



A Review on Optimization and Damage Simulation in Cylinders for Green Hydrogen Storage

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Abstract

This review article addresses the optimization and damage simulation in Type III and IV composite cylinders for the safe and efficient storage of green hydrogen, a promising energy alternative. The text details the multiple failure modes that can compromise the structural integrity of these high-pressure tanks, such as manufacturing defects, hydrogen embrittlement, permeation, cracks, and delamination. To mitigate these risks, the study highlights the importance of design optimization thru advanced computational simulations, using software such as ANSYS and ABAQUS and failure criteria like Tsai-Wu and Hashin, which allow predicting the burst pressure and identifying critical points in the structure. The integration of experimental tests with these numerical simulations is, therefore, fundamental to developing lighter and more reliable cylinders, ensuring the safety of hydrogen storage systems, especially in risk scenarios such as fires.

Keywords Green hydrogen · composite pressure cylinders · Type III and Type IV vessels · numerical simulation · failure modes · Tsai-Wu and Hashin failure criteria · hydrogen storage safety

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1 Introduction

The growing demand for alternative and sustainable energy sources has positioned hydrogen as a promising fuel in a low-carbon economy. Considered a viable alternative to fossil fuels, hydrogen stands out for its abundance, high energy density, and for being a clean energy source, generating only water as a byproduct of its combustion. Its versatility allows for applications in various sectors, such as transportation, thru fuel cell vehicles, power generation in gas turbines, and industrial processes, such as ammonia production and petroleum refining [1–4]. In fuel cells, hydrogen reacts with oxygen to generate electricity, releasing only water, which represents an ideal solution for applications that prioritize sustainability and emission reduction. Despite its advantages, one of the main challenges for its widespread use is efficient and safe storage, given its low energy density. In its gaseous form at atmospheric pressure, hydrogen occupies a very large volume, making storage a critical issue. To overcome this problem, the most common approaches are storage in liquid form at cryogenic temperatures or under high pressure in a gaseous state. The storage of gaseous hydrogen at high pressure is currently one of the most viable options, as it allows for rapid loading and unloading, with low energy consumption and an excellent operating temperature range.

Currently, high-pressure hydrogen storage is the most popular method due to its low cost, maturity, and ease of use. High-pressure tanks are divided into five subfamilies [5] (Fig. 1).

Over time, different types of pressure vessels have been developed for the storage of gas under high pressure. Based on classifications from the American Society of Mechanical Engineers (ASME) and the International Organization for Standardization (ISO), these vessels were grouped into four main categories. Types I and II are metallic vessels, with Type I consisting of steel cylinders with operating pressures typically below 100–200 bar, widely used in vehicular applications [6]. Types III and IV, on the other hand, are manufactured with composite materials and have gained popularity in fuel cell electric vehicles (FCEVs). Type III is composed of an internal metallic cylinder (liner) wrapped in a layer of fiber and resin composite, while Type IV has an internal polymer cylinder with multiple layers of carbon fibers oriented in different directions [7]. A more recent alternative, Type V, has no liner and is entirely constructed of composite material. Type IV tanks are increasingly used due



Fig. 1 Different method of hydrogen storage [5]

to their excellent strength-to-weight ratio and high resistance to fatigue and corrosion, supporting pressures up to 700 bar [8, 9]. On the other hand, Type III tanks have disadvantages such as higher weight, higher manufacturing costs, and fatigue problems in the metal liner [10]. Although Type V vessels are 10–20% lighter than Type IV vessels, their development still faces challenges related to cost and limited operational pressure, currently being used mainly in aerospace applications [10].

With the expansion of the use of Type III and IV pressure vessels, concerns arise about their structural integrity. The failure of a storage system can cause severe economic losses and impact the large-scale acceptance of hydrogen. Damage to these vessels can occur due to manufacturing defects, impact, fatigue, or service conditions, and an undetected failure can lead to a catastrophic rupture [11, 12]. The main failure modes vary according to the type of vessel: for Type III, they are rupture and fatigue of the metallic liner; for Type IV, they are rupture, collapse of the polymeric liner, and hydrogen leakage [10]. The permeation of hydrogen thru the polymer in Type IV can compromise its mechanical properties, especially under rapid decompression conditions, resulting in blisters, cracks, and premature failures [13]. For Type V, rupture is also the main mode of failure. Rupture is the most dangerous behavior for vessels of types III, IV, and V, mainly caused by damage to the composite wrap [14]. Given these risks, research on damage mechanisms is essential to improve the integrity and reliability of storage systems.

The use of composite materials, such as carbon fiber reinforced polymers (CFRP), is fundamental to increasing the strength and reducing the weight of cylinders, allowing the construction of lightweight tanks with high resistance to pressure and corrosion [5]. However, its non-isotropic behavior makes the prediction of mechanical performance more complex. Impact and fatigue resistance can be a limiting factor in certain scenarios [15], and modeling the interaction between the fibers and the matrix is a challenge for failure analysis [16]. The manufacturing process is also critical, with the winding technique of the composite layers (longitudinal, circumferential, and spiral) playing a crucial role in the structural resistance of the vessel. Given the complexity of these systems, the optimization of design and manufacturing is essential. Advanced simulation techniques, such as topological optimization and fatigue analysis, show promising results for creating lighter, safer, and more efficient cylinders, identifying critical points in the structure without significantly increasing the cost [17]. Although various computational techniques are used to model and analyze Type III and IV cylinders, there is no single approach that solves all the challenges. The choice of method depends on the type of failure, the loading conditions, and the manufacturing specificities, with the combination of different approaches being common for a more robust analysis.

This article includes a survey of the literature on Type III and IV hydrogen cylinder failure modes. With a focus on the effects of high pressure and temperature on the acceleration of these processes, the study will examine the most prevalent failure causes. We'll look at the most popular structural modeling and simulation tools and the regulations governing efficiency and safety testing. Recent research on optimizing these cylinders to lower the likelihood of failures will also be examined in the review. Lastly, we will talk about how the manufacturing process affects the development of flaws, how to identify them experimentally, and how effective these methods are at averting failures.

2 Analysis of Failure Modes in Type III and IV Hydrogen Cylinders

The Table 1 summarizes the main failure modes observed in composite structures, with special emphasis on systems with liners and fiber reinforcements. Each failure mode is briefly described, highlighting the physical mechanisms involved, such as microscopic defects (voids), hydrogen ingress and diffusion (permeation and hydrogen embrittlement), delamination, cracks, interlaminar failures, impact, among others. Furthermore, the table provides bibliographic references that support each description, classified as experimental studies, numerical studies, or both. This systematization provides a comprehensive view of the critical factors affecting the structural integrity of composite materials and serves

