SeMA Journal
https://doi.org/10.1007/s40324-026-00427-w

Hydrogen as an energy vector: challenges in storage and transport with special emphasis on metal-based solutions

Antonio La Gatta[1] · Luca La Gatta[2] · Vincenzo Vespri[3]

Received: 19 November 2025 / Accepted: 9 April 2026

Abstract
Hydrogen has long been considered a potential cornerstone of the future energy system, especially in the context of the transition away from fossil fuels. Its appeal lies in its abundance, its clean combustion (producing only water as a by-product), and its versatility as both a fuel and a feedstock. However, the practical use of hydrogen as an energy vector is hindered by fundamental challenges related to its physical and chemical properties. Its very low atomic mass makes hydrogen an energy carrier with low volumetric density; liquefaction is energetically costly due to the extremely low boiling point, and compression requires pressures of several hundred atmospheres, raising issues of safety and efficiency. Furthermore, hydrogen transport is problematic: its tiny molecular size leads to permeation through pipes, and it can induce embrittlement and cracking in metals such as steel. Alternative strategies, such as binding hydrogen into compounds like ammonia, provide partial solutions but bring their own limitations, including energy-intensive synthesis. A promising avenue of research involves solid-state hydrogen storage using metals or alloys, notably palladium, which exhibits exceptional absorption properties. The aim of this article is to discuss these issues from a mathematical and physical perspective, highlighting the analytical and modeling challenges that arise when hydrogen is considered as a key element of the energy transition .

Keywords Hydrogen economy · Energy vector · Storage · Transport · Palladium · Magnesium · Transition metals · Mathematical challenges

V. Vespri: Member of G,N.A.M.P.A. (Istituto Nazionale di Alta Matematica).

✉ Vincenzo Vespri
vincenzo.vespri@unifi.it

Antonio La Gatta
a.lagatta@innovazione.gov.it

Luca La Gatta
lucalagatta21@gmail.com

1 Dipartimento per la Trasformazione Digitale, Largo Pietro di Brazzà 86, 00187 Roma, Italy

2 Politecnico di Milano, Piazza Leonardo da Vinci, 32, 20133 Milano, Italy

3 Dipartimento di Matematica e Informatica, Università di Firenze, Viale Morgagni 67/a, 50134 Firenze, Italy

Published online: 20 May 2026

Mathematics Subject Classification 80A20 (Thermodynamics) · 74A50 (Hydrogen embrittlement) · 35Q79 (PDEs in connection with energy models) · 76M45 (PDEs in fluid mechanics, hydrogen flow)

Contents

1 Introduction

The role of hydrogen as a potential energy vector has been a matter of discussion for several decades, often oscillating between high expectations and sobering recognition of its limitations. The concept entered the public debate with renewed vigor following the publication of Jeremy Rifkin's influential book *The Hydrogen Economy* [32], which popularized the vision of a society powered by hydrogen as a clean and ubiquitous energy source. Since then, hydrogen has repeatedly been identified by policymakers, researchers, and industry stakeholders as a possible keystone in the shift away from fossil fuels. Yet, despite this persistent enthusiasm, hydrogen has not yet fulfilled its promise in mainstream energy systems.

The reasons for this gap between vision and reality are deeply rooted in the fundamental physics and chemistry of hydrogen. As the lightest element in the periodic table, hydrogen carries significant disadvantages as a practical energy vector. While it is true that hydrogen has a high gravimetric energy density (120 MJ/kg), its volumetric energy density is extremely low under ambient conditions. A mole of hydrogen weighs only 2 grams, making it one of the least efficient carriers per unit of volume. For hydrogen to be useful in applications requiring compact storage and efficient transport—such as powering vehicles or feeding industrial processes—it must either be liquefied or compressed.

Liquefaction, however, poses formidable challenges. Hydrogen's boiling point at 1 atm is 20.3 K, which requires cryogenic technology. Achieving and maintaining such temperatures is energetically costly and often inefficient on a large scale. On the other hand, compression demands very high pressures, often up to 700 bar for vehicular storage, which raises issues of energy cost, infrastructure safety, and material durability. Thus, neither liquefaction nor compression provides an entirely satisfactory solution.

A further difficulty lies in the transport of hydrogen. Its small molecular size allows it to permeate through many materials, including the metals commonly used in pipelines. Moreover, hydrogen can induce embrittlement in steel, leading to crack propagation and structural failures. This effect, widely known as *hydrogen embrittlement*, represents a serious obstacle to repurposing existing natural gas infrastructure for hydrogen transport. While the use of composite materials and advanced alloys can mitigate some risks, the overall challenge remains unresolved.

Another approach to hydrogen transport and storage involves chemical carriers. Ammonia (NH_3) is often highlighted as a promising candidate: it is easier to liquefy than hydrogen, has a well-established infrastructure, and can release hydrogen through catalytic decomposition. However, ammonia synthesis itself is highly energy-intensive, relying heavily on the Haber–Bosch process, which consumes around 1–2% of the world's total energy supply. While biological nitrogen fixation demonstrates a more efficient pathway through enzymes such as nitrogenase, scaling such biological processes to industrial levels is still an open challenge. In addition, the toxicity and handling risks of ammonia complicate its direct use as a widespread energy vector.

Against this background, solid-state hydrogen storage using metals and alloys has emerged as a highly promising avenue of research. Certain metals—notably palladium, magnesium, and titanium—exhibit the remarkable ability to absorb hydrogen into their lattice structures, forming metal hydrides. Among these, palladium is particularly attractive due to its extraordinary hydrogen absorption capacity, storing hydrogen at near-ambient conditions and releasing it reversibly. Palladium hydrides have been studied since the 19th century, and their peculiar thermodynamic and structural properties continue to provide insights into both applied and fundamental science.

This article aims to explore the intricate mathematical challenges that emerge in the modeling, analysis, and optimization of hydrogen as an energy vector. A first line of inquiry concerns the development of accurate models for hydrogen diffusion in metals, where lattice strain, crystalline defects, and possible phase transitions play a decisive role in determining the transport properties of the material. Closely related to this is the need to understand the coupling between mechanical stress and hydrogen migration, a phenomenon that underlies the dangerous processes of embrittlement and crack propagation in structural components.

Another central problem involves the quantitative assessment of the energetic trade-offs among the various storage strategies–compression, liquefaction, and solid-state adsorption–each governed by distinct thermodynamic constraints and efficiency considerations. From a mathematical perspective, these problems often lead to nonlinear systems of partial differential equations describing hydrogen absorption and desorption dynamics, particularly in metals such as palladium that exhibit strong hysteresis and phase-change behavior.

Finally, the stability of hydrogen-bearing compounds, including ammonia and metal hydrides, must be analyzed through coupled thermodynamic and kinetic models, which allow one to predict the conditions under which such compounds remain viable for storage and transport applications. Together, these topics define a coherent mathematical framework that links continuum mechanics, thermodynamics, and nonlinear analysis in the service of a sustainable hydrogen economy.

The scope of this paper is not to provide final solutions to these problems, but rather to highlight the mathematical structure underlying them and to clarify why they are central to the feasibility of the hydrogen economy. While the hydrogen narrative has often been dominated by technological optimism, our focus will be on the rigorous exploration of the barriers that mathematics and physics reveal. By doing so, we aim to provide a critical foundation upon which both theoretical advances and practical applications may build.

In what follows, Section 2 will outline the physical and chemical characteristics of hydrogen that make it a challenging energy carrier. Section 3 will examine the conventional strategies of liquefaction and compression, emphasizing their mathematical modeling aspects. Section 4 will discuss issues of hydrogen transport, particularly the phenomenon of embrittlement in metals. Section 5 will address ammonia as a chemical carrier, weighing its potential and limitations. In addition, Section 5 will briefly discuss hydrogen peroxide (H_2O_2) as a possible alternative energy vector. Although less frequently considered in contemporary energy policy debates, hydrogen peroxide presents interesting thermodynamic and storage properties, including liquid-phase stability at ambient conditions and high oxygen content, which make it relevant in propulsion systems and potentially in distributed energy applications. Section 6 will turn to solid-state hydrogen storage, with a special focus on palladium, and Section 7 will present the mathematical models relevant to absorption and desorption processes. Finally, Section 8 will offer some concluding remarks on the future of hydrogen research within the broader energy transition.

2 Physical and chemical characteristics of hydrogen as an energy carrier

Hydrogen is widely regarded as a promising vector for sustainable and decarbonized energy systems, yet its intrinsic physical and chemical properties make large-scale deployment highly challenging. In this section, we summarize the most relevant characteristics that affect its storage, transport, and utilization.

Hydrogen is the lightest element, with atomic number $Z = 1$ and atomic mass

$$M_{\mathrm{H}} \approx 1.008\,\mathrm{g/mol}.$$

Under standard temperature and pressure (STP: $T = 273.15\,\mathrm{K}$, $p = 1\,\mathrm{atm}$), its density is

$$\rho_{\mathrm{H}_2,\mathrm{STP}} \approx 0.0899\,\mathrm{kg/m^3},$$

about fourteen times lower than that of air. This extremely low density complicates storage and distribution, as large volumes or high pressures are required [23, 39].

Hydrogen also exhibits the highest specific energy by weight among known fuels. The lower heating value (LHV) is

$$\mathrm{LHV}(H_2) \approx 120\,\mathrm{MJ/kg},$$

nearly three times higher than gasoline on a mass basis [9]. However, when expressed per unit volume under ambient conditions, the corresponding energy density is

$$E_v(H_2,\ 1\,\mathrm{bar}) = \rho_{\mathrm{H}_2} \cdot \mathrm{LHV}(H_2) \approx 0.0108\,\mathrm{MJ/L},$$

which is far lower than for conventional hydrocarbon fuels. This large discrepancy between gravimetric and volumetric energy densities represents a major barrier to the practical adoption of hydrogen as an energy carrier [38].

To achieve practical energy densities suitable for storage and transport, hydrogen must be maintained either in a compressed gaseous form or as a cryogenic liquid. In the compressed-gas configuration, hydrogen is typically stored at pressures in the range of $p \approx 350$–$700\,\mathrm{bar}$, which yields a volumetric energy density of approximately

$$E_v(700\,\mathrm{bar}) \approx 5.6\,\mathrm{MJ/L}.$$

Achieving and maintaining such high pressures, however, requires a considerable energy input, estimated to be about 10–15% of the stored energy content [23].

