster hydrogen desorption
- Better temperature uniformity

The main disadvantage is that additional fins occupy reactor volume, slightly reducing the total hydrogen storage capacity.

Helical Coil Heat Exchanger Reactor

Helical coil heat exchangers are among the most effective thermal management techniques used in magnesium hydride reactors. In this design, a helical tube carrying a heat transfer fluid passes through the reactor.

During hydrogen absorption, coolant flowing through the coil removes excess reaction heat.

During hydrogen desorption, hot fluid circulating inside the coil supplies the thermal energy required to release hydrogen.

This design provides:

- Excellent temperature control
- Faster hydrogen charging
- Uniform reactor temperature
- Reduced thermal stresses

Several numerical studies have demonstrated that helical coil reactors outperform conventional cylindrical reactors under identical operating conditions.

Shell-and-Tube Reactors

Shell-and-tube reactors are commonly employed for medium and large hydrogen storage systems. The hydride material is placed either inside multiple tubes or within the shell, while the heat transfer fluid circulates through the remaining passages.

Advantages include:

- Excellent heat removal
- Large heat transfer area
- Suitable for industrial applications
- Uniform hydrogen distribution

These reactors are particularly suitable for stationary hydrogen storage systems requiring large storage capacities.

Tube Bundle Reactor

Tube bundle reactors consist of multiple parallel tubes filled with magnesium hydride.

Compared with single-cylinder reactors, tube bundle systems provide:

- Greater surface-to-volume ratio
- Faster heat transfer
- Better temperature uniformity
- Improved hydrogen charging rates

However, fabrication complexity increases significantly because of the larger number of pressure-resistant tubes.

Table 6. Comparison of Reactor Configurations

Reactor Type	Heat Transfer	Manufacturing	Storage Capacity	Overall Performance
Cylindrical	Low	Easy	High	Moderate
Finned	High	Moderate	Moderate	High
Helical Coil	Very High	Moderate	High	Excellent
Shell-and-Tube	Excellent	Complex	High	Excellent
Tube Bundle	Excellent	Complex	Moderate	Excellent

Advanced Thermal Management Techniques

Thermal management remains one of the most significant challenges in magnesium-based hydrogen storage systems. Researchers have proposed several methods to enhance thermal conductivity within the hydride bed.

These include:

- Expanded graphite
- Carbon nanotubes
- Graphene nanoplatelets
- Copper foam
- Aluminum foam
- Metallic fins
- Embedded heat exchanger tubes
- Composite hydride materials
- Additively manufactured lattice structures

The integration of these materials significantly improves heat dissipation, resulting in faster hydrogen absorption and desorption.

VIII. NANOSTRUCTURED MAGNESIUM HYDRIDES

Nanotechnology has emerged as one of the most effective strategies for improving hydrogen storage performance. Reducing magnesium particle size to the nanometer scale shortens hydrogen diffusion paths, increases surface area, and introduces crystal defects that facilitate hydrogen transport.

Common nanostructuring techniques include:

- High-energy ball milling
- Mechanical alloying
- Chemical reduction
- Vapor deposition
- Spark plasma sintering

Nanostructured magnesium hydrides exhibit:

- Faster hydrogen absorption
- Lower desorption temperatures
- Improved cycling stability
- Enhanced catalyst dispersion

Despite these advantages, nanoparticle agglomeration and oxidation remain significant challenges that require careful material processing and storage.

IX. FINITE ELEMENT ANALYSIS (FEA) IN REACTOR DESIGN

Finite Element Analysis has become an indispensable tool in the design of metal hydride reactors. FEA enables researchers to evaluate structural integrity, thermal behaviour, and stress distribution under different operating conditions without extensive experimental testing.

Typical FEA investigations include:

- Temperature distribution
- Thermal stress analysis
- Pressure vessel integrity
- Deformation due to cyclic loading
- Safety factor evaluation

The use of FEA significantly reduces development time and manufacturing costs while improving reactor reliability.

Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is widely used to analyze hydrogen flow behaviour, heat transfer, and coolant distribution within metal hydride reactors.

CFD simulations help optimize:

- Hydrogen flow paths
- Coolant channel design
- Heat exchanger geometry
- Temperature distribution

- Pressure losses

By combining CFD with FEA, researchers can simultaneously evaluate thermal and structural performance, enabling more efficient reactor optimization.

Artificial Intelligence in Reactor Optimization

Artificial Intelligence (AI) and Machine Learning (ML) have recently emerged as powerful tools for optimizing hydrogen storage systems.

Applications include:

- Predicting hydrogen absorption rates
- Optimizing catalyst composition
- Designing reactor geometries
- Real-time thermal management
- Fault detection and predictive maintenance

AI-driven optimization reduces computational time compared with conventional trial-and-error approaches and accelerates the development of next-generation hydrogen storage technologies.

X. RESEARCH GAPS

Although considerable progress has been achieved in magnesium-based hydrogen storage systems, several scientific and engineering challenges continue to restrict commercialization.

Thermal Conductivity

Magnesium hydride possesses relatively low thermal conductivity, resulting in significant temperature gradients during hydrogen charging and discharging. Although expanded graphite, metal foams, and internal heat exchangers improve thermal performance, achieving uniform temperature distribution remains a major challenge.

Slow Hydrogen Sorption Kinetics

Hydrogen diffusion through the MgH_2 layer remains relatively slow, increasing hydrogen charging and discharging times. Catalyst addition improves reaction kinetics; however, catalyst stability and long-term effectiveness require further investigation.

High Desorption Temperature

Hydrogen release from MgH_2 generally requires temperatures above 300°C .

Reducing this temperature while maintaining storage capacity remains one of the most important research objectives.

Reactor Scale-Up

Many published studies focus on laboratory-scale reactors.

Industrial-scale hydrogen storage introduces additional challenges including:

- Heat removal
- Mechanical integrity
- Uniform hydrogen distribution
- Manufacturing cost
- Long-term durability

Material Stability

Repeated hydrogen absorption and desorption cycles can lead to:

- Particle agglomeration
- Powder degradation
- Catalyst deactivation
- Structural expansion

These factors reduce long-term reactor performance.

XI. FUTURE RESEARCH OPPORTUNITIES

Research Area	Expected Benefit
Advanced Catalysts	Faster hydrogen kinetics
Nanostructured MgH ₂	Reduced desorption temperature
Hybrid Heat Exchangers	Improved thermal management
AI Optimization	Faster reactor design
Additive Manufacturing	Complex internal cooling structures
Digital Twin Technology	Real-time reactor monitoring
Renewable Integration	Sustainable hydrogen economy

XII. CONCLUSION

Magnesium-based metal hydride reactors represent one of the most promising technologies for safe and efficient solid-state hydrogen storage. Their exceptionally high hydrogen storage capacity, abundance, and relatively low cost make magnesium hydride an attractive material for future hydrogen energy systems. However, practical implementation remains constrained by slow hydrogen sorption kinetics, poor thermal conductivity, and high hydrogen desorption temperatures.

This review has summarized recent advances in reactor design, thermal management techniques, catalyst-assisted enhancement, nanostructured materials, and computational optimization methods. Advanced reactor configurations incorporating internal heat exchangers, metallic fins, phase change materials, expanded graphite, and metal foams have demonstrated significant improvements in hydrogen charging and discharging performance. Furthermore, computational techniques such as Finite Element Analysis, Computational Fluid Dynamics, Artificial Intelligence, and Machine Learning have accelerated reactor optimization while reducing experimental costs.

Despite remarkable progress, several challenges remain before magnesium-based hydrogen storage systems can achieve widespread commercialization. Future research should focus on hybrid thermal management systems, intelligent reactor control, advanced catalyst development, additive manufacturing, and renewable energy integration. The combination of these emerging technologies is expected to facilitate the development of highly efficient, compact, and economically viable hydrogen storage systems capable of supporting the global transition toward sustainable energy.

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