Table 1 Failure mode

Failure mode	Description	Reference
Empty	Persistent microscopic defects that occur during the manufacturing process	[18–22] (Experimental) [23] (Numerical) [24] (Experimental/Numerical)
Bubbles	Air pockets between the liner and the wrap	[25] (Experimental/Numerical)
Hydrogen Embrittlement (HE)	Diffusion of atomic hydrogen into the metal	[26–28] (Experimental) [29] (Experimental/Numerical)
Permeation	Entry of atomic hydrogen into the material matrix	[30] (Experimental/Numerical) [31] (Numerical) [32] (Experimental)
High tension in the fiber	Amount of hydrogen that can be absorbed by the material increases	[33] (Experimental/Numerical)
Cracks	Influence on stress-strain behavior	[22] (Experimental) [34] (Numerical) [35] (Experimental/Numerical)
Delamination	Separation of composite layers	[28, 36, 37] (Experimental) [38, 39] (Experimental/Numerical)
Matrix Cracks	These cracks are caused by tensile stresses perpendicular to the fibers (or by shear stresses along the fibers).	[40, 41] (Experimental)
Fiber Breakage	Fiber breakage occurs when the applied stress exceeds the tensile strength of the fibers	[42] (Experimental) [39] (Experimental/Numerical)
Fiber/Matrix Debonding	Fiber/matrix detachment involves the separation of fibers from the surrounding matrix	[43, 44] (Experimental) [45] (Numerical)
Interlaminar shear failure	Occurs due to shear stresses between layers	[46] (Experimental/Numerical)
Environmental Damage SCC (General - Both Types)	Degradation assisted by the external environment, such as stress corrosion cracking (SCC) or other environmental effects on the structure	[47] (Experimental)
Impact Damage	Damage caused by external impact (e.g., fall, collision)	[48] (Experimental/Numerical)
Interface Failure Liner/Composite	Detachment or failure of adhesion between the liner and the composite overlay	[49] (Numerical)
Leak in BOSS structure	Hydrogen leak at the metal connection (BOSS) between the liner and the external valve	[50, 51] (Numerical)
Decompression in polymeric liners	Caused by high internal stresses	[52] (Experimental/Numerical)
Risks of spontaneous ignition and leaks	Risk of spontaneous ignition and leaks due to its flammability	[28] (Experimental)

as an important basis for design analyses, failure prevention, and the development of new materials.

The safe and efficient storage of hydrogen at high pressure is a fundamental pillar for enabling the hydrogen economy, especially in mobile applications such as fuel cell vehicles. Type III and IV tanks, which employ advanced composite materials to combine lightness and high mechanical strength, represent the forefront of this technology. However, the structural integrity of these components is susceptible to a variety of failure modes that can originate both during the manufacturing process and throughout their operational lifespan. A thorough understanding of these damage mechanisms is, therefore, indispensable to ensure the safety and reliability of storage systems. The following text presents a detailed analysis of the main degradation phenomena that affect these tanks, based on a review of recent scientific literature, addressing everything from microstructural defects, such as voids and bubbles, to macroscopic failures, such as delamination, cracks, and the effects of hydrogen embrittlement.

The safety and efficiency of hydrogen storage in high-pressure vessels, particularly Type III and Type IV composite tanks, are critically dependent on managing defects introduced during manufacturing and material interaction during service. A thorough understanding of these damage mechanisms is indispensable for design analysis and failure prevention.

In the context of hydrogen storage tanks, Voids are defined as persistent microscopic defects that occur during the manufacturing process, consisting of unfilled spaces within the composite material or at the liner interfaces [18, 20, 21]. These defects, caused by incomplete resin impregnation, inadequate fiber wettability, or suboptimal curing conditions, negatively impact the material by reducing the effective fiber volume fraction and acting as initiation points for critical failure mechanisms like interlaminar delamination and fiber-matrix interface decohesion [20, 21]. They compromise structural performance not only under static loads but also increase susceptibility to failures during dynamic operations such as rapid refueling [19].

Ueda et al. [18] conducted a systematic classification of voids in Type IV tanks, detailing their origins and causes, which is crucial for developing effective mitigation techniques. For non-destructive evaluation, Zhu et al. [21] validated the microwave technique using the reflection coefficient S_{11} , demonstrating its sensitivity to distinguishing between voids and cracks. Regarding mitigation, maintaining a high fiber volume fraction through precise control of winding parameters is essential [53], with optimized dome design and winding adjustments playing a crucial role in reducing stress concentrations and defect propagation [54]. Techniques like the *Random Vibration-Assisted Vacuum Processing (RVAVP)* [55] and improved wettability (Turner et al. [56]) are effective strategies.

The term bubbles (porosity), while sometimes used synonymously with voids, typically refers to localized gas pockets that are often transient. They form during liquid infusion due to inadequate wettability or rapid resin flow [56]. Unlike permanent voids, bubbles can be minimized through optimized processing techniques like the application of vibration or vacuum, which promote better resin flow and fiber impregnation [55]. Although both are critical, voids are more detrimental to long-term structural integrity and fatigue behavior due to their permanent nature and distribution throughout the laminate [20, 21, 53].

Hydrogen interaction with the polymeric liner of Type IV tanks leads to a critical operational failure mode: blistering and structural collapse. This phenomenon begins with the permeation of high-pressure hydrogen into the polymeric material. During subsequent rapid

depressurization, the trapped hydrogen expands, generating high internal pressures that manifest as cracks and blisters in the liner [25]. The in-depth experimental investigation by Feng et al. [25] on Type IV tanks elucidated the underlying mechanisms of blistering and the factors influencing its occurrence. The study noted that the application of adhesives at the interface does not eliminate bubble formation but may slow their propagation under load.

Voids are the most critical manufacturing defects, acting as primary initiators of failure, and their mitigation must focus on optimizing manufacturing controls like winding tension and utilizing high-sensitivity non-destructive testing (NDT). Conversely, blistering in Type IV liners is a dominant operational failure mechanism resulting from hydrogen permeation and rapid decompression, underscoring the need for selecting polymers with low diffusivity and carefully calibrating liner thickness.

The integrity of high-pressure storage tanks is fundamentally challenged by mechanisms arising from the interaction between pressurized hydrogen and the structural materials, leading to catastrophic failure potential [57, 58]. Hydrogen Embrittlement (HE) is a critical failure mode predominantly affecting the metallic liners of Type III tanks (aluminum or steel alloys). This process involves the diffusion of hydrogen atoms into the crystalline structure, causing microstructural changes that severely reduce ductility, fracture toughness, and mechanical strength, particularly under repeated loading cycles [58–60]. Studies by Chen et al. [59] and Reda et al. [60] consolidate the understanding that HE facilitates crack propagation from pre-existing microcracks, severely compromising structural integrity and necessitating leak prevention [26]. The complexity of these mechanisms intensifies under extreme operational conditions like high pressure and rapid thermal variations, which accelerate hydrogen diffusion and material deterioration [58]. Mitigation strategies involve careful material selection, surface treatments, and the application of anti-diffusion barriers [57, 60].

In parallel, Permeation is the necessary condition for hydrogen to be adsorbed, dissociate, and diffuse through both metallic and polymeric structures [61]. This atomic flow concentrates hydrogen at critical microstructural points, accelerating crack formation [62]. While permeation contributes to HE in metals, in Type IV tanks, it is crucial to the functional failure of the polymeric liner, such as the liner collapse studied by Pépin et al. [30, 62] and the blistering analyzed by Jin et al. [52]. The relationship between permeation and embrittlement is critical, as diffusion facilitates the nucleation and propagation of microcracks under cyclic loads, reducing ductility and energy absorption capacity [63]. An integrated approach combining numerical modeling, experimental tests, and microstructural research is vital for developing safer tanks, requiring strict control over material selection and operational processes to reduce hydrogen concentration at critical points [61, 63].

Structural integrity is further threatened by macroscopic progressive damage mechanisms within the composite layers, largely dictated by stress management and environmental factors. High Stresses on Fibers, resulting from high internal pressure, are fundamental to performance. Multiscale analyses demonstrate that the progressive failure of fiber bundles and interface decohesion are determining mechanisms under high-stress conditions [20, 64]. The management of these stresses is critical for Type IV tanks, where optimization of stress trajectories and residual state control (Sapre et al. [53]) is essential for maintaining structural integrity during operational cycles. Papula et al. [65] reinforced this by improving simulation models to predict tensile failure based on fiber strength dispersion.