Alternatively, hydrogen can be stored as a cryogenic liquid, obtained by cooling below its normal boiling temperature

$$T_b = 20.27\,\mathrm{K},$$

resulting in a higher volumetric energy density of roughly

$$E_v(\mathrm{LH_2}) \approx 8.5\,\mathrm{MJ/L}.$$

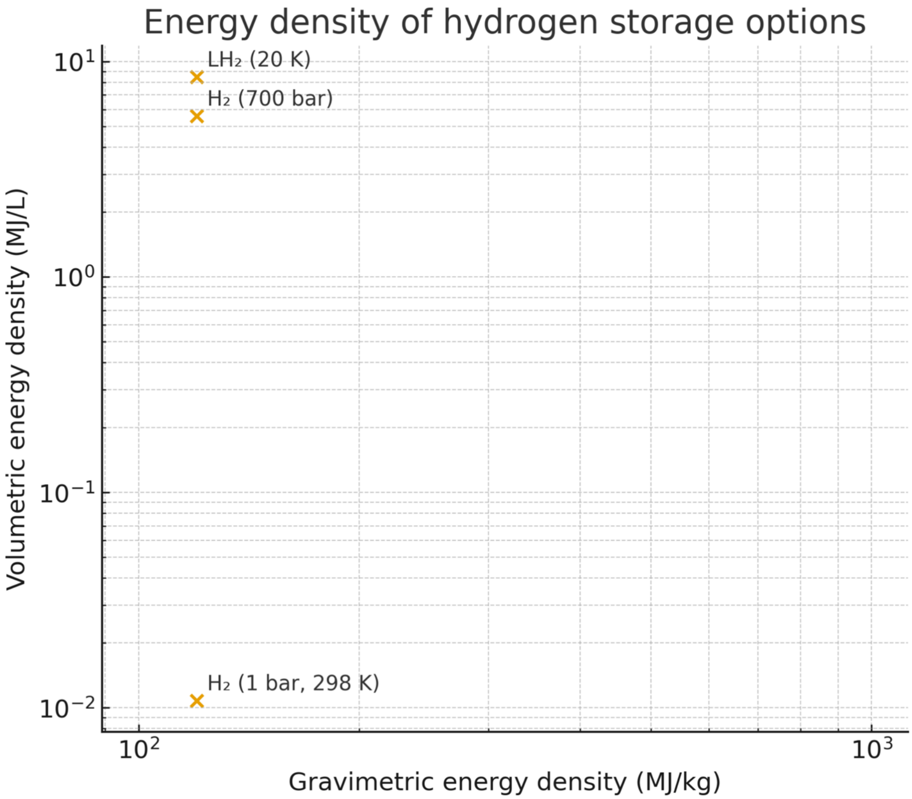

Fig. 1 Gravimetric vs. volumetric energy density for hydrogen in different storage states. All points share the same gravimetric value (∼120 MJ/kg), while volumetric energy density varies by orders of magnitude: H_2 (1 bar, 298 K) ≈ 0.0108 MJ/L; H_2 (700 bar) ≈ 5.6 MJ/L; LH_2 (20 K) ≈ 8.5 MJ/L. Adapted from [8]

This approach, while advantageous in terms of compactness, is energetically demanding: the liquefaction process typically consumes between 30% and 40% of the lower heating value (LHV) and is further affected by boil-off losses during storage and transport [15]. Consequently, both storage methods involve a delicate balance between energy efficiency, safety, and infrastructure requirements, representing one of the key challenges in the deployment of a large-scale hydrogen economy.

Hydrogen is also highly flammable, with a wide flammability range in air:

$$4\% < \text{Vol.}\%\ H_2 < 75\%,$$

and an extremely low minimum ignition energy,

$$E_{\text{ign}} \approx 0.02\,\text{mJ}.$$

These characteristics raise significant safety concerns during storage, handling, and transport [34, 46].

Because of its small molecular size ($d_{\text{H}_2} \approx 0.289\,\text{nm}$), hydrogen diffuses rapidly through many materials. The diffusion coefficient in metals can be modeled as

$$D(T) = D_0\ \exp\left(-\frac{E_a}{RT}\right),$$

where D_0 is the pre-exponential factor, E_a is the activation energy, R the gas constant, and T the absolute temperature. This diffusion behavior can lead to hydrogen embrittlement and material degradation, critical challenges for pipeline and storage infrastructure design [18, 28].

In summary, hydrogen combines exceptionally high specific energy with very low density and demanding storage requirements. Its flammability, diffusivity, and interactions with materials further complicate its safe and efficient use as an energy carrier. Consequently, technological advances in compression, liquefaction, solid-state storage, and materials science remain essential to enable a viable hydrogen economy [8, 23].

3 Conventional strategies for hydrogen liquefaction and compression: mathematical modeling aspects

This section provides a mathematical modelling framework for understanding the fundamental processes of hydrogen liquefaction and compression. Equations of state, thermodynamic cycle analysis, and irreversibility modelling serve as the foundation for optimising these conventional strategies. The theoretical insights derived here set the stage for the subsequent sections addressing advanced hydrogen storage methods.

As discussed in the previous section, hydrogen, despite its remarkably high gravimetric energy density, poses substantial challenges as an energy carrier due to its extremely low volumetric density under ambient conditions. These physical characteristics make the storage and transportation of hydrogen technically complex and energetically demanding. To address these limitations, two conventional strategies are predominantly employed:

1. *Liquefaction*, in which hydrogen is cooled to cryogenic temperatures near 20.3 K at atmospheric pressure, thereby increasing its volumetric energy density by nearly an order of magnitude compared to the gaseous state. This process, however, requires a considerable energy input and involves sophisticated cryogenic infrastructure.
2. *Compression*, where hydrogen gas is stored at very high pressures, typically within the range 350−700 bar, to achieve sufficient volumetric energy density for practical applications such as vehicular fuel storage and industrial supply networks. This approach, while technologically mature, still entails significant energy expenditure and stringent safety requirements.

Both processes involve substantial energy expenditure motivating ongoing research into alternative carriers and solid-state storage technologies. Both processes are governed by thermodynamic, fluid-dynamic, and transport phenomena that can be analysed and optimised through mathematical modelling. Let us begin with the problems connected with hydrogen liquefaction, which is based on reducing the temperature of gaseous hydrogen to below its critical temperature $T_c = 33.2$ K and then condensing it at atmospheric pressure ($p \approx 1$ bar). Unlike natural gas, which has a comparatively high boiling point, hydrogen liquefaction requires advanced cryogenic cycles to reach such ultra-low temperatures [1]. The general principle of hydrogen liquefaction relies on a combination of thermodynamic processes that collectively enable efficient temperature reduction and phase transition to the liquid state. A key mechanism is the *isentropic expansion*, in which hydrogen experiences a significant temperature drop as it expands through a turbine or expander, performing mechanical work while conserving entropy. Complementary to this is the *Joule–Thomson (JT) effect*, an essentially isenthalpic process in which the gas cools upon expansion through a throttling valve, with its enthalpy remaining nearly constant during the transition [5]. Finally, effective *heat*

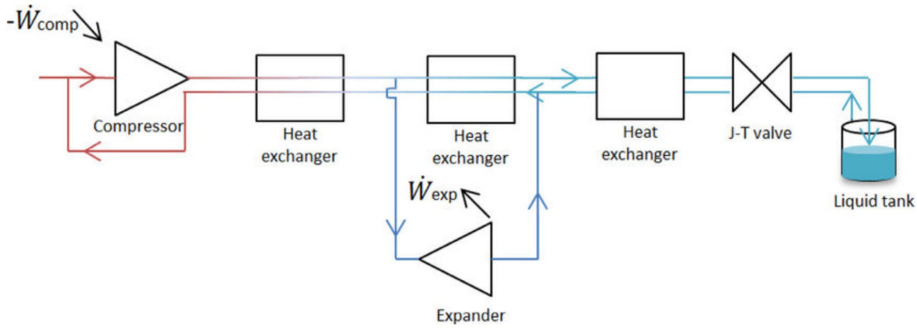

Fig. 2 Schematic of the Claude cycle for hydrogen liquefaction. Compressed hydrogen is pre-cooled in a heat exchanger, expanded in a turbine for partial liquefaction, and then further cooled via a Joule-Thomson valve before liquid–vapour separation. Thermodynamic states (T_i, p_i) correspond to the enthalpy relations above

exchange with pre-cooled streams plays a critical role in maintaining high thermodynamic efficiency. This is typically achieved through regenerative refrigeration cycles that employ liquid-nitrogen or mixed-refrigerant pre-cooling stages to progressively lower the temperature of the hydrogen stream before expansion [40]. Together, these coupled processes form the foundation of modern cryogenic hydrogen liquefaction systems, where advanced control and optimisation of expansion and heat-exchange stages determine overall system performance.

The liquefaction work can be derived from the First Law of Thermodynamics. The specific work of liquefaction, w_{liq}, can be expressed as:

$$w_{\text{liq}} = \int_{s_0}^{s_f} T\, ds = h_{\text{in}} - h_{\text{out}} - T_0\,(s_{\text{in}} - s_{\text{out}}),$$

where h is the specific enthalpy, s the specific entropy, and T_0 the ambient temperature. This relation highlights the dependence on entropy reduction and thus on irreversibilities present in the cycle.

The "classic" Claude cycle is widely applied to hydrogen liquefaction. It involves pre-cooling using liquid nitrogen, isentropic expansion in turbines, and final Joule–Thomson expansion. The efficiency is limited by:

$$\eta = \frac{L}{W_{\text{in}}},$$

where L is the latent heat of liquefaction per unit mass and W_{in} is the input work. Mathematically, the turbine-expansion stage can be modelled as:

$$h_{\text{out}} = h_{\text{in}} - \eta_{\text{turb}}\,(h_{\text{in}} - h_{\text{is}}),$$

where h_{is} is the isentropic enthalpy and η_{turb} is the turbine efficiency. The JT-expansion stage is modelled as an isenthalpic process:

$$h_{\text{out}} = h_{\text{in}}, \quad \Delta T = \frac{1}{C_p}\left[T\left(\frac{\partial v}{\partial T}\right)_p - v\right]\Delta p,$$

where C_p is the specific heat capacity at constant pressure, and v the specific volume. For hydrogen, the JT coefficient is "positive only below ~ 200 K", making pre-cooling essential [1].

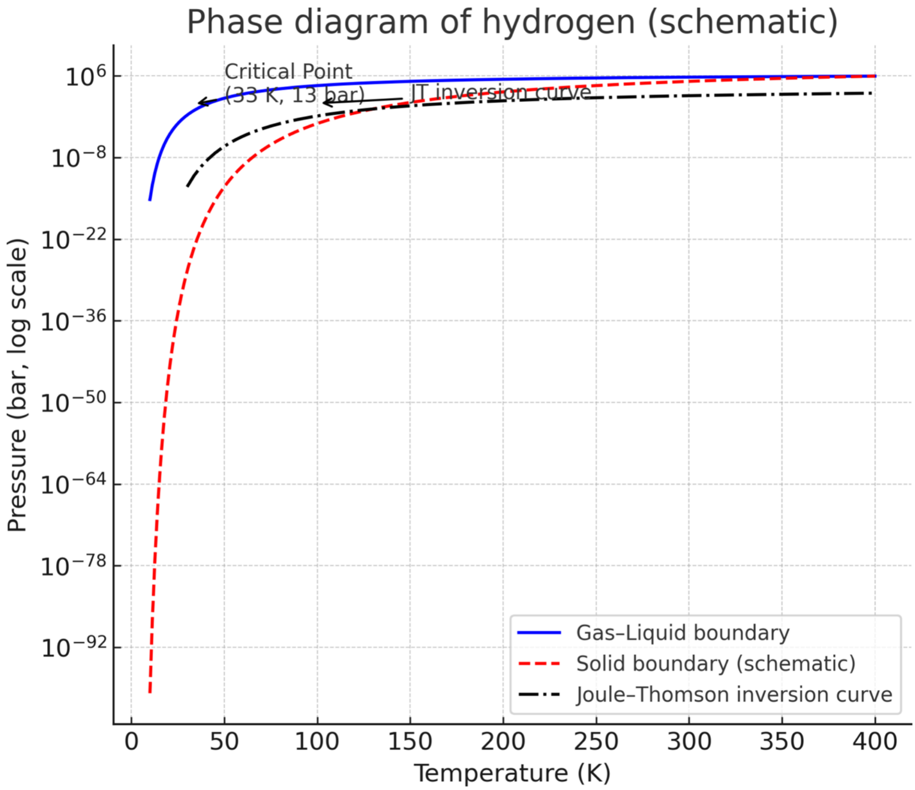

Fig. 3 Phase diagram of hydrogen (schematic). The critical point occurs at $T_c = 33\,\mathrm{K}$ and $p_c = 13\,\mathrm{bar}$. Below the Joule–Thomson inversion curve, isenthalpic expansion results in cooling, which enables hydrogen liquefaction in Claude-type cryogenic cycles

We now turn to the mathematical modeling of hydrogen compression, a process designed to achieve pressures typically in the range of $350-700\,\mathrm{bar}$, as required for vehicular and industrial storage applications. The analysis relies primarily on accurate thermodynamic equations of state (EOS) for hydrogen at high pressures, which provide the fundamental relationship among pressure, temperature, and density in the compressible regime. In practical systems, compression is carried out through multi-stage compressors equipped with inter-cooling mechanisms, and a precise estimation of the mechanical work input at each stage is essential for evaluating overall system performance. The associated heat transfer processes during inter-cooling play a crucial role in reducing gas temperature and enhancing energetic efficiency, thereby mitigating mechanical stress on the compressor and limiting entropy generation throughout the cycle [19]. From a mathematical standpoint, these phenomena are described by coupled nonlinear equations linking thermodynamics, fluid mechanics, and heat transfer, offering a fertile ground for optimization and model-based control in advanced hydrogen storage technologies.