The appearance of Cracks in the structure is a critical safety concern. Cracks can originate from embrittlement mechanisms, stress corrosion, and thermal effects. Ham et al. [66]

highlighted that cryogenic temperatures can lead to embrittlement of the epoxy matrix and weakening of the fiber-resin interface, resulting in cracks and delamination. Furthermore, *delayed cracking* is associated with localized phase transformations, such as the austenite-to-martensite transformation in some steels, which accelerates crack propagation under the action of hydrogen [67]. Operational dynamics, particularly rapid filling, induce thermal shocks and residual stresses that increase the potential for microcrack nucleation [68].

Delamination represents a progressive separation of composite layers, often initiated by microscopic defects or high interface stresses generated by differences in thermal expansion coefficients and cyclic loads [69, 70]. Concurrently, Matrix Cracks are initiated by local stress concentrations under high pressure and thermal variations [71]. Studies using criteria like Puck and finite element models demonstrate that the propagation of these microcracks is highly dependent on interface quality and stress distribution [72]. Nimdum et al. [24] also pointed out that gaps at the composite-metal interface can cause localized bending and non-linear behavior during pressurization.

Numerical analysis and computational modeling are indispensable for understanding and mitigating these complex failure modes. Finite Element Methods (FEM) coupled with hydrogen diffusion simulations allow for accurate estimation of stress intensity factors and the critical area for crack evolution [73, 74].

- **Progressive Damage Models (PDM):** Ge dt al. [23] developed a 3D PDM using ABAQUS to simulate void-induced damage, enabling accurate estimates of the rupture pressure. This approach is supported by Zhang et al. [29], who advocate for numerical simulation to predict failure propagation.
- **Multiscale and Criterion-Based Modeling:** Lin et al. [39] combined micromechanical modeling, the Puck failure criterion, and FEM with a UDSLFD subroutine for progressive damage analysis in Type III vessels, achieving high accuracy in burst pressure prediction ($\sim 5\%$ error). Moskvichev [34] employed a numerical model incorporating elasto-plastic effects to analyze stress states and crack propagation in metallic liners.
- **Manufacturing Heterogeneity:** Harada et al. [36] addressed the non-homogeneity in fiber packing by using the Weibull distribution to quantify variations and predict rupture pressures in Type III vessels.
- **Interface Optimization:** Motaharinejad et al. [37] highlighted the importance of controlling the polymer-metal interface in Type IV cylinders, although their method was primarily experimental.

Ensuring the structural integrity of Type III and IV tanks is a multifaceted challenge. The most reliable strategy lies in the integration of advanced computational tools, particularly multi-scale modeling frameworks that incorporate Progressive Damage Modeling (PDM) through constitutive approaches such as the Puck criterion, validated by experimental characterization. This validation must explicitly account for microstructural defects (e.g., voids) and environmental influences (HE exposure, cryogenic effects). Such an integrated approach is essential to address the inherent complexities of composite anisotropy and to accurately predict long-term durability and safety under operational conditions.

The damage processes and influencing factors of various forms of failure are shown in Fig. 2 [75].

3 Simulation

Table 2 provides a detailed overview of the programs used in the simulation and evaluation of Type III and IV hydrogen storage cylinders. The table organizes each program according to its application area—from structural simulation and materials modeling to computational fluid dynamics (CFD) and failure analysis. Each item provides a description of the purpose of the program and the types of analysis it supports, along with related bibliographic references. This collection of information is a useful resource for researchers and engineers choosing the appropriate tools for modeling, optimization, and evaluation of composite pressure vessels under various environmental and loading conditions.

The structural and operational reliability of Type III and IV hydrogen storage tanks is increasingly assessed and optimized through advanced numerical simulation, significantly reducing the reliance on costly and time-consuming experimental testing. This modeling encompasses Finite Element Analysis (FEA) for structural integrity, Computational Fluid Dynamics (CFD) for thermomechanical behavior during operation, and hybrid approaches for design optimization.

FEA, primarily using software like ABAQUS and ANSYS, is fundamental for predicting rupture pressure and identifying critical failure modes.

- ABAQUS-Centric Studies:** Li et al. [93] employed high-fidelity ABAQUS models and Hashin criteria (via USDFLD subroutines) to simulate failure in Type IV domes. Hu et al. [95] used ABAQUS with UMAT subroutines to implement a progressive damage model, validating localized dome reinforcement (DR) to shift the failure mode to a safer pattern and achieve mass reduction. Similarly, Nebe et al. [97] utilized ABAQUS and the CompDam progressive damage model, achieving excellent agreement with experimental data from DIC and acoustic emission, with failure initiating in the matrix/

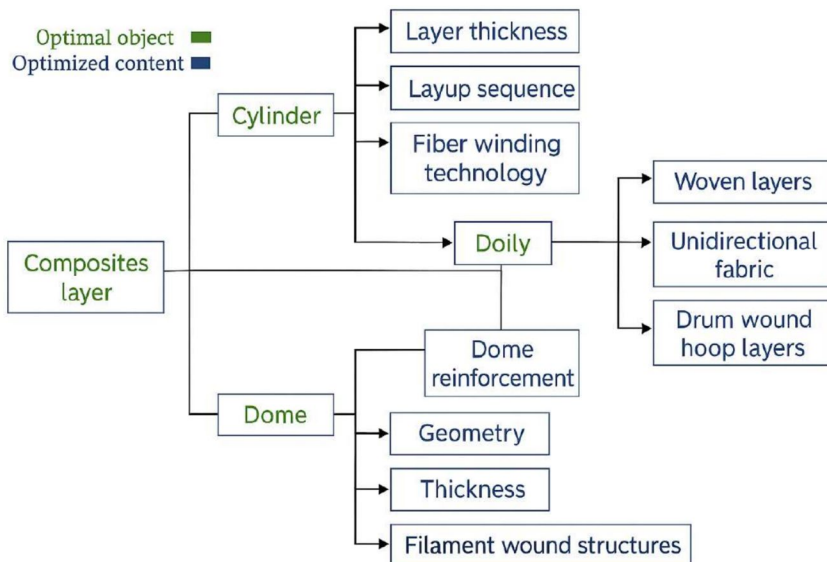


Fig. 2 Three aspects of failure analysis: burst pressure, fatigue failure and impact failure [75]

Table 2 Software tools for hydrogen cylinder (Type III/IV) simulation and analysis

Software	Software Description (in context of application)	Reference
Ansys APDL	ANSYS APDL is a structural simulation tool with parametric language and high analytical control.	Type III and IV [76] Type III [34, 77–79]
Ansys ACP	Modeling of multilayer composite materials with different winding angles. Calculation of failure factor (IRF) to predict failures by delamination, fiber and matrix rupture.	Type III and IV [80, 81] Type III [82] Type IV [83, 84] Type V [85]
SolidWorks	Create 3D CAD models of pressure vessels.	Type I, III and IV [80] Type IV [86]
FreeFlyer	Determine temperature variations that vessels face in space.	Type I, III and IV [80]
LS-DYNA	Explicit simulation of compressive loading and damage evolution.	Type IV [87, 88] Type III [35]
LS-OPT	Parametric optimization software used for calibration of constitutive models and sensitivity analysis coupled to LS-DYNA.	Type III [35]
Matlab	Post-processing tools for result analysis.	Type III and IV [76] [89] Type III [35, 90, 91]
Abaqus	Performs high-fidelity finite element simulations, modeling stress distribution and failures.	Type IV [30, 92–101] Type III [33, 39, 102–112] Type III and IV [113–115]
Ansys Fluent	CFD simulation tool to model thermal and fluid dynamic behavior.	Type III [116–119] Type IV [120, 121] Type III and IV [122–125]
Ansys material designer	Used to perform homogenization of composite material properties with different fiber volume fractions (FVF).	Type III [33]
Static Structural	Stress and strain simulation	Type III [82] Type IV [86] [83]
OpenFOAM	Free open-source computational fluid dynamics (CFD) software	Type III and IV [126] Type IV [127]
FLACS	For hydrogen dispersion and explosion simulation	Type III and IV [89]
Ansys CFX	Computational Fluid Dynamics (CFD) software	Type III and IV [128] Type III [129, 130]
Gasflow	Software that uses numerical methods to analyze the behavior of moving gases	Type III [130]
ZEBULON	Advanced finite element analysis (FEA) software	Type IV [24]
COMSOL	Used to model and simulate physical phenomena and processes in various engineering and science fields	Type III [131]

delamination and culminating in fiber rupture in the cylindrical region. Lin et al. [39] applied a multiscale approach combined with the Puck criterion in ABAQUS, achieving an average error of only 5% in predicting Type III burst pressure. Hu et al. [96] also employed ABAQUS with UMAT for Type IV vessels, demonstrating the impact of lay-up sequences on stress concentration, porosity, and rupture resistance.

- ANSYS and Multi-Criterion Analysis:** Studies utilizing ANSYS Workbench, often with the Composite PrepPost (ACP) module, focus on structural performance and material comparisons. Sharma and Neogi [38] used ANSYS (ACP) to validate their analytical model for optimizing Type IV composite thickness, applying multiple failure criteria (Tsai-Wu, Hashin, etc.). Siddiqui et al. [86] used ANSYS Structural to evaluate different fiber materials (Kevlar, S-glass, T700) for Type IV cylinders, concluding Kevlar offered the best performance. Sharma et al. [82] and Chethan Kumar et al. [81] employed ANSYS Static Structural and ACP to predict burst pressure and evaluate structural de-

formation in both Type III and IV tanks, validating results against analytical models and standards. Kang et al. [76] found, using ANSYS, that failure begins with matrix cracking in spiral layers and progresses to brittle fracture of hoop fibers in the critical cylindrical region.

- **Impact and Dynamic Loading:** Wen et al. [35] used LS-DYNA with the GISSMO ductile damage model and a submodeling technique to accurately predict damage evolution in Type III metallic liners under localized compressive loads, identifying that critical damage begins on the inner face where the stress state is predominantly tensile. Weerts et al. [87] also used LS-DYNA, employing thick shell elements and cohesive zones, to predict the mechanical behavior and failure modes of Type IV cylinders under impact conditions.

Simulation tools are heavily leveraged for design optimization and assessing long-term performance:

- **Hybrid Optimization:** Li et al. [93] proposed a hybrid approach combining FEA (ABAQUS) with Artificial Neural Networks (ANN). By generating a large simulation database, they trained the ANN to efficiently predict damage, resulting in significant optimization of winding parameters that increased the experimental rupture pressure from 1450 bar to 1570 bar.
- **Manufacturing Process Control:** Błachut et al. [33] combined ABAQUS/ANSYS with experiments to show that increasing fiber tension during filament winding significantly increases fiber volume fraction (45% to 63%) and gravimetric efficiency (up to 6%) in Type III tanks, despite introducing new failure risks.
- **Fatigue Life Prediction:** Zhang et al. [103] used a coupled ABAQUS Fe-safe approach with the modified Brown-Miller criterion to estimate the fatigue life of the Type III aluminum liner under cyclic loading, identifying optimal lay-up sequences to maximize durability by controlling alternating stresses. Shrivastava et al. [104] used Abaqus and linear elastic fracture mechanics (LEFM) to predict crack propagation life in Type III metallic liners, demonstrating that the autofrettage process and optimal stacking sequences can extend the lifespan to over 6000 cycles.
- **Material Selection and Standards Compliance:** Saha et al. [94] used ABAQUS axisymmetric shell models to evaluate burst pressure for Type IV cylinders with various natural and synthetic fiber combinations. Sharma et al. [83] employed ANSYS to simulate standardized tests (ISO 11439), incorporating thermal degradation and the Hashin criterion to predict structural performance under extreme operating conditions.

CFD simulations, primarily using ANSYS Fluent and OpenFOAM, are essential for assessing critical thermal behavior during fast refueling and external fire scenarios.

- **Rapid Refueling Analysis:** Monteiro et al. [122] used ANSYS Fluent to simulate the fast filling process, finding that Type IV tanks reach higher internal temperatures due to the low thermal conductivity of the polymer liner, which can compromise system integrity. Li et al. [123] also used ANSYS Fluent for transient modeling, validating their results with experimental data and demonstrating that pre-cooling and flow control are effective strategies to mitigate thermal peaks and ensure structural safety (Wu et al.

[117]). Gonin et al. [126] used OpenFOAM to capture complex phenomena like thermal stratification and hot spots in Type III and IV tanks, providing a basis for optimizing filling protocols.

- **Extreme Environment Modeling:** Reda et al. [80] presented a detailed analysis of Type I, III, and IV vessels for space environments, concluding that Type IV is the most advantageous in terms of lightness and structural integrity under absolute vacuum and severe thermal variations. Molkov et al. [124] used ANSYS Fluent (LES approach) to simulate the rupture of tanks in fire scenarios, demonstrating that hydrogen combustion significantly amplifies the resulting shock wave pressure, highlighting the critical role of thermal failure modes.
- **Discharge Dynamics:** Kim et al. [118] and [116] used ANSYS Fluent to model hydrogen discharge, confirming that the Redlich-Kwong gas model coupled with the SST turbulence model is most reliable for predicting non-ideal gas behavior and critical temperature drops (down to -235°C), which can induce structural risks in the metal liner of Type III tanks via differential thermal contraction.

The systematic application of these advanced numerical tools—FEA for structural prediction, CFD for operational safety, and hybrid methods for optimization—is essential for the continued development of high-pressure hydrogen storage. The integration of simulation with experimental validation has proven to be an accurate and cost-effective approach for predicting critical failure modes, optimizing lay-up sequences, and ensuring compliance with stringent safety standards.

The simulation landscape is highly effective, with ABAQUS and ANSYS dominating structural FEA, often enhanced by custom subroutines (UMAT/USDFLD) for progressive damage (Hashin, Puck) and the ACP module for composites. CFD (ANSYS Fluent/OpenFOAM), using the Redlich-Kwong equation of state and SST turbulence models, is the gold standard for thermal failure analysis during rapid refueling and fire. The most promising future direction lies in the integration of these techniques with Machine Learning (e.g., ANN) to leverage large simulation databases, accelerating the optimization of critical manufacturing parameters like winding angle and fiber tension.

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High-fidelity FEA models are paramount for safe and optimized designs. Zhang et al. [98] proposed an integrated approach for a 700 bar Type IV tank, focusing on precise thickness prediction in the dome using modeling techniques like cubic spline functions to avoid accumulation during filament winding. Their ABAQUS-based simulation, which included buckling and progressive damage analysis (Tsai-Wu criterion), validated that optimal internal pressure during manufacturing (1.1 to 1.5 bar) is crucial for preventing liner buckling and achieving a high safety factor (2.5, with estimated rupture pressure of 1750 bar). Similarly, Villalonga et al. [99] designed a fully thermoplastic Type IV cylinder using Polyamide 6 (PA6) reinforced with carbon fiber, leveraging the Abaqus Wound Composite plugin

for winding architecture and stress analysis, investigating failure modes such as transverse cracks and delamination.