For an ideal gas, the work of isothermal compression from p_1 to p_2 is:

$$W_{\mathrm{iso}} = n\,R\,T\,\ln\left(\frac{p_2}{p_1}\right),$$

where n is the number of moles and R the universal gas constant. For adiabatic compression with heat-capacity ratio $\gamma = C_p/C_v$, the work is:

$$W_{\text{ad}} = \frac{n\,R\,T}{\gamma - 1}\left[\left(\frac{p_2}{p_1}\right)^{\frac{\gamma-1}{\gamma}} - 1\right].$$

Hydrogen, however, deviates from ideal-gas behaviour at high pressures. Real-gas effects are modelled using equations of state such as the Peng–Robinson equation of state (PR-EOS):

$$p = \frac{R\,T}{v - b} - \frac{a(T)}{v\,(v + b) + b\,(v - b)},$$

where $a(T)$ and b are species-dependent constants. For hydrogen:

$$a(T) = 0.45724\frac{R^2 T_c^2}{p_c}\,\alpha(T), \quad b = 0.07780\frac{R T_c}{p_c},$$

$$\alpha(T) = \left[1 + (0.37464 + 1.54226\,\omega - 0.26992\,\omega^2)\,(1 - \sqrt{T/T_c})\right]^2,$$

where ω is the acentric factor. This EOS allows accurate modelling of $p\!-\!v\!-\!T$ behaviour at elevated pressures.

Industrial hydrogen compression typically uses multiple stages with inter-cooling. The optimum pressure ratio per stage r for n stages can be derived by minimising work:

$$r = \left(\frac{p_{\text{final}}}{p_{\text{initial}}}\right)^{1/n}.$$

The total work for n stages is:

$$W_{\text{tot}} = n \cdot \frac{\gamma}{\gamma - 1}\,RT_0\left[\left(r^{\frac{\gamma-1}{\gamma}}\right) - 1\right].$$

This illustrates how splitting compression into stages with cooling reduces work and improves efficiency.

Both liquefaction and compression are affected by irreversibilities due to friction, non-ideal expansion, and finite-temperature heat transfer. The entropy generation rate $\dot{S}_{\text{gen}}$ can be modelled as:

$$\dot{S}_{\text{gen}} = \dot{m}\,(s_{\text{out}} - s_{\text{in}}) \; - \sum \frac{\dot{Q}}{T},$$

where $\dot{m}$ is the mass flow rate and $\dot{Q}$ the heat flux. Minimising $\dot{S}_{\text{gen}}$ is central to process optimisation.

From a modelling standpoint, the treatment of hydrogen storage processes such as liquefaction and compression requires a detailed coupling of thermodynamics, fluid dynamics, and optimisation theory. Liquefaction, in particular, involves cryogenic thermodynamics combined with regenerative heat exchange and gas expansion dynamics, where the accurate prediction of enthalpy and entropy variations is essential for system design. Compression, on the other hand, relies on equations of state (EOS) valid at high pressures, enabling the evaluation of real-gas effects and the optimisation of multi-stage compressor configurations.

Experimental and industrial data indicate that the energy demand for hydrogen liquefaction typically ranges between $\sim\, 10 - 13\,\text{kWh/kg}$, whereas compression up to 700 bar requires approximately $\sim 3-4\,\mathrm{kWh/kg}$. Mathematical models play a central role in refining both processes, reducing operational costs and maximising thermodynamic efficiency through predictive control and optimisation algorithms.

The current frontier of research increasingly relies on advanced computational methods. High-fidelity simulations based on computational fluid dynamics (CFD) allow a detailed characterisation of cryogenic heat exchangers, capturing transient heat and mass transfer phenomena that strongly influence overall performance. In parallel, nonlinear optimisation techniques are employed to enhance the efficiency of mixed-refrigerant cycles, while machine-learning-assisted surrogate models are emerging as powerful tools for the accurate prediction and control of thermodynamic properties within complex equations of state.

Together, these advanced mathematical and computational frameworks are expected to play a pivotal role in the design and optimisation of next-generation hydrogen storage and distribution systems, bridging the gap between theoretical modelling and industrial-scale implementation.

4 Hydrogen transport and the phenomenon of embrittlement in metals

Hydrogen is often referred to as the *"fuel of the future"*, but its transport and storage raise unique scientific and engineering challenges. Chief among these is the phenomenon of hydrogen embrittlement (HE), a process by which metals lose ductility and fracture prematurely in the presence of hydrogen. This section examines the physics, mathematics, and engineering of hydrogen embrittlement, with emphasis on fracture mechanics, historical case studies, and numerical simulation approaches.

Hydrogen can be transported through several technological pathways that differ in physical state, infrastructure requirements, and energy efficiency. In its simplest form, hydrogen is conveyed as a *compressed gas* at pressures reaching up to 70 MPa, a method well-suited for short- to medium-distance distribution and refueling applications. Alternatively, it may be transported as *liquefied hydrogen* (LH_2) at cryogenic temperatures of approximately 20 K, which allows for significantly higher volumetric energy density but requires advanced insulation and boil-off management systems to minimize losses. A third option involves the use of *chemical or infrastructural carriers*, where hydrogen is delivered either directly through dedicated pipelines in its gaseous form or indirectly via hydrogen-rich compounds such as ammonia or metal hydrides. Each of these transport modalities presents distinct thermodynamic, economic, and safety considerations, and their relative feasibility depends strongly on the intended scale, distance, and integration within broader energy networks.

Pipelines remain the most economically attractive option for large-scale transport. However, when hydrogen diffuses into pipeline steel or other metallic infrastructures, mechanical properties can be severely altered.

Hydrogen embrittlement is the process by which hydrogen atoms infiltrate metallic lattices and induce premature material failure under stress. The general manifestation is a loss of ductility, fracture toughness, and fatigue resistance. As one authoritative review puts it: *Hydrogen embrittlement (HE) corresponds to the abrupt degradation of mechanical properties of materials in the presence of hydrogen* [27].

Let us denote by σ_c the critical stress leading to fracture in the presence of hydrogen, and by σ_0 the critical stress in its absence. One may define a *hydrogen-induced reduction factor*:

$$R_H = \frac{\sigma_c}{\sigma_0}, \qquad 0 < R_H < 1,$$

where values closer to zero represent severe embrittlement.

Several mechanisms have been proposed in the literature to explain the phenomenon of hydrogen embrittlement, each highlighting a different aspect of the interaction between hydrogen and metallic microstructures. One widely discussed hypothesis is the *hydrogen-enhanced localized plasticity* (HELP) mechanism, according to which the presence of hydrogen lowers the energy barrier for dislocation motion, thereby facilitating localized slip and promoting heterogeneous plastic deformation. A second explanation, known as *hydrogen-enhanced decohesion* (HEDE), suggests that hydrogen reduces the cohesive strength between atomic planes and at grain boundaries, ultimately weakening interfacial bonds and promoting crack initiation and propagation. Finally, the *hydrogen-induced phase transformation* (HIPT) mechanism postulates that hydrogen stabilizes brittle hydride phases that can nucleate under mechanical stress, leading to loss of ductility and premature fracture. Although these models are not mutually exclusive, their relative contribution depends strongly on the microstructural characteristics of the alloy, the stress state, and the environmental conditions under which hydrogen absorption occurs. The interplay of these mechanisms depends on material microstructure, hydrogen concentration, temperature, and applied stress state [6].

Hydrogen transport within a metallic lattice is generally modelled by diffusion equations. Consider Fick's second law:

$$\frac{\partial C}{\partial t} = D\nabla^2 C,$$

where:

- $C(\mathbf{x}, t)$ is the hydrogen concentration at point $\mathbf{x}$ and time t,
- D is the diffusion coefficient, which depends on temperature and stress state.

In the presence of hydrostatic stress σ_h, diffusion can be stress-driven, as expressed by:

$$\frac{\partial C}{\partial t} = \nabla \cdot \left[D\nabla C - \frac{D\,V_H\,C}{R\,T}\,\nabla\sigma_h \right],$$

where V_H is the partial molar volume of hydrogen, R is the gas constant, and T is temperature. This term couples mechanical loading with hydrogen transport [7].

Hydrogen embrittlement has been implicated in numerous catastrophic failures of steel pipelines, pressure vessels, and structural components, underscoring its significance as both a scientific and engineering challenge. Historical case studies provide essential context for the development and validation of mathematical and physical models describing hydrogen-induced degradation.

One of the earliest documented events occurred in the mid-1960 s with the failure of sections of high-pressure natural-gas pipelines in Kansas, USA. These transcontinental pipelines suffered sudden and brittle ruptures, and subsequent metallurgical investigations revealed that dissolved hydrogen–originating primarily from cathodic protection and welding processes–had accelerated crack propagation. The fracture surfaces exhibited intergranular morphology, characteristic of hydrogen-induced cracking, providing early empirical support for the emerging theories of hydrogen embrittlement.

A second major episode was reported in Europe during the early 1980 s, when experimental high-pressure hydrogen pipelines constructed in France and Germany for early hydrogen-economy research began to exhibit unexpected fatigue cracks. These failures prompted the first systematic applications of fracture-mechanics principles to hydrogen-affected materials and ultimately contributed to important revisions in pipeline design standards, including updates to ASME and ISO codes aimed at mitigating hydrogen-related risks.

Further insights came from Japan in the 1990 s, during the rapid development of liquid-hydrogen infrastructure to support both aerospace and energy applications. Instances of cracking in cryogenic storage tanks and associated distribution pipelines revealed the critical interplay among low temperatures, high pressures, and hydrogen diffusion kinetics. These observations confirmed that hydrogen embrittlement is not confined to a single temperature or pressure regime but arises from a complex coupling between mechanical stress, material microstructure, and environmental exposure. Together, these case histories illustrate the progressive understanding of hydrogen-induced failure and the continuing need for integrated mathematical, thermodynamic, and materials-science models to predict and prevent such phenomena in modern hydrogen systems. These cases underline the urgency of rigorous mathematical models for predicting failure. Let us denote by J_H the hydrogen flux:

$$J_H = -D\nabla C + \frac{D\,V_H\,C}{R\,T}\;\nabla\sigma_h,$$

which shows that both concentration-gradients and stress-gradients drive hydrogen diffusion.

The probability of fracture initiation can be modelled using a critical concentration criterion:

$$C(\mathbf{x}, t)\;\geq\;C_{\mathrm{crit}}\quad\Rightarrow\quad\text{fracture initiation},$$

where C_{crit} is the threshold hydrogen concentration for crack nucleation.

Alternatively, one may use a fracture-mechanics approach. The effective stress intensity factor K_{eff} in the presence of hydrogen is expressed as:

$$K_{\mathrm{eff}} = K_I - \alpha\,C,$$

where K_I is the applied stress intensity factor and α is a material-dependent hydrogen sensitivity coefficient. Crack propagation occurs when:

$$K_{\mathrm{eff}}\;\geq\;K_{IC,H},$$

with $K_{IC,H}$ being the hydrogen-reduced fracture toughness.