The complexity of structural assessment is managed through a hierarchy of models. Van der Heijden et al. [113] proposed a systematic hierarchy combining analytical, semi-analytical, and detailed 3D FE simulations in Abaqus. This approach accurately represents critical regions like the dome-cylinder transition, allowing for precise failure prediction (delamination, matrix, and fiber rupture) while balancing precision and computational cost, making it highly applicable to vehicle design stages.

CFD simulations are essential for assessing thermal safety, a critical operational failure mode. Xu et al. [127] presented a coupled numerical modeling of transient heat transfer in Type IV cylinders exposed to fire (impingement). Using the FireFOAM solver (OpenFOAM) with Large Eddy Simulation (LES), they demonstrated that cylinder failure is predominantly caused by the thermal degradation of the composite, with internal temperature sufficient to melt the polymeric liner before structural rupture. The study emphasized the non-uniformity and transience of the heat flow, highlighting that localized maximum heat flux is more critical than the average flow. For the routine operational risk, Kim et al. [120] utilized a coupled thermo-fluid-structural approach (ANSYS Fluent/Transient Thermal) to analyze rapid refueling in Type IV tanks. Their results confirmed that the filling rate and low thermal conductivity of the polymer liner can generate critical internal temperatures (above 85°C), posing a risk of liner degradation and structural compromise due to adiabatic compression. This reinforces the necessity of pre-cooling and flow control protocols.

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The designer must take into account the general characteristics, such as tank capacity, working pressure, material attributes, and safety factors. A complete design cycle of a composite hydrogen tank is illustrated in Fig. 3 [132].

4 Failure Criteria

The Table 3 shows the main failure criteria used primarily for the structural analysis of composite materials, with practical guidance on the various configuration requirements for pressurized cylinders. The potential for application to different types of structures (Types I, II, III, and IV) is demonstrated.

The structural safety assessment of high-pressure composite pressure vessels, particularly Types III and IV, requires the rigorous application of failure criteria that consider the

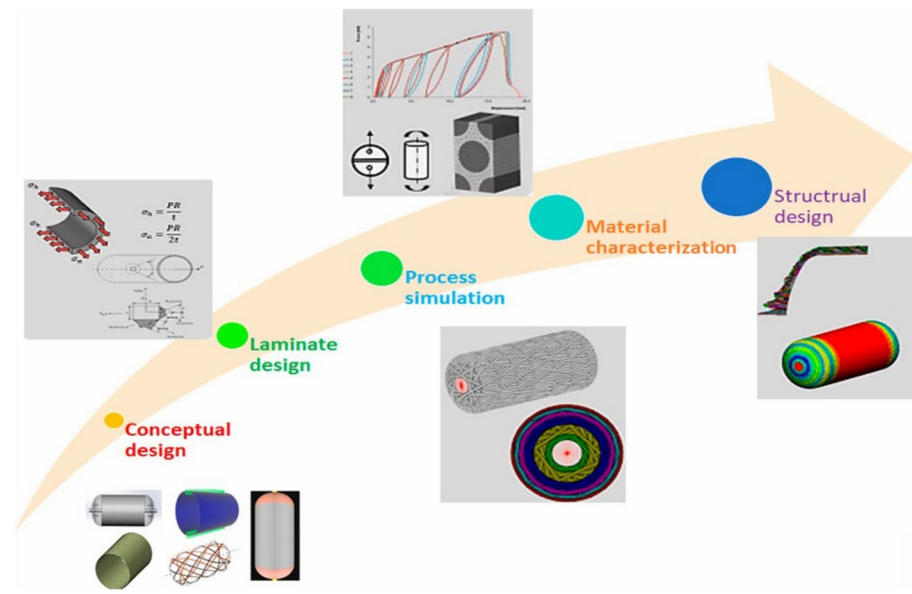


Fig. 3 Design methodology of hydrogen storage vessels [132]

anisotropic nature of the materials and the complex multiaxial stress states. The main focus lies on Progressive Damage Models (PDM), which are capable of simulating the gradual degradation of material properties up to final rupture (LPF), since the Rupture Pressure (LPF) can be more than 60% higher than the First Ply Failure Pressure (FPF) [138, 140].

The most effective criteria for PDM are those that distinguish between failure modes, decoupling the behavior of the fiber and the matrix under tension and compression. The Hashin criterion is widely validated for Type IV and Type III vessels and identifies four distinct intralaminar damage modes [93, 96]. Studies such as those by Sharma and Neogi [38] confirmed that Hashin showed the best correlation with actual hydrostatic burst tests (error less than 5%), being an essential criterion for modeling matrix failure under high-temperature conditions [83]. Similarly, the Puck criterion is recognized for its superior ability to identify the critical fracture plane, resulting in remarkable accuracy in rupture pressure prediction (error less than 0.2% when combined with the CompDam model) [97]. The implementation of these criteria in numerical simulations, such as that performed by Song Lin et al. [39] in Abaqus, often requires the development of custom subroutines (UDSLFD or UMAT) to integrate stiffness degradation based on failure modes.

For predicting First Ply Failure (FPF) and for design optimization, interactive criteria like Tsai-Wu and Tsai-Hill are widely used due to their consideration of interactions between stress components [82, 98, 134]. For example, Sharma et al. [82] indicated that the Tsai-Wu criterion showed higher correlation with experimental data, correctly identifying the failure initiation region in Type III cylinders, and the work by Takalkar et al. [137] used it to optimize the winding angle to $\pm 35^\circ$. Non-interactive criteria, such as Maximum Stress, while simple and useful for qualitative analyses [79], tend to result in overdesign of the material [138].

Table 3 Failure criteria

Model	Description	Cylinder
Tsai-Wu	A failure theory used for composite materials, especially fiber-reinforced unidirectional laminates.	Type III [79, 82, 102, 133–135] Type IV [38, 92, 98, 136, 137] Type III and IV [6, 8, 76, 138–140]
Von Mises	A model that determines when a ductile material begins to plastically deform (yield).	Type III [103, 134, 141, 142] Type IV [92, 94] Type III and IV [6, 33, 80]
Fick and Henry Laws	Describe mass transport phenomena, specifically diffusion and gas solubility in liquids, respectively.	Type IV [92]
Rankine Stress	States that material failure occurs when the maximum principal stress (tension) reaches the yield strength or ultimate strength of the material.	Type III and IV [76, 80, 139, 140] Type III [79, 133]
Inverse Reserve Factor (IRF)	Indicates the ratio between applied load and structural load capacity, showing how close the structure is to reaching its limit or failing.	Type III and IV [80]
Cohesive Zone Model (CZM)	A simulation approach for quasi-brittle fracture that represents a damage zone near the crack tip, relating tractions to displacement jumps at interfaces during crack propagation.	Type III and IV [5]
Hashin Failure Criterion	A theory used to predict failure in composite materials, distinguishing between fiber and matrix failure.	Type III and IV [5, 8, 138, 140] Type III [108–110, 133, 134, 142, 143] Type IV [38, 83, 93, 96, 144]
GISSMO Model	An incremental damage model that considers stress state to predict failure in ductile materials, especially in stamping simulations and impact analysis.	Type III [35]
Tsai-Hill	A failure theory for composite materials that considers interaction between different stress components, such as tension, compression, and shear.	Type III [79, 82, 133] Type IV [38, 137] Type III and IV [8, 138–140]
Brown-Miller Criterion	A model used to analyze failure in ductile materials, especially under complex loading conditions such as multiaxial stresses and cyclic variation.	Type III [103]
Hoffman	Mathematical models that predict when a composite material will fail under load.	Type III [79, 82, 102] Type III and IV [8, 138–140]
Puck Failure Criterion	Considers different failure modes, such as matrix or fiber fracture, and their interaction, accounting for failure plane orientation and acting stresses.	Type III [39] Type IV [97] Type III and IV [8]
Tresca Criterion	A failure criterion used to predict yielding in ductile materials.	Type III [141]

Regarding interlaminar failures (delamination), simulation requires Cohesive Zone Models (CZM) to represent the initiation and propagation of cracking between layers [5]. These models are complemented by intralaminar criteria such as Hashin, in a hybrid approach that simulates the degradation of mechanical properties through Damage Variables from Continuum Damage Mechanics (CDM), as detailed by Rafiee et al. [142].

For liners, whether metallic (Type III) or polymeric (Type IV), specialized criteria are necessary. The Von Mises criterion is widely employed for ductile materials, such as the liner's aluminum, in the evaluation of equivalent stresses and plasticization [33, 141], and is

also used to assess the resistance of polymeric liners to structural collapse [92]. For damage under dynamic loads and localized impact, the GISSMO (Generalized Incremental Stress State dependent damage Model) is highly effective, capturing material degradation under multiaxial stress states and disproportionate loadings [35]. For evaluating the fatigue life of the Type III metallic liner, the Brown-Miller equation modified by Morrow is used, which is suitable for capturing the cumulative effects of stresses in critical regions [103].

The structural integrity of polymeric liners in Type IV vessels presents unique failure modes, such as blistering due to hydrogen diffusion and rapid depressurization. The prediction of these phenomena is carried out through coupled models that combine gas diffusion laws (Fick's and Henry's) with mechanical strength criteria such as Von Mises and Tsai-Wu [92]. Furthermore, analysis in extreme environments, such as space conditions or elevated temperatures, requires the application of specialized criteria like the Inverse Reserve Factor (IRF) and consideration of changes in matrix stiffness and brittleness, which favor delamination and microcracking [80].

The reliability of simulation methodologies is reinforced by adopting a multi-criteria approach and experimental validation. Studies demonstrate that the combination of different criteria (e.g., Von Mises with the Average Shear Stress Yield - ASSY theory) can lead to discrepancies less than 8% compared to theoretical values [94]. The World-Wide Failure Exercise (WWFE) reinforced that no single theory is universally accurate, but highlighted the Puck, Hashin, and Tsai approaches as the most promising, recommending that designers combine conservative methods (like Puck) with interactive criteria (like Tsai-Wu) and actively consider residual thermal stresses and coupling with finite element tools. The critical conclusion is that the structural analysis of high-pressure hydrogen vessels requires the use of Progressive Damage Models based on mode-distinguishing criteria (Hashin and Puck), implemented with custom subroutines for PDM, and that liner safety be evaluated by specialized criteria (GISSMO, Brown-Miller, Fick's/Henry's models), ensuring the integrity of the structure under all operational conditions.

The application of precise failure criteria is essential for the structural assessment of composite pressure vessels, especially Type III and IV vessels used in high-pressure hydrogen storage. The current trend strongly favors mode-distinguishing criteria for accurate Progressive Damage Modeling (PDM), which simulates the gradual reduction of material properties following localized failure, promoting stress redistribution among intact layers. The Hashin criterion is widely recognized for its ability to distinguish between distinct tensile and compressive failure modes in both the fiber and matrix, allowing for the identification of dominant mechanisms at each loading stage [110, 143]. Han and Chang [109] demonstrated its effectiveness in Type III vessels subjected to free-fall impact (488 J), successfully predicting matrix fracture and delamination without fiber rupture, thereby reinforcing the vessel's functionality under service pressure as long as the main fibers remained uncompromised. This progressive approach, often implemented through custom subroutines based on Continuum Damage Mechanics (CDM), links stiffness degradation to the specific fracture energy of each mode, where matrix cracking is often the predominant mode due to its lower energy resistance [110].

Further refining the PDM approach, Leh et al. [144] proposed a progressive failure model based on the Hashin-Rotem criteria for Type IV vessels, capable of simulating the gradual degradation of elastic properties under load evolution. This model considers distinct failure modes—fibers, matrix, and interface—and is crucial for predicting both safe failures (in the

cylindrical section) and unsafe failures (in the caps), the latter being undesirable due to ballistic risk. Model calibration with experimental data showed good correlation with rupture tests, emphasizing the importance of parameters like longitudinal elastic modulus (E_L) and matrix damage variables (d_T) in predicting burst pressure. In the context of thermomechanical behavior, Hu et al. [143] applied Hashin's criterion to Type III cylinders under transient thermal loads, indicating that matrix failure, particularly in the outer layers exposed to heat, constitutes the primary degradation mechanism.

In multiaxial stress states, particularly for predicting rupture pressure and optimizing design, interactive criteria that account for the coupling between orthogonal stress components are essential. The Tsai-Wu criterion stands out for incorporating quadratic and linear stress interactions, offering greater accuracy in estimating the rupture pressure compared to simpler criteria like Maximum Stress, Hoffman, or Tsai-Hill, especially in three-dimensional stress states [79]. For Type III cylinder design, Mostafa et al. [135] used Tsai-Wu to identify the fiber winding angle (optimal performance around 65°) as the critical parameter determining structural integrity. Similarly, Dae-Sung Son et al. [102] utilized Tsai-Wu and Hoffman, confirming the effectiveness of considering stress interactions and showing that the transverse direction is most susceptible to failure, particularly in the dome-cylinder transition regions. Their analysis also validated that the ideal autofrettage pressure (1070 bar) ensures structural safety by preventing failures in both the aluminum liner and the composite layers through the management of residual stresses.

The complexity inherent in composite failure prediction was comprehensively highlighted by the World-Wide Failure Exercise (WWFE), a landmark initiative introduced by Hinton, Kaddour, and Soden [145]. The exercise was motivated by a lack of confidence in existing methodologies and the absence of a universal definition of failure, systematically evaluating nineteen distinct theoretical approaches across 14 multiaxial test cases. The comparative analysis revealed significant discrepancies between initial and final failure envelopes, with variations exceeding 1000% in matrix-dominated cases [146]. This enormous dispersion is largely attributed to methodological differences, such as the consideration or omission of residual thermal stresses, the adoption of micromechanical models, and post-failure degradation strategies. The study classified theories into categories, noting that interactive theories (e.g., Tsai-Wu, Cuntze, Mayes) show strong sensitivity to stress interactions.

The WWFE's quantitative assessment established that theories integrating robust progressive failure modeling and treatment of nonlinearities, such as Cuntze and Bogetti, achieved a better overall correlation with experimental evidence [147]. The four highest-ranked theories achieved predictions within 50% of experimental values in more than 75% of cases, emphasizing the critical importance of robust post-failure models to capture real laminate behavior up to final rupture. The exercise reinforced the need for continuous experimental validation to consolidate more reliable design criteria and provided crucial guidelines for designers, advocating for the integration of reliable analytical tools with computational design environments and the necessity of further research into critical areas such as post-failure modeling and thermal effects [148].