In reality, hydrogen does not diffuse uniformly; it is trapped at lattice defects such as dislocations, vacancies, and grain boundaries. The McNabb–Foster model extends diffusion theory by distinguishing between *lattice hydrogen* C_L and *trapped hydrogen* C_T:

$$\frac{\partial C_L}{\partial t} = D\nabla^2 C_L - k_t\,C_L + k_d\,C_T,\quad \frac{\partial C_T}{\partial t} = k_t\,C_L - k_d\,C_T,$$

where k_t and k_d are trapping and detrapping rates. This model highlights how microstructural heterogeneity governs hydrogen distribution [13].

For a hydrogen pipeline under internal pressure p, the hoop stress is:

$$\sigma_\theta = \frac{p\,r}{t},$$

where r is the inner radius and t the wall thickness. Combining this with stress-assisted diffusion leads to localized hydrogen accumulation near the inner wall.

Failure probability can be estimated using reliability models, where the hazard function $h(t)$ depends on both stress and hydrogen concentration:

$$h(t) = h_0\exp\left(\beta_1\,\sigma_\theta + \beta_2\,C\right),$$

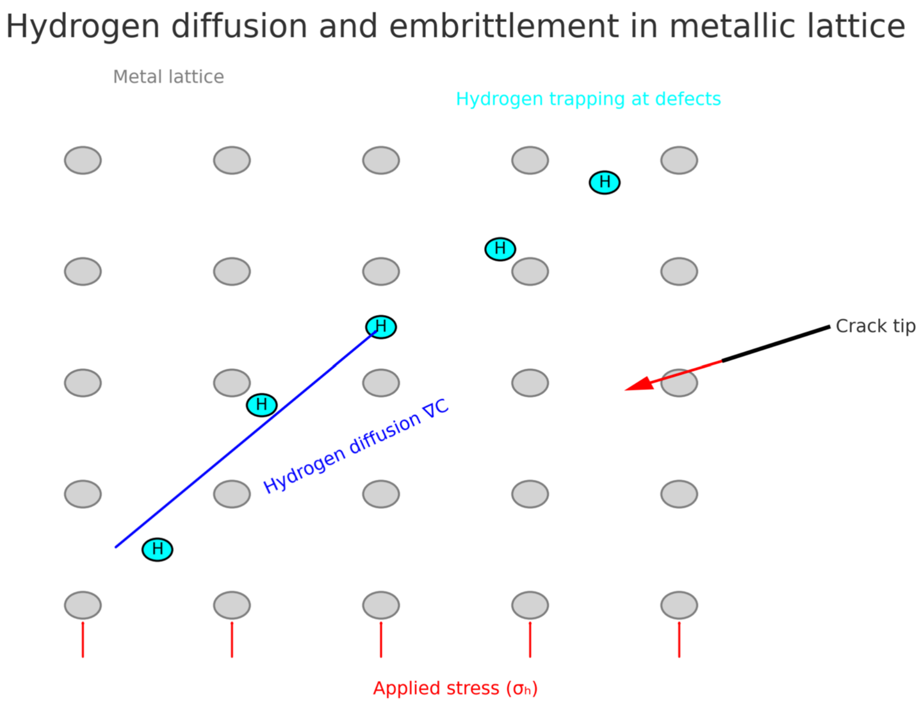

Fig. 4 Schematic representation of hydrogen diffusion and embrittlement in metallic materials. Hydrogen atoms diffuse through the metal lattice following concentration gradients (∇C) and are driven by hydrostatic stress gradients ($\nabla \sigma_h$) toward crack-tips and defect regions, where they reduce cohesion and promote brittle fracture

with β_1, β_2 material-dependent constants and h_0 the baseline hazard.

In practical transport applications, pipelines and vessels experience cyclic loading. The fatigue life N_f under a hydrogen environment can be modelled as:

$$N_f = N_0 \exp(-\gamma C),$$

where N_0 is the fatigue life without hydrogen and γ a material constant. This exponential reduction reflects the dramatic effect of hydrogen on fatigue resistance.

Several strategies have been developed to mitigate the effects of hydrogen embrittlement. Material selection plays a crucial role, with austenitic stainless steels and nickel-based alloys demonstrating significantly lower susceptibility to hydrogen-induced cracking. Surface coatings, such as palladium or ceramic layers, act as barriers that limit hydrogen ingress and reduce the risk of localized embrittlement. Careful control of operating conditions, including maintaining lower mechanical stresses and avoiding abrupt pressure transients, further contributes to mitigating damage. In addition, microstructural engineering aimed at reducing defect density and controlling grain boundaries can limit hydrogen trapping sites, thereby enhancing the overall resistance of metals to embrittlement.

Mathematically, mitigation reduces either the effective diffusion coefficient D_{eff} or the trapping term k_t in the transport equations.

Fatigue crack growth rate in air is governed by the Paris law:

$$\frac{da}{dN} = C\,(\Delta K)^m,$$

with ΔK the stress intensity range, and C, m empirical constants. In hydrogen, experimental results suggest an acceleration of crack growth. A modified Paris law is:

$$\frac{da}{dN} = C\,(\Delta K)^m\left(1 + \alpha\, c^{\beta}\right),$$

where α, β are constants capturing the embrittlement effect, and c the local hydrogen concentration.

Predicting hydrogen-assisted fracture requires solving coupled diffusion–mechanics problems. Finite element modelling (FEM) is the dominant tool. The coupled equations to be solved are:

$$\nabla\cdot\sigma + f = 0, \qquad \frac{\partial c}{\partial t} = D\nabla^2 c - \nabla\cdot\left(\frac{D\,V_H}{R\,T}\,c\,\nabla\sigma_h\right).$$

Weak-form discretisation yields:

$$\mathbf{K}_u\mathbf{u} = \mathbf{F}, \qquad \mathbf{M}_c\dot{\mathbf{c}} + \mathbf{K}_c\mathbf{c} = \mathbf{Q}(\mathbf{u}, \mathbf{c}),$$

where $\mathbf{K}_u$ is the structural stiffness matrix, $\mathbf{M}_c$ the mass matrix for diffusion, $\mathbf{K}_c$ the diffusion stiffness, and $\mathbf{Q}$ the stress-assisted diffusion term.

Recent research employs phase-field models to capture crack initiation and growth under hydrogen exposure. The free energy functional is:

$$\Psi = \int_\Omega \left(g(\phi)\,W(\varepsilon) + G_c\,\gamma(\phi, \nabla\phi) - \chi\,c\right)\,d\Omega,$$

where ϕ is the crack-phase field, $g(\phi)$ a degradation function, and G_c the fracture toughness. The preceding analysis has highlighted the multifaceted nature of hydrogen embrittlement in metallic systems, combining diffusion physics, fracture mechanics, numerical modelling, and mitigation strategies. Now, we provide a synthesis of these insights and outline design guidelines for hydrogen transport infrastructures such as pipelines, storage tanks, and pressure vessels.

Hydrogen embrittlement is governed by the coupled processes of diffusion and stress-assisted trapping, together with fracture-mechanics mechanisms that dictate crack growth. The general diffusion equation with stress coupling is:

$$\frac{\partial C}{\partial t} = D\nabla^2 C - \nabla\cdot\left(\frac{D\,V_H}{R\,T}\,C\,\nabla\sigma_h\right),$$

where C is the hydrogen concentration, D the diffusion coefficient, V_H the partial molar volume, R the gas constant, T the absolute temperature, and σ_h the hydrostatic stress. This equation couples the transport of hydrogen with stress fields, explaining why crack-tips and plastically-deformed zones act as strong sinks for hydrogen.

Fracture mechanics provides the quantitative criterion for failure. The effective stress intensity factor under hydrogen influence is:

$$K_{\text{eff}} = K_I - \Delta K_H(C,\, t),$$

where K_I is the applied mode I stress intensity and ΔK_H represents the hydrogen-induced reduction in fracture resistance. Empirical studies show that ΔK_H increases with local hydrogen concentration and exposure time [7].

The Paris law for fatigue crack growth is modified in hydrogen environments as:

$$\frac{da}{dN} = C_H \, (\Delta K)^m,$$

with $C_H > C_0$, the coefficient in inert environments, reflecting hydrogen's acceleration of crack growth rates [6].

Historical pipeline failures reveal recurring characteristics in the mechanisms of hydrogen-induced damage. Cracks typically initiate at welds or at inclusions, where stress concentrations coincide with maximal hydrogen accumulation. The onset of failure is often delayed, underscoring the significance of time-dependent diffusion processes. Furthermore, environmental factors such as pressure cycling and temperature fluctuations exacerbate crack propagation, highlighting the complex interplay between material, hydrogen, and operating conditions. These observations reinforce the predictive value of models that couple hydrogen diffusion with fracture mechanics and fatigue analysis.

Finite element (FE) modelling of coupled diffusion–stress problems has matured into a robust tool for predicting embrittlement. For instance, the weak formulation solved by FE codes reads:

$$\int_\Omega \frac{\partial C}{\partial t} \, w \, d\Omega \; + \; \int_\Omega D \, \nabla C \cdot \nabla w \, d\Omega \; - \; \int_\Omega \frac{D \, V_H}{R \, T} \, C \, \nabla \sigma_h \cdot \nabla w \, d\Omega \; = \; 0,$$

for all weighting functions w. Numerical simulations allow parametric studies of pressure levels, load-cycles, and alloy microstructures, yielding safety factors beyond analytical limits.

From the integration of theoretical analysis, numerical simulation, and empirical field data, several design principles for hydrogen transport systems become evident. Material selection should prioritise steels with proven resistance to hydrogen embrittlement, favouring tempered martensitic or ferritic steels with low hydrogen diffusivity. Microstructural control through appropriate heat treatments can reduce trap densities and minimise the presence of susceptible phases, such as retained austenite. The application of diffusion-resistant coatings, including nickel, palladium, or multilayer ceramics, serves to slow hydrogen ingress. Welding protocols must minimise hydrogen introduction, utilising low-hydrogen consumables and post-weld heat treatments, while stress concentrators should be minimised through careful design that avoids sharp corners and ensures smooth weld transitions. Continuous inspection and monitoring, employing in-situ hydrogen sensors and acoustic-emission techniques, provide early detection of crack initiation. Finally, finite-element-based simulations coupling hydrogen diffusion and fracture mechanics should be incorporated as part of the certification process for new pipeline designs.

Thus, the effective design of hydrogen transport infrastructure requires a holistic framework that integrates models for diffusion–stress coupling to predict local hydrogen concentrations, fracture-mechanics criteria, including J-integral and Paris-law adaptations, to quantify crack initiation and propagation, numerical simulation as a verification tool, and empirical validation through case studies and accelerated testing.

Future research must focus on multiscale models bridging atomistic simulations of hydrogen–lattice interactions with continuum-scale fracture mechanics, thus enabling predictive and safe design for the coming hydrogen economy.

5 Ammonia as a chemical hydrogen carrier

Ammonia represents a compelling chemical carrier for hydrogen, with well-established production and transport technologies. Mathematical models integrating thermodynamics, reaction kinetics and transport phenomena allow rigorous evaluation of energy efficiency and system design. While challenges remain–particularly in decomposition kinetics, toxicity, environmental impact, and industrial production cost–advanced catalysts and integrated engineering designs provide viable pathways for ammonia-based hydrogen distribution [12, 44].

The key reaction for hydrogen release is the decomposition of ammonia:

$$2\,\mathrm{NH_3} \;\rightarrow\; \mathrm{N_2} + 3\,\mathrm{H_2}, \quad \Delta H_r^\circ = 92.4\ \mathrm{kJ/mol}. \tag{1}$$

This endothermic reaction governs the thermodynamic feasibility of ammonia as a hydrogen carrier.

The rate of hydrogen release from ammonia is typically modeled using Arrhenius-type kinetics:

$$\frac{dC_{\mathrm{NH_3}}}{dt} = -k(T)\, C_{\mathrm{NH_3}}^n, \quad k(T) = A\exp\Big(-\tfrac{E_a}{RT}\Big), \tag{2}$$

where $C_{\mathrm{NH_3}}$ is the ammonia concentration, n is the reaction order, A is the pre-exponential factor, E_a is the activation energy, R is the universal gas constant, and T is absolute temperature [36].

Catalysts (e.g. Ru, Ni or Co-based) significantly enhance the decomposition rate, reducing the required operating temperature and reactor volume [22, 36].

Consider a continuous reactor decomposing ammonia at a molar flow rate $F_{\mathrm{NH_3}}^{\mathrm{in}}$. The mass balance is:

$$\frac{dF_{\mathrm{NH_3}}}{dz} = -\, r_{\mathrm{NH_3}}(T,\, C_{\mathrm{NH_3}}), \tag{3}$$

where $r_{\mathrm{NH_3}}$ is the local reaction rate per unit reactor length z. The corresponding hydrogen production rate is:

$$F_{\mathrm{H_2}}(z) = \frac{3}{2}\Big(F_{\mathrm{NH_3}}^{\mathrm{in}} - F_{\mathrm{NH_3}}(z)\Big). \tag{4}$$

The energy balance within the reactor, including the endothermic decomposition and heat supply, is:

$$\rho\, C_p \frac{dT}{dz} = Q_{\mathrm{supplied}} - \Delta H_r\, r_{\mathrm{NH_3}}(T,\, C_{\mathrm{NH_3}}), \tag{5}$$

where ρ is the gas density, C_p the specific heat, and Q_{supplied} the heat flux from external sources or embedded heaters.

Ammonia can be stored and transported as a liquid under moderate pressures, offering a volumetric energy density superior to compressed hydrogen gas:

$$\rho_{E,\mathrm{NH_3}} = \rho_{\mathrm{NH_3}} \times \mathrm{wt\%\,H} \times LHV_{\mathrm{H_2}} \approx 9.5\ \mathrm{MJ/L}, \tag{6}$$

where $LHV_{\mathrm{H_2}} = 120\ \mathrm{MJ/kg}$ is the lower heating value of hydrogen.

For pipeline transport, the flow of liquid ammonia is governed by the Navier–Stokes equations:

$$\nabla\cdot\mathbf{v} = 0, \tag{7}$$

$$\rho\,(\mathbf{v}\cdot\nabla)\,\mathbf{v} = -\nabla p + \mu\nabla^2\mathbf{v} + \mathbf{f}, \tag{8}$$

with $\mathbf{v}$ the velocity field, p the pressure, μ the dynamic viscosity, and $\mathbf{f}$ body forces. Temperature and pressure must be maintained to prevent vaporization and maintain laminar or turbulent flow regimes within design specifications.

The overall energy efficiency of using ammonia as a hydrogen carrier is:

$$\eta = \frac{E_{H_2,\,\text{recovered}}}{E_{NH_3,\,\text{synthesis}} + E_{\text{transport}} + E_{\text{cracking}}}. \tag{9}$$

Each term must account for energy losses during synthesis (Haber–Bosch process), liquefaction or compression, transport, and catalytic decomposition [35].

Interestingly, despite the relative simplicity of the NH_3 molecule and the wide production in nature by animal metabolism, producing ammonia industrially remains energy-intensive and expensive. The Haber–Bosch process requires high pressures (150–250 bar) and temperatures (400–500 °C), consuming large amounts of energy, typically sourced from fossil fuels, which increases both cost and carbon footprint [21].

In contrast, biological systems, such as nitrogen-fixing bacteria, can synthesise ammonia under ambient conditions with remarkable efficiency, using enzyme-mediated pathways that operate at room temperature and atmospheric pressure. This stark contrast underlines the counterintuitive nature of using ammonia as a hydrogen carrier: while chemically feasible, the energy cost of industrial production may offset the advantages of transport and storage efficiency. Consequently, any large-scale application must carefully balance the energy input for synthesis against the recovered hydrogen energy to ensure net efficiency and sustainability.

This explains why, despite its clear advantages, the use of ammonia as a hydrogen carrier still faces several significant challenges. The energy-intensive synthesis via the Haber–Bosch process requires high temperatures and pressures, which result in a substantial CO_2 footprint unless the hydrogen employed is renewable [21]. The decomposition kinetics of ammonia necessitate the use of catalysts and elevated temperatures in the range of 400–600 °C [22]. Additionally, storage and transport demand careful containment due to ammonia's toxicity and corrosiveness, as it can permeate seals and pipelines. Finally, environmental concerns arise from the potential formation of nitrogen oxides during combustion or incomplete cracking, which must be minimised to ensure safe and sustainable operation.

Consider now a system linking ammonia production, transport and hydrogen recovery. The overall mass and energy balance can be expressed as:

$$\frac{dF_{\text{NH}_3}}{dt} = -\, r_{\text{NH}_3}(T,\, C_{\text{NH}_3}), \tag{10}$$

$$\frac{dF_{\text{H}_2}}{dt} = \frac{3}{2}\, r_{\text{NH}_3}(T,\, C_{\text{NH}_3}), \tag{11}$$

$$\frac{dE_{\text{sys}}}{dt} = -\,\Delta H_r\, r_{\text{NH}_3}(T,\, C_{\text{NH}_3}) + Q_{\text{input}} - Q_{\text{loss}}, \tag{12}$$

where E_{sys} is the total energy within the system and Q_{input}, Q_{loss} are heat supplied and losses, respectively.

Coupled numerical simulations solve these differential equations under operational constraints, including reactor dimensions, flow rates, catalyst loading and thermal management. Optimization techniques determine the best combination of pressure, temperature, and residence time to maximise hydrogen yield while minimising energy consumption.

In summary, ammonia stands out as one of the most promising and technically mature chemical hydrogen carriers among the conventional options. Its high hydrogen density, well-established production and handling infrastructure, and compatibility with existing transport systems make it an attractive candidate for large-scale deployment [21, 35].

Nevertheless, despite these clear advantages, the pathway toward a fully efficient and economically viable ammonia-based hydrogen economy remains challenging. The energy penalties associated with synthesis, cracking, and purification, together with safety and environmental constraints, still hinder its competitiveness against alternative carriers and direct hydrogen use. Therefore, while ammonia represents perhaps the most promising of the traditional hydrogen carriers, the technology has yet to achieve the industrial and economic maturity required for widespread implementation. Continued advances in catalyst design, process integration, and renewable-energy-driven synthesis are essential to unlock its full potential in the global hydrogen transition. [24]

Another possibility is represented by Hydrogen peroxide that is not a hydrogen carrier in the conventional sense, since it does not release H_2, yet it can function as a liquid *energy vector* through controlled decomposition or electrochemical conversion. From a thermochemical perspective, hydrogen peroxide decomposes exothermically according to

$$2,\, H_2O_2(l) \rightarrow 2,\, H_2O(l) + O_2(g), \tag{13}$$

and, using standard enthalpies of formation from NIST and ATcT [4, 31], the reaction enthalpy is

$$\Delta H^\circ \approx -196.9\ \mathrm{kJ} \quad (\approx -98.5\ \mathrm{kJ/mol}\ H_2O_2), \tag{14}$$

corresponding to roughly 2.9 MJ/kg. Unlike ammonia, therefore, hydrogen peroxide releases heat rather than requiring it for activation, although its gravimetric energy density remains significantly lower than that of NH_3 or H_2. A distinctive feature of H_2O_2 is its dual redox character, since it can act both as oxidant and reductant, enabling direct hydrogen peroxide fuel cells (DHPFCs) [30]. In such systems the anodic and cathodic half-reactions are given by

$$\text{Anode:}\quad H_2O_2 \rightarrow O_2 + 2H^+ + 2e^-,\ \text{Cathode:}\qquad H_2O_2 + 2H^+ + 2e^- \rightarrow 2H_2O, \tag{15}$$

with a theoretical open-circuit voltage of approximately 1.09 V. Recent research has focused on the electrochemical synthesis of H_2O_2 via the two-electron oxygen reduction reaction ($2e^-$-ORR) under mild conditions [41], potentially enabling distributed production powered by renewable electricity. From the standpoint of safety and storage, hydrogen peroxide is chemically reactive and susceptible to catalytic decomposition; industrial bulk storage guidelines, which typically limit concentrations to solutions $\leq$ 70 wt.%, emphasize strict material compatibility and thermal management requirements [11]. Consequently, whereas ammonia poses primarily toxicological challenges, hydrogen peroxide presents a different risk profile associated with instability and oxidative hazards. In conclusion, ammonia remains one of the most technically mature chemical hydrogen carriers, supported by well-established synthesis, storage, and transport infrastructures, although it is constrained by the high energy demand of the Haber–Bosch process and the thermal requirements of catalytic cracking. Hydrogen peroxide, by contrast, should be regarded as an exothermic liquid energy vector rather than a true hydrogen carrier: it enables innovative electrochemical architectures and mild-condition synthesis pathways, yet it offers lower energy density and stricter stability constraints. From a systems-engineering perspective, ammonia appears more suitable for large-scale hydrogen logistics, while hydrogen peroxide may occupy niche roles in distributed or hybrid electrochemical systems. Rigorous thermodynamic modeling, kinetic analysis, and integrated energy-balance optimization remain essential to determine which vector–ammonia, hydrogen peroxide, or alternative compounds–is most appropriate under specific operational, economic, and environmental constraints.

6 Solid-state hydrogen storage: focus on palladium

Solid-state hydrogen storage represents a promising approach for safe, compact and high-density hydrogen containment. Among various metal hydrides, palladium (Pd) exhibits unique absorption characteristics, high reversibility and ease of hydrogen dissociation, making it a prototypical material for hydrogen-storage studies [16, 29]. This section explores the thermodynamics, kinetics, mechanical behaviour, numerical simulations and engineering applications of palladium-based hydrogen-storage systems, with rigorous mathematical modelling.

Palladium can absorb up to approximately 0.6 hydrogen atoms per Pd atom under ambient conditions, forming PdH_x hydrides. The hydrogen-absorption mechanism involves surface dissociation, lattice diffusion and formation of solid-solution and hydride phases. The general reaction is:

$$\mathrm{Pd} + \frac{\mathrm{x}}{2}\mathrm{H_2} \rightleftharpoons \mathrm{PdH_x}\,, \tag{16}$$

where x is the hydrogen-to-metal ratio [16].

The equilibrium between hydrogen gas and palladium hydride is described by the Van't Hoff equation:

$$\ln P_{H_2} = -\frac{\Delta H}{RT} + \frac{\Delta S}{R}\,, \tag{17}$$

where P_{H_2} is the equilibrium hydrogen pressure, ΔH is the enthalpy change of hydride formation, ΔS is the entropy change, R the universal gas constant and T the absolute temperature [42].

The plateau region in the pressure-composition isotherms (PCI) reflects the coexistence of the α (solid-solution) and β (hydride) phases. The hydrogen capacity is maximised in the β phase, whereas absorption/desorption hysteresis occurs due to lattice strain and phase-boundary effects [20].

Also the hydrogen diffusion in palladium is governed by Fick's laws. For a spherical Pd particle of radius R, the diffusion equation is:

$$\frac{\partial C}{\partial t} = D\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right)\right), \tag{18}$$

where $C(r, t)$ is the hydrogen concentration, D is the diffusion coefficient and r is the radial coordinate.