The fundamental equation for the Tsai-Wu failure criterion, applied by Jaber et al. [149] and Nachtane et al. [150] to determine the strength limit and burst pressure in hydrogen tanks, is expressed by the Eq. 1:

$$F_1\sigma_1 + F_2\sigma_2 + F_{11}\sigma_1^2 + F_{22}\sigma_2^2 + F_{66}\sigma_6^2 + 2F_{12}\sigma_1\sigma_2 = 1 \quad (1)$$

Where:

- σ_1 and σ_2 are the normal stresses in the principal axes (longitudinal and transverse to the fibers);
- σ_6 represents the in-plane shear stress;
- F_i and F_{ii} are the material strength coefficients, calculated from experimental tensile (X_t, Y_t), compressive (X_c, Y_c), and shear (S) strengths (e.g., $F_{11} = 1/(X_t X_c)$ and $F_{22} = 1/(Y_t Y_c)$);
- F_{12} is the interaction term between normal stresses, generally assumed as $F_{12} = -0.5\sqrt{F_{11}F_{22}}$ for composite materials.

Material failure is predicted at the moment the sum on the left side of the equation reaches or exceeds unity (1).

The assessment of structural integrity in composite overwrapped pressure vessels (COPVs) for hydrogen storage relies on the application of phenomenological criteria that define the material's strength envelope. Beyond interactive approaches, the Tsai-Hill Criterion is widely utilized for considering distortion energy, predicting failure when the combined stress ratio exceeds unity according to the following relationship, Eq. 2:

$$\frac{\sigma_{11}^2}{X^2} - \frac{\sigma_{11}\sigma_{22}}{X^2} + \frac{\sigma_{22}^2}{Y^2} + \frac{\sigma_{12}^2}{S^2} \geq 1 \quad (2)$$

Additionally, the Maximum Stress Criterion provides a more conservative and simplified perspective by independently evaluating whether any individual stress component exceeds the material's strength limits, as defined by Eq. 3:

$$\max\left(\frac{\sigma_{11}}{X}, \frac{\sigma_{22}}{Y}, \left|\frac{\sigma_{12}}{S}\right|\right) \geq 1 \quad (3)$$

In these formulations, σ_{11} and σ_{22} represent the normal stresses in the longitudinal and transverse axes, respectively, while σ_{12} denotes the in-plane shear stress. The parameters X , Y , and S correspond to the material's ultimate strength limits in tension/compression and shear. According to Nachtane et al. [150], the convergence of these analytical models with finite element simulations identifies that failure is frequently governed by low transverse matrix strength or high shear stresses, with the failure index (I_F) serving as the determining metric for optimizing tank wall thickness and winding angles.

Structural integrity modeling of composite pressure vessels has significantly advanced with the implementation of the Puck failure criterion, as detailed by Lin et al. [39]. Unlike global phenomenological criteria, Puck's formulation allows for a rigorous segregation between fiber failure (FF) and inter-fiber failure (IFF), the latter being based on the physics of fracture within the action plane. The exposure effort for the FF mode ($f_{E,FF}$) is governed by the following relationship:

$$f_{E,FF} = \frac{1}{\pm R_{\parallel}^{t,c}} \left[\sigma_{11} - \left(\nu_{\perp\parallel} - \nu_{\perp\parallel f} \cdot m_{of} \frac{E_{\parallel}}{E_{\parallel f}} \right) \cdot (\sigma_{22} + \sigma_{33}) \right] \quad (4)$$

where σ_{ii} represents the stress tensor components, $R_{\parallel}^{t,c}$ denotes the longitudinal tensile and compressive strengths, and the term $(\nu_{\perp\parallel} - \nu_{\parallel\perp} \cdot m_{of} \frac{E_{\parallel}}{E_{\parallel f}})$ couples the Poisson effect and the transverse stress magnification ($m_{of} = 1.1$) between the fiber and matrix. For the IFF mode ($f_{E,IFF}$), the criterion introduces slope parameters ($p_{\perp\psi}^{t,c}$) that modulate the fracture plane shear strength ($R_{\perp\psi}^A$) as a function of the acting normal stress, capturing the micro-crack closure effect under transverse compression ($\sigma_n < 0$). This multiscale approach, validated by Lin et al. [39] through computational subroutines, demonstrated superior predictive capability for the burst pressure in 35 MPa reservoirs, showing experimental agreement with an average error of only 5.4%.

In conclusion, the structural integrity of high-pressure hydrogen vessels mandates an approach that transcends simple failure prediction. The ideal methodology integrates mode-distinguishing progressive models like Hashin or the more accurate Puck criterion with interactive criteria such as Tsai-Wu for a comprehensive First Ply Failure analysis. Crucially, the model must incorporate factors identified by the WWFE and specific pressure vessel studies, including residual stresses induced by autofrettage and the effects of coupled thermal loading, thereby ensuring a reliable and safe design that accounts for the full evolution of damage up to the ultimate rupture pressure.

5 Optimization

Table 4 provides a broad overview of the main structural optimization techniques used for structural optimization of pressure vessels, highlighting the methods used, the software employed, the associated benefits, and the type of cylinder considered in each study. It should be noted that various strategies have been proposed, ranging from classic methods like the Arc-type dome transition design implemented in Abaqus to more sophisticated artificial intelligence techniques like optimization based on artificial neural networks (ANN) and modified evolutionary algorithms.

The optimization of composite pressure vessels for hydrogen storage is a multidisciplinary field that employs everything from classical analytical theories to artificial intelligence algorithms. The following studies illustrate the diversity of methodologies used to enhance the performance, safety, and cost efficiency of these critical components.

Optimization in the design of composite pressure vessels, particularly Types III and IV, is systematically classified across methodologies ranging from foundational analytical models to advanced computational intelligence, with a constant need for comparative analysis and critical evaluation. The initial phase of structural sizing relies on classical analytical methods, primarily the Netting Theory, which simplifies the structure by assuming that mechanical load resistance is provided exclusively by the reinforcement fibers, thus neglecting the matrix contribution [53, 98].¹ This method provides analytical equations for determining the thickness of helical and circumferential layers. Advancements include the use of a stress equilibrium coefficient to extend the Netting Theory to the dome section [95] and the introduction of cubic spline functions with variable polar radii to improve fiber distribution in the dome region, reducing material accumulation near the openings [98]. Although fast, the Netting Theory requires robust validation through Finite Element Analysis (FEA) to

Table 4 Summary of studies on structural optimization of hydrogen cylinders

Optimization method	Software	Advantage	Cylinder
Arc-type dome transition design method	Abaqus	Reduces stress in the transition and increases burst pressure	Type IV [151]
Double-Double (DD)	ANSYS LS-DYNA	High efficiency in explicit simulations	Type IV [6]
Constitutive parameter calibration	LS-OPT	High local accuracy with reduced computational cost	Type III [35]
Non-dominated Sorting Genetic Algorithm II	EasyPBC + ABAQUS + WOUNDSIM + Python	Time reduction via multivariate prediction and automated simulation	Type IV [152]
Multiphase (structure + manufacturing)	ANSYS + VERICUT VCP/VCS	Weight reduction, defect control	Type IV [153]
Global Search Optimization (via ANN)	Python (with custom scripts)	High efficiency in exploring solution space; avoids lengthy simulations	Type IV [93]
Netting theory	Abaqus	Estimates ideal thickness of composite layers with safety and lightness	Type IV [53, 95, 96, 98]
Parametric inverse problem	Not specified	High accuracy in reproducing experimental data; allows graphical nomogram construction for safety engineering	Type III and Type IV [154]
K-means++ with PCA	AEWin (Physical Acoustics)	Efficient damage mechanism identification; non-destructive analysis; good clustering accuracy	Type IV [155]
Modified Differential Evolution	Not specified	High accuracy, avoids local minima, easy tuning	Type III [134]

account for matrix effects, complex stress states, and thermal coupling, as demonstrated by Sapre et al. [53] whose FEA results showed a difference of less than 6% compared to experimental burst pressure data. The critical evaluation is that while the Netting Theory is an efficient initial sizing tool, it is conservative and insufficient for predicting true structural failure and damage progression.