The diffusion coefficient D depends on concentration and temperature, typically expressed as:

$$D(C, T) = D_0 \exp\!\left(-\tfrac{E_a}{RT}\right) f(C), \tag{19}$$

where D_0 is a pre-exponential factor, E_a is the activation energy, and $f(C)$ captures the concentration dependence due to lattice occupancy and phase interactions [14].

Very important in the process is the hydride formation that involves coupled chemical potential and phase equilibrium. The chemical potential of hydrogen in the metal lattice is:

$$\mu_H = \mu_H^0 + RT\,\ln a_H, \tag{20}$$

where a_H is the activity of hydrogen, linked to hydrogen concentration via non-ideal solution models [29].

The Gibbs free energy for a two-phase system is minimised to predict equilibrium compositions:

$$G = (1-\theta)\,G_\alpha + \theta\,G_\beta, \tag{21}$$

$\Delta H = 30\,\mathrm{kJ/mol}$

$\Delta S = 90\,\mathrm{J/(mol{\cdot}K)}$

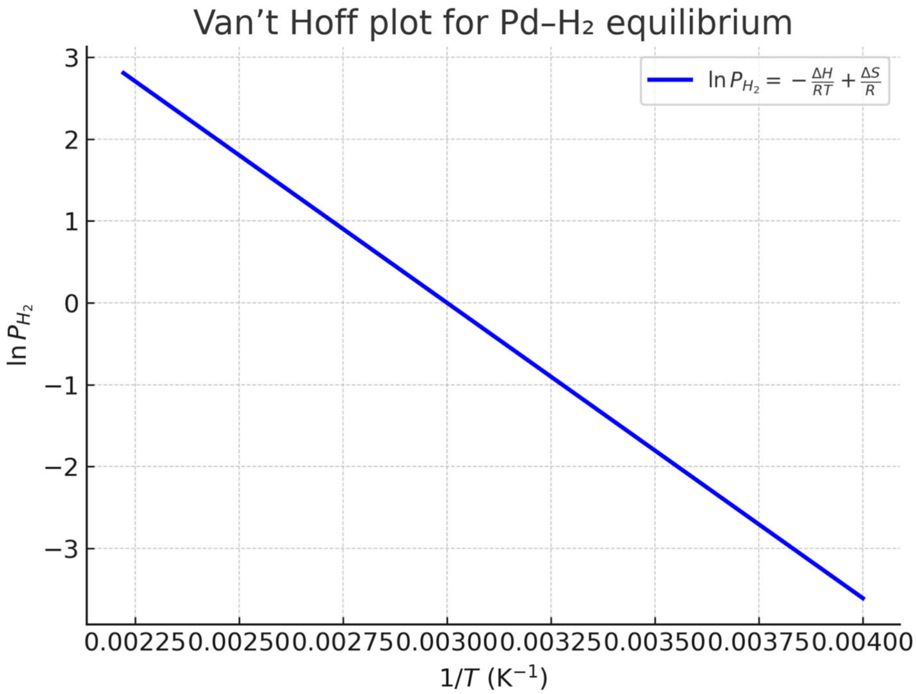

Fig. 5 Van't Hoff plot for the Pd–H_2 system. The slope yields the enthalpy of hydride formation (e.g. $\Delta H \approx$ 30 kJ/mol), and the intercept provides the entropy term (e.g. $\Delta S \approx 90$ J/(mol K)). Experimental data typically show near-linear behaviour within this temperature range (250–450 K)

with θ the fraction of hydride phase. Mechanical stress due to lattice expansion introduces additional energy terms:

$$G_{\text{total}} = G + \frac{1}{2}\int_V \sigma_{ij}\,\varepsilon_{ij}\,\mathrm{d}V, \tag{22}$$

where σ_{ij} and ε_{ij} are the stress and strain tensors, accounting for volumetric expansion of PdH_x [14].

Hydrogen absorption induces volumetric expansion ($\Delta V/V \approx 10\%$), generating stress within the metal lattice. The diffusion–stress coupling is described by:

$$\frac{\partial C}{\partial t} = \nabla\cdot\left(D\,\nabla C - \frac{D\,\Omega}{R\,T}\,C\,\nabla\sigma_h\right), \tag{23}$$

where Ω is the partial molar volume of hydrogen and σ_h is the hydrostatic stress. High stresses can lead to dislocations, embrittlement or cracking, limiting reversibility [14].

Consider a 1 mm radius Pd sphere absorbing hydrogen at 300 K. Using $D = 1\times10^{-9}$ m^2/s and $\Delta H_r = 30$ kJ/mol, numerical integration yields a saturation time of $\approx 1000s$ and a

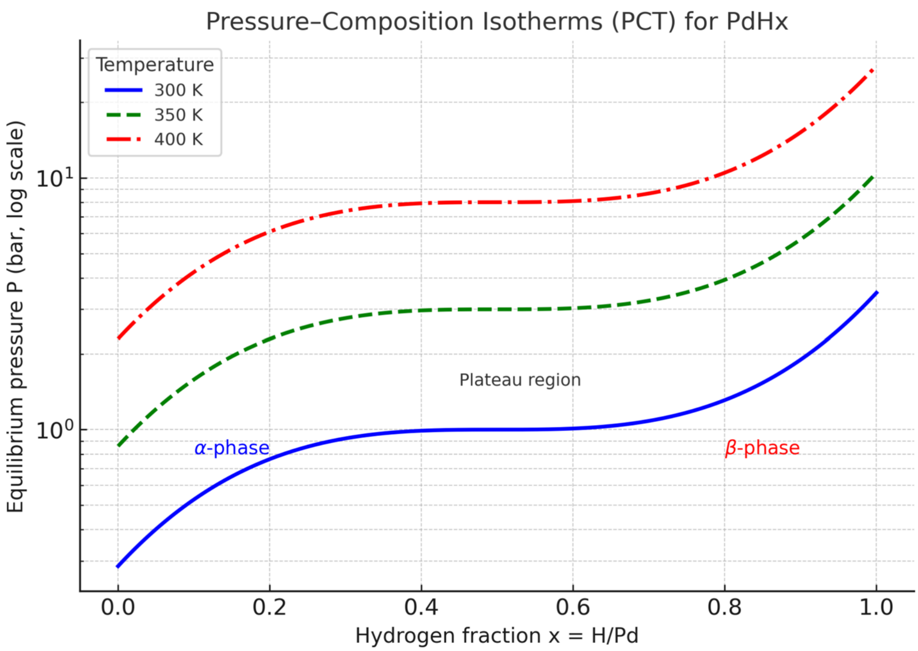

Fig. 6 Pressure–composition isotherms (PCT) for PdH_x at 300 K, 350 K and 400 K. The plateau region corresponds to the coexistence of the α (solid solution) and β (hydride) phases. The plateau pressure increases with temperature, consistent with the Van't Hoff relationship

surface hydrogen concentration approaching the equilibrium value given by the Van't Hoff relation. Stress analysis indicates a peak hydrostatic stress of $\approx$ 0MPa near the particle surface during the plateau region.

The PCT curves characterise storage capacity under varying conditions. For a given temperature, the equilibrium pressure P is derived from the Van't Hoff equation and phase fraction θ:

$$P(T,\theta) = P_0 \exp\left(-\frac{\Delta H}{RT} + \frac{\Delta S}{R}\right) f(\theta), \tag{24}$$

where $f(\theta)$ accounts for non-ideal interactions. Plotting P vs $x = \text{H/Pd}$ provides the plateau pressure and hysteresis insights.

During repeated absorption/desorption cycles, heat removal/addition is critical. The transient energy balance for a Pd bed of volume V is:

$$\rho C_p \frac{dT}{dt} = Q_{\text{in}} - k A \frac{\Delta T}{L} + \Delta H_r \frac{dC}{dt}, \tag{25}$$

where Q_{in} is external heat input, A is surface area, L characteristic length and ΔT temperature difference. Efficient heat exchange prevents localised overheating and capacity loss.

The use of palladium for hydrogen storage presents several notable advantages. Palladium offers a high volumetric hydrogen density compared to gaseous storage and allows for reversible absorption and desorption at moderate pressures. Its thermodynamics are well characterised, supported by extensive experimental data, while the kinetics of hydrogen uptake and release are predictable and can be controlled through temperature and particle size.

However, several limitations must also be considered. The high cost of palladium restricts its large-scale application [14], and repeated lattice expansion can lead to mechanical degradation [14]. Furthermore, kinetic limitations arise at low temperatures in the absence of catalysts [42], and thermal management during absorption/desorption cycles requires additional energy input.

Consequently, engineering design of palladium-based hydrogen storage systems necessitates optimisation of particle size and porosity to enhance diffusion rates, the alloying of palladium with other metals such as silver or gold to reduce cost and improve mechanical stability [3], and the implementation of efficient heat-exchange systems to manage the enthalpy of absorption and desorption. Integration with fuel cells ensures a continuous hydrogen supply.

In conclusion, palladium-based solid-state hydrogen storage remains a benchmark system combining high reversibility and compactness. Coupled numerical simulations, pressure-composition-temperature (PCT) modelling, and stress analysis enable design optimisation and predictive performance evaluation. Future research on palladium alloys, nanoscale morphologies, and hybrid hydride systems aims to enhance storage capacity, reduce costs, and improve long-term stability, positioning solid-state hydrogen storage as a viable component of the emerging hydrogen economy.

7 Mathematical models for absorption and desorption processes

Let us now examine the mathematical framework governing hydrogen absorption and desorption phenomena. The coupled mass, heat, and momentum transport processes underlying hydrogen uptake and release in storage media can be represented by comprehensive mathematical models. A representative energy balance is given by:

$$\rho\, C_p \frac{\partial T}{\partial t} \;=\; k\, \nabla^2 T \;+\; (-\Delta H)\; R_H(C_H, T), \tag{26}$$

where ρ is the density, C_p the specific heat, k the thermal conductivity, and ΔH the reaction enthalpy of absorption or desorption. The term $R_H(C_H, T)$ denotes the local reaction rate of hydrogen uptake or release. This type of equation is widely adopted in studies of metal-hydride hydrogen storage systems. [17, 33]

Coupling mass and energy balances enables prediction of transient temperature and concentration fields during absorption/desorption cycles, and thus is essential for design and optimisation of hydrogen storage systems.

In hydride systems and other hydrogen-carrier materials, PCT curves (Pressure-Composition-Time) characterize the storage behaviour. A simplified kinetic model for the hydrogen fraction $x = C_H / C_{\max}$ evolves according to:

$$\frac{dx}{dt} = k(T)\left[\, x_{\text{eq}}(P, T) - x \,\right], \tag{27}$$

where $x_{\text{eq}}(P, T)$ denotes the equilibrium hydrogen fraction determined by thermodynamics. This first-order dynamical equation can be solved numerically to represent the time-dependent loading or unloading of hydrogen in the storage media [26].

In solid-state hydrogen storage materials, lattice expansion associated with hydride formation induces mechanical stress, which in turn can influence diffusion and reaction kinetics. The diffusion equation may be modified accordingly as:

$$\frac{\partial C_H}{\partial t} = \nabla \cdot \left(D\, \nabla C_H \;-\; \frac{D\, \Omega}{R\, T}\, C_H\, \nabla \sigma_h \right), \tag{28}$$

where D is the diffusion coefficient, Ω the partial molar volume of hydrogen in the host, and σ_h the hydrostatic stress. Finite element modelling of such coupled diffusion-stress fields has been applied in recent years [2].

Finite difference, finite volume and finite element methods are commonly used to solve this kind of coupled diffusion–reaction–energy equations. Implicit time-stepping schemes are often preferred for stability in stiff systems. For instance:

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\,\frac{C_{i+1}^{n+1} - 2\,C_i^{n+1} + C_{i-1}^{n+1}}{(\Delta r)^2} \;+\; R_H(C_i^{n+1}, T_i^{n+1}), \tag{29}$$

and simultaneously:

$$T_i^{n+1} = T_i^n \;+\; \frac{\Delta t}{\rho\, C_p}\left(k\,\frac{T_{i+1}^{n+1} - 2\,T_i^{n+1} + T_{i-1}^{n+1}}{(\Delta r)^2} \;-\; \Delta H\, R_H(C_i^{n+1}, T_i^{n+1})\right). \tag{30}$$

These methods allow the tracking of spatial and temporal evolutions of both concentration and temperature fields in hydrogen-storage media [17].

As a specific example, consider the absorption of hydrogen into a spherical palladium hydride particle of radius $R = 1$ mm at $T = 300$ K, with $D = 1 \times 10^{-9}$ m^2/s and $\Delta H = 30$ kJ/mol. Using the coupled diffusion–reaction model described above, numerical integration can yield the saturation time, hydrogen concentration profiles, surface fluxes and the associated temperature rise. A stress analysis based on the diffusion–stress coupling equation can predict the maximum hydrostatic stress and identify potential regions of mechanical failure.

Absorption and desorption processes are intrinsically multi-scale, ranging from atomic-level site occupancy and chemical potentials, through mesoscale diffusion and phase-transformation phenomena, up to macroscopic system behaviour of storage tanks and heat-management systems. The hierarchical coupling can be represented schematically:

$$\mu_H^{\text{atomistic}} \;\rightarrow\; R_H(C_H, T) \;\rightarrow\; \frac{\partial C_H}{\partial t} \;\rightarrow\; \text{system-scale } P\!-\!T\!-\!x \text{ evolution.} \tag{31}$$

Recent reviews highlight the importance of integrating atomistic, mesoscopic and continuum models for accurate predictions [2].

The approach based on mathematical models offers several significant strengths. These models provide predictive capability that supports the optimisation of hydrogen storage system design, while also enhancing quantitative understanding of the underlying kinetics, diffusion processes, and thermal effects. Furthermore, such models are versatile, being applicable across solid, liquid, and gaseous hydrogen carrier systems.

Nevertheless, important limitations exist. Accurate predictions depend critically on precise material parameters, such as the diffusion coefficient D, reaction rate constants k, and enthalpy changes ΔH, all of which can vary substantially with system conditions. Full-scale three-dimensional coupled models are often computationally demanding, which can limit their applicability in real-time or operational contexts. Additionally, simplifying assumptions, such as isothermal behaviour, ideal activities, or homogeneous media, may reduce model fidelity when applied under extreme or highly heterogeneous conditions.

Summarising, mathematical modelling of absorption and desorption processes integrates diffusion, reaction kinetics, thermodynamics and stress effects into unified frameworks. Numerical simulations enable prediction of transient behaviour, optimisation of storage media and design of practical hydrogen-storage systems. Coupled models, validated against experimental data, are essential for advancing efficient, safe and scalable hydrogen storage technologies.

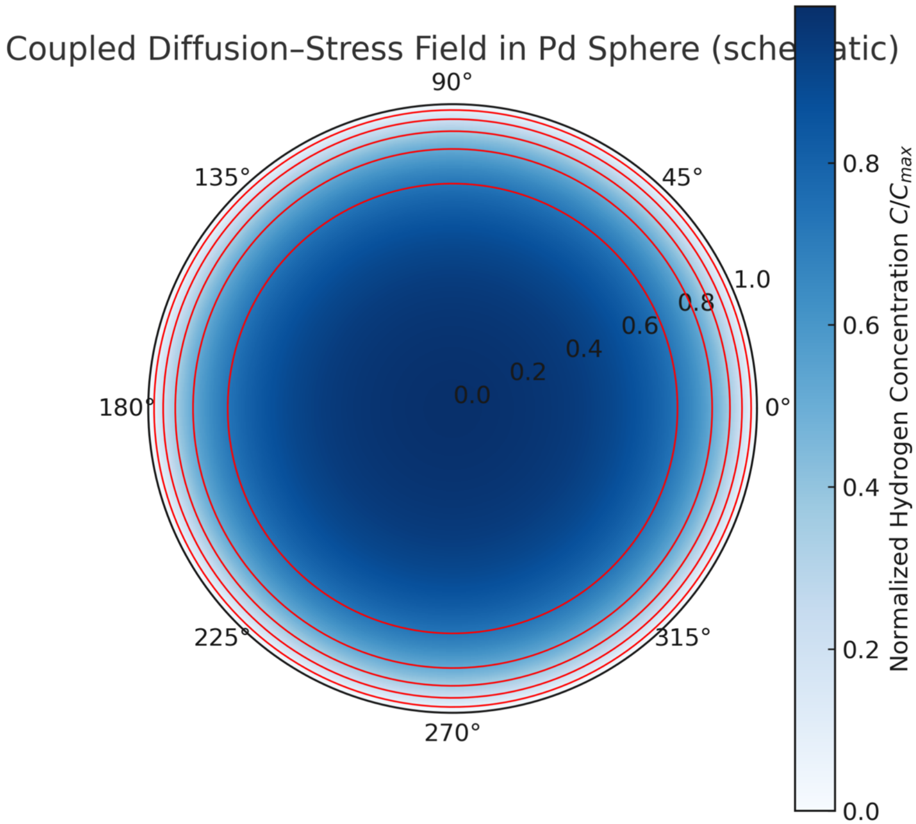

Fig. 7 Coupled diffusion–stress field in a Pd sphere during hydrogen absorption (schematic). The color map represents the normalized hydrogen concentration (C/C_{max}), while red contour lines indicate hydrostatic stress levels (σ_h). The highest stress occurs near the outer surface where hydrogen accumulation and lattice expansion are greatest

8 Concluding remarks on the future of hydrogen research in the energy transition

The transition to a sustainable energy system demands the rigorous integration of multiple technological pathways, among which hydrogen occupies a central role as a flexible and clean energy carrier. The preceding sections have examined the physical, chemical and engineering aspects of hydrogen storage and transport, emphasising the challenges associated with gaseous, liquid and solid-state systems. In this concluding section, we synthesise these insights, highlight the indispensable role of mathematics in designing and predicting hydrogen systems, and discuss why we believe that metal-based storage, particularly with palladium, represents one of the most promising avenues for the future.

Hydrogen has emerged as a key enabler of decarbonisation across multiple sectors–including transport, industry and grid balancing. Its versatility lies in its ability to be produced from renewable electricity via water electrolysis, stored, and then reconverted into energy using fuel cells or controlled combustion:

$$2\,H_2 + O_2 \;\rightarrow\; 2\,H_2O + \text{Energy}. \tag{32}$$

However, the realisation of a hydrogen-based energy infrastructure faces several technical and economic challenges–especially in storage, transport and large-scale delivery.

Mathematics serves as the backbone for understanding and optimising hydrogen systems. The absorption and desorption processes, transport phenomena, thermal management and stress evolution can all be described by rigorous differential equations. For instance, the generalised diffusion–reaction equation for solid-state storage reads:

$$\frac{\partial C_H}{\partial t} = \nabla\cdot\left(D\,\nabla C_H - \frac{D\,\Omega}{R\,T}\,C_H\,\nabla\sigma_h\right) + R_H(C_H, T), \tag{33}$$

where all terms capture coupled physics including concentration gradients, stress effects and reaction kinetics. Numerical solutions of these equations using finite element or finite difference methods enable predictive modelling and system design.

Similarly, thermodynamic constraints are captured via Van't Hoff relationships, PCT isotherms, and chemical-potential formulations:

$$\ln P_{H_2} = -\frac{\Delta H}{R\,T} + \frac{\Delta S}{R}. \tag{34}$$

These mathematical frameworks allow us to forecast equilibrium pressures, reaction rates and temperature dependencies, providing a quantitative basis for the selection and optimisation of storage materials.

Among the myriad of hydrogen-storage strategies, metal hydrides–and specifically palladium-based systems–present distinct advantages. Palladium's ability to reversibly absorb hydrogen, forming PdH_x, with well-characterised thermodynamics and kinetics, renders it a prime candidate for efficient storage [25, 43]. The benefits include high volumetric density, intrinsic safety and compatibility with existing fuel-cell systems. The challenges–material cost, mechanical degradation and thermal management–can be systematically addressed via mathematical modelling and numerical optimisation. Alloying with other metals, nano-structuring and optimised thermal control are strategies under active research.

The multi-physics nature of hydrogen storage–including diffusion, reaction and stress–requires integrated mathematical models. For example, coupling energy and mass balances yields:

$$\rho\,C_p\frac{\partial T}{\partial t} = k\,\nabla^2 T + (-\Delta H)\,R_H(C_H, T), \tag{35}$$

$$\frac{\partial C_H}{\partial t} = \nabla\cdot\left(D\,\nabla C_H - \frac{D\,\Omega}{R\,T}\,C_H\,\nabla\sigma_h\right) + R_H(C_H, T). \tag{36}$$

Solving these coupled partial-differential equations allows the optimisation of particle size, geometry and cycle conditions to maximise hydrogen uptake while minimising stress-induced damage. Furthermore, predictive simulations can guide experimental design, reducing costly trial-and-error efforts.

Metal-based hydrogen storage systems can be integrated with renewable energy sources to buffer intermittency. For example, excess electricity from wind or solar can drive electrolysis to produce hydrogen, which is then stored in palladium-based systems. Upon demand, hydrogen is released and converted back to electricity via fuel cells:

$$\text{Renewable Electricity} \;\rightarrow\; H_2 \;\rightarrow\; \mathrm{PdH}_x \;\rightarrow\; H_2 \;\rightarrow\; \text{Fuel Cell} \;\rightarrow\; \text{Electricity}. \tag{37}$$

The predictive capability of mathematical models ensures optimal matching between storage capacity, reaction rates and energy demand [8].

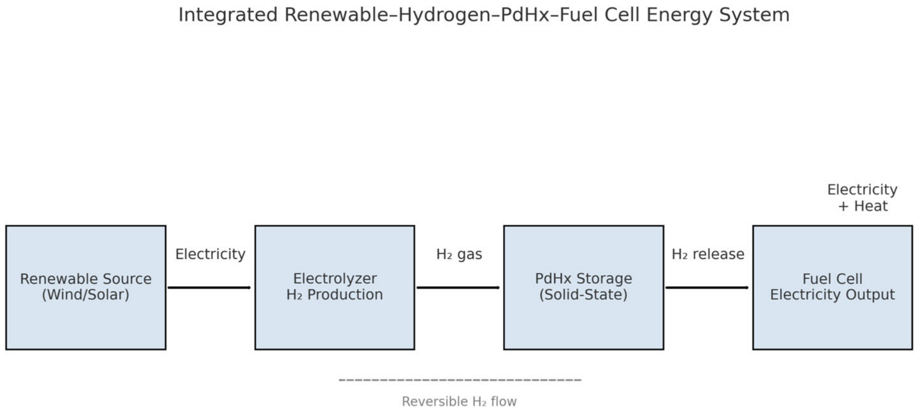

Fig. 8 Integrated renewable–hydrogen–PdH_x–fuel cell energy system. Electricity from renewable sources powers electrolysis to produce H_2, which is absorbed in a palladium-based solid-state storage system. Upon demand, hydrogen is released and converted back to electricity via fuel cells, closing the reversible energy cycle

The future of hydrogen research is increasingly focused on the integration of advanced materials innovation with rigorous mathematical modelling. Promising directions involve the development of low-cost palladium alloys to reduce economic barriers, the nano-engineering of metal hydrides to improve reaction kinetics and mitigate mechanical stress, and the advancement of multi-scale modelling approaches that bridge atomic, particle, and system scales. In parallel, the integration of hydrogen storage systems with smart grids and renewable energy sources enables dynamic operation, while life-cycle analysis coupled with thermodynamic and kinetic models facilitates optimisation of system performance.

Palladium-based storage approaches offer several advantages, including high volumetric hydrogen density, reversible absorption and desorption with inherent safety, compatibility with fuel-cell and broader energy storage systems, and predictable thermodynamics and kinetics that can be reliably modelled. Despite these strengths, significant challenges remain before large-scale industrial deployment is feasible. High material costs, particularly for pure palladium, mechanical degradation from repeated lattice expansion and contraction, thermal management requirements associated with exothermic and endothermic cycles, and scaling limitations for large energy-storage applications all constitute barriers that must be addressed (Figs. 1, 2, 3, 4, 5, 6, 7 and 8).

In conclusion, the advancement of hydrogen as an energy vector is tightly linked to both the development of advanced storage materials and the rigorous application of mathematical modelling. Palladium-based and other metal hydride systems offer a compelling combination of high density, reversibility, and safety, while predictive modelling enables optimisation, scaling, and design verification. By integrating materials science, numerical simulation, and system-level engineering, research can progress toward a hydrogen-based energy economy that is efficient, sustainable, and practically deployable.

Author Contributions The first two authors contributed to the modelling aspects of the work, while the third author assisted them in formulating the models from a mathematical perspective.

Funding Open access funding provided by Università degli Studi di Firenze within the CRUI-CARE Agreement.

Data availability No datasets were generated or analysed during the current study. The article is based on theoretical analysis, mathematical modelling, and literature review

Declarations

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

References

1. Al Ghafri, S.Z.S., et al.: Hydrogen liquefaction: a review of the fundamental physics, engineering practice and future opportunities. Energy Environ. Sci. **15**, 2690–2731 (2022)
2. Alvares, E., Sellschopp, K., Wang, B., Kang, S., Klassen, T., Wood, B.C., Heo, T.W., Jerabek, P., Pistidda, C.: Multiscale modeling of metal-hydride interphases-quantification of decoupled chemo-mechanical energies. Comput. Mater. **10**, 14 (2024)
3. Andersson, C., Zimmerman, J., Fritzsche, J., Rabkin, E., Langhammer, C.: Hydride formation pressures and kinetics in individual Pd nanoparticles with systematically varied levels of plastic deformation. Nat. Commun. **16**, 9242 (2025)
4. Active Thermochemical Tables (ATcT), version 1.118. *Hydrogen peroxide (H_2O_2): enthalpy of formation*. Argonne National Laboratory. Available at: https://atct.anl.gov/Thermochemical%20Data/version%201.118/species/?species_number=817 (accessed 2026-02-20)
5. Atkins, P.W., de Paula, J.: Atkins' Phys. Chem., 11th edn., pp. 79–82. Oxford University Press, Oxford (2018)
6. Barnoush, A., Vehoff, H.: Recent developments in the study of hydrogen embrittlement: Hydrogen effect on dislocation nucleation. Acta Materalia. **58**, 5274–5285 (2010)
7. Barrera, O., et al.: Understanding and mitigating hydrogen embrittlement of steels: a review of experimental, modelling and design progress from atomistic to continuum. J. Mater. Sci. Technol. **53**, 6251–6290 (2018)
8. Beyazit, N.I.: Comparative study of hydrogen storage and metal hydride systems: future energy storage solutions. Processes **13**, 1506 (2025). https://doi.org/10.3390/pr13051506
9. Bossel, U.: Does a hydrogen economy make sense? Proc. IEEE **94**(10), 1826–1837 (2006)
10. Cao, C., Wen, B., Fang, Y., Hou, Z., Wang, Q., Zhang, T., Huang, L., Chen, Q., Zhang, L., Zhao, Y., Lüddeke, C.T.: A comprehensive comparison of green ammonia and green methanol from a full chain: production, transportation, storage and utilization. Carbon Neutr. Syst. **1**, 8 (2025)
11. Cefic Peroxygens Sector Group, Hydrogen Peroxide Subgroup: Bulk Storage Guideline, v06, (2021). Available at: https://www.peroxygens.org/wp-content/uploads/2021/06/Peroxygens-BSGuidelines-V06.pdf (accessed 2026-02-20)
12. Chatterjee, S., Parsapur, R.K., Huang, K.W.: Huang limitations of ammonia as a hydrogen energy carrier for the transportation sector. ACS Energy Lett. **6**, 4390–4394 (2021)
13. Chen, Y.S., et al.: Hydrogen trapping and embrittlement in metals – a review. Int. J. Hydrog. Energy **136**, 789–821 (2025)
14. Das, S.S., Kopnov, G., Gerber, A.: Kinetics of the lattice response to hydrogen absorption in Thin Pd and CoPd films. Molecules **25**, 359 (2020)
15. Demirbas, A.: Future hydrogen economy and policy. Energy Sour Part B **12**(2), 172–181 (2017). https://doi.org/10.1080/15567249.2014.950394
16. Flanagan, T.B., Oates, W.A.: The palladium-hydrogen system. Annu. Rev. Mater. Sci. **21**, 269–304 (1991)

17. Gadre, S.A., Ebner, A.D., Al-Muhtaseb, S.A., Ritter, J.A.: Practical modeling of metal hydride hydrogen storage systems. Ind. Eng. Chem. Res. **42**, 1713–1722 (2003)
18. Gangloff, R.P., Somerday, B.P.: Gaseous hydrogen embrittlement of materials in energy technologies Volume 1: The problem, its characterisation and effects on particular alloy classes. Elsevier, Netherlands (2012)
19. Ghorbani, B., Zendehboudi, S., Saady, N.M.C., Duan, X., Albayati, T.M.: Strategies To improve the performance of hydrogen storage systems by liquefaction methods: a comprehensive review. ACS Omega **8**, 18358–18399 (2023)
20. Griessen, R., Strohfeldt, N., Giessen, H.: Thermodynamics of the hybrid interaction of hydrogen with palladium nanoparticles. Nature **15**, 311–317 (2016)
21. Hafiz, S.A., Zaid, Y., Waqar, A.K., Ali, F.: Sustainable pathways to ammonia: a comprehensive review of green production approaches. Clean Energy **8**, 60–72 (2024)
22. Han, T., Wei, L., Shaohua, X., Yuxi, L., Hongxing, D., Jiguang, D.: Catalyst design for ammonia decomposition: an overview. Ind, Chem Mater **3**, 311–331 (2025)
23. International Energy Agency, Global Hydrogen Review 2022, IEA Publications, Paris, (2022)
24. bin Jumah, S.: A comprehensive review of production, applications, and the path to a sustainable energy future with hydrogen. RSC Adv. **36**, 26400 (2024)
25. Klopčič, N., Grimmer, I., Winkler, F., Sartory, M., Trattner, A.: A review on metal hydride materials for hydrogen storage. J. Energy Storage **72**, 108456 (2023)
26. Larpruenrudee, P., Bennett, N.S., Luo, Z., Hossain, M.J., Haque, N., Sauret, E., Fitch, R., Islam, M.S.: A review on the overall performance of metal hydride-based hydrogen storage systems. Energies **18**, 1291 (2025)
27. Li, Q., Ghadiani, H., Jalilvand, V., Alam, T., Farhat, Z., Islam, M.A.: Hydrogen impact: a review on diffusibility, embrittlement mechanisms, and characterization. Materials **17**, 965 (2024)
28. Li, H., Niu, R., Li, W., Lu, H., Cairney, J., Chen, Y.S.: Hydrogen in pipeline steels: recent advances in characterization and embrittlement mitigation. J. Nat. Gas Sci. Eng. **105**, 104709 (2022)
29. Lischka, M., Groß, A.: Hydrogen on palladium: a model system for the interaction of atoms and molecules with metal surfaces, Technische Universität München, preprint (2002). Available at: https://www.uni-ulm.de/fileadmin/website_uni_ulm/nawi.inst.250/publications/HPd_review.pdf
30. McDonnell-Worth, C.J., MacFarlane, D.R.: Progress towards direct hydrogen peroxide fuel cells (DHPFCs) as an energy storage concept. Aust. J. Chem. **71**(10), 781–788 (2018). https://doi.org/10.1071/CH18328
31. NIST Chemistry WebBook, SRD 69. Water (H_2O): Condensed phase thermochemistry data. National Institute of Standards and Technology. Available at: https://webbook.nist.gov/cgi/cbook.cgi?ID=C7732185&Mask=2 (accessed 2026-02-20)
32. Rifkin, J.: The hydrogen economy: the creation of the worldwide energy web and the redistribution of power on earth. TarcherPerigee Editor. (2003)
33. Roubíček, T., Tomassetti, G.: Thermomechanics of hydrogen storage in metallic hydrides: modeling and analysis. arXiv preprint, (2013) arXiv:1309.3227
34. Sandia National Laboratories, Hydrogen Safety, Codes, and Standards, (2018) Edition. Available at: https://energy.sandia.gov/programs/sustainable-transportation/hydrogen/hydrogen-safety-codes-and-standards/
35. Serpell, O., Hsain, Z., Chu, A., Johnsen, W.: Ammonia's role in a net-zero hydrogen economy. The Kleinman Center for Energy Policy's 2022 report
36. Takahashi, A., Fujitani, T.: Kinetic analysis of decomposition of ammonia over nickel and ruthenium catalysts. J. Chem. Eng. Japan **49**, 22–28 (2016)
37. Tian, Y., Deng, D., Xu, L., Li, M., Chen, H., Wu, Z., Zhang, S.: Strategies for sustainable production of hydrogen peroxide via oxygen reduction reaction: from catalyst design to device setup. Nano-Micro Lett. **15**, 122 (2023). https://doi.org/10.1007/s40820-023-01067-9
38. Turner, J., Sverdrup, G., Mann, M.K., Maness, P.C., Kroposki, B., Ghirardi, M., Evans, R.J., Blake, D.: Renewable hydrogen production. Int. J. Energy Res. **32**, 379–407 (2008)
39. U.S. Department of Energy, Hydrogen Storage., Hydrogen and Fuel Cell Technologies Office, (2020) Available at: https://www.energy.gov/eere/fuelcells/hydrogen-storage
40. Yin, L., Ju, Y.: Review on the design and optimization of hydrogen liquefaction systems. Front. Chem. Sci. Eng. **14**, 530–544 (2020)
41. Yu, A., Liu, S., Yang, Y.: Recent advances in electrosynthesis of H_2O_2 via two-electron oxygen reduction reaction. Chem. Commun. **60**, 5232–5244 (2024). https://doi.org/10.1039/D4CC01476F
42. Wadell, C., Pingel, T., Olsson, E., Zorič, I., Zhadov, V.P., Langhammer, C.: Thermodynamics of hydride formation and decomposition in supported sub-10 nm Pd nanoparticles. Chem. Phys. Lett. **603**, 75–81 (2014)

43. Wang, Q., Zhang, S., Guo, J., Chen, P.: Advances in highly hydrided palladium. Front. Mater. (2024). https://doi.org/10.3389/fmats.2024.1365526
44. Zhai, L., Liub, S., Xiang, Z.: Ammonia as a carbon-free hydrogen carrier for fuel cells: a perspective. Ind. Chem. Mater. **1**, 332–342 (2023)
45. Zhang, T., Uratani, J., Huang, Y., Xu, L., Griffiths, S., Ding, Y.: Hydrogen liquefaction and storage: recent progress and perspectives. Renew. Sustain. Energy Rev. **176**, 113204 (2023)
46. Züttel, A.: Hydrogen safety and hazards, in: Hydrogen Science and Engineering, Wiley-VCH, (2020)