FEA serves as the industry standard for detailed optimization, enabling the analysis of complex phenomena such as progressive damage and the influence of specific geometries. Optimization approaches based on FEA often vary the lay-up sequence or geometric param-

eters to enhance burst pressure.2 Hu et al. [96] used a Hashin-based progressive damage model (PDM) via a UMAT subroutine in ABAQUS to show that the lamination sequence can influence rupture pressure by up to 15%. Similarly, Tian et al. [151] used the Hashin criterion within a PDM to optimize the arc-type dome transition and ply-drop positioning, achieving a 16% increase in theoretical burst pressure and validating the prediction with an error of less than 4%. The Tsai-Wu criterion is also widely adopted for PDM, facilitating the identification of failure modes and the subsequent matrix stiffness degradation [98]. Beyond static analysis, dynamic explicit simulation is employed, as seen in the work by Barbosa and Gomes [6] using ANSYS LS-DYNA with the Double-Double (DD) model, which offers design flexibility and computational efficiency for structures where impact and explosion resistance are critical. The conclusion is that FEA, coupled with PDM based on mode-distinguishing criteria like Hashin or Tsai-Wu, is essential for accurate failure prediction and local optimization.

The cutting edge of optimization is represented by the integration of computational intelligence and stochastic methods, which are crucial for exploring complex design spaces and non-intuitive solutions. Evolutionary algorithms are a key class of this methodology: Ayakdaş et al. [134] utilized the Modified Differential Evolution Method (MDE) for global search to minimize the structural failure index in Type III tanks, incorporating multiple constraints such as Tsai-Wu, Hashin-Rotem, and Maximum Stress criteria.3 For multi-objective problems, Donghai Hu et al. [152] presented an advanced model combining the NSGA-II evolutionary algorithm with the TOPSIS multi-criteria evaluation technique, leading to a 32% weight reduction and a 56% cost reduction. Hybrid models, such as those combining FEA with Artificial Neural Networks (ANN), significantly increase efficiency by training the ANN to rapidly predict damage states across thousands of winding angle configurations, as demonstrated by Li et al. [93], who achieved an increase in rupture pressure from 1450 bar to 1580 bar. These advanced methods offer a robust framework for simultaneous optimization across performance, cost, and safety.

A final, critical category of optimization involves integrating structural design with manufacturing constraints and external safety factors, moving beyond purely mechanical performance. Rozova et al. [156] developed a multi-objective parametric optimization for vessels with unequal polar openings, solving the structural and weight minimization problem through the use of non-geodesic trajectories, which are vital for achieving the optimal fiber angle distribution under complex geometric requirements.4 The manufacturing feasibility is addressed by Oromiehie et al. [153], who integrated structural FEA (ANSYS/Tsai-Wu) with Automated Fiber Placement (AFP) simulation software (VERICUT) to generate precise fiber deposition paths, leading to a total weight reduction of 18%. Furthermore, optimization techniques are applied to improve the accuracy of the damage models themselves: Liu et al. [35] used LS-OPT software for the classical optimization of constitutive parameters for the GISSMO damage model, ensuring a high-fidelity representation of the Type III liner's response to impact. Safety assessment under external events is also optimized, as Kashkarov et al. [154] employed a parametric inverse problem to calibrate a physical model describing shock wave propagation from hydrogen tank rupture in fires. Finally, Meemary et al. [157] addressed Structural Health Monitoring (SHM) by using a Puck 3D-based PDM model to validate the progressive failure in instrumented composite rings, considering the effect of embedded fiber optic sensors, which is essential for developing reliable SHM strategies in high-performance composite components.5 The conclusion is that reliable design

requires a multidisciplinary optimization approach that holistically integrates structural, manufacturing, and safety requirements

6 Safety of High-Pressure Hydrogen Tanks in Fire Scenarios

The increasing adoption of hydrogen as an energy carrier in automotive and industrial applications poses significant challenges to the safety of storage systems. In particular, high-pressure hydrogen tanks are subject to severe risks in fire scenarios, which can result in catastrophic failures with significant human and material consequences. This chapter presents a comprehensive analysis of the main experimental and numerical studies on the behavior of type III and IV tanks in fire situations, focusing on structural safety, fire propagation, and emerging protection technologies.

The study of high-pressure hydrogen tanks in fire scenarios is crucial for safety engineering, focusing primarily on the failure mechanisms and consequence mitigation for Type III and Type IV composite pressure vessels. Early experimental investigations by Zalosh [158] provided detailed quantification of catastrophic events involving tanks without pressure relief devices (PRDs), establishing the benchmarks for risk assessment. Catastrophic rupture of a Type IV tank was observed after 6.5 minutes of fire exposure, resulting in a 7.7-meter fireball and fragment projection up to 80 meters. A Type III tank rupture took longer (12.3 minutes) but yielded a larger fireball (24 meters) and fragment projection exceeding 100 meters. Shock wave overpressure measurements were consistent with theoretical models, although analysis revealed that vehicle geometry affects propagation, requiring the use of virtual distances for accurate prediction. Furthermore, the study quantified the severe thermal threat, measuring radiant heat flux up to 210 kW/m^2 at 15 meters, emphasizing the necessity of effective pressure relief to prevent such explosions [158–160]. Risk quantification methodologies, such as the TNT equivalent mass method, have been validated to delineate risk zones based on overpressure, fragment range, and explosion energy [13, 154].

Experimental and numerical analyses have refined the understanding of fire response and the critical role of Thermal Pressure Relief Devices (TPRDs). Tamura et al. [161] developed an innovative propane burner to simulate localized fire scenarios, addressing the limitation of engulfing fire tests which fail to represent real-world accidents where fire may not directly impinge upon the TPRD. Comparative tests showed that localized fire can be more severe, potentially leading to rupture without device activation, a finding corroborated by Ruban et al. [162], who also noted that resistance time is not significantly different between partial and total fire exposure. Importantly, the research revealed that initial gas pressure exerts a greater influence on rupture time than the exposed fire area. Crucially, the use of a TPRD with a reduced orifice diameter (0.5 mm) was shown to prevent rupture by promoting a controlled leak, dramatically reducing the flame length from up to 18 meters to approximately 1.5 meters, thus mitigating risks and potentially reducing required safety distances [162, 163].

Numerical modeling using Computational Fluid Dynamics (CFD) has been essential in elucidating the thermal and mechanical behavior. Zheng et al. [119, 125] demonstrated that due to the low thermal conductivity of composite layers, temperature and internal pressure increases are insignificant during the initial period of fire exposure, especially when the fire is distant from the PRD. The CFD work highlighted the highly non-uniform temperature

distribution on the tank surface, peaking in the central region, which standardizes thermal sensor placement. A critical finding is that TPRD activation is primarily governed by external heat exposure rather than internal gas temperature increase. The degradation of the composite material is a key failure factor, starting with resin pyrolysis around 330°C [164], with the residual mechanical strength being strongly correlated with the thickness of the uncharred layer [165].

The analysis of failure modes indicates that internal pressure is decisive for the rupture mechanism: lower pressures tend to result in leaks, while higher pressures lead to explosive rupture [164]. Even when the TPRD activates effectively, Li et al. [166] observed that the critical failure pressure is consistently reduced compared to the cold hydraulic rupture pressure. Halm et al. [100] successfully integrated experimental tests with numerical simulations to predict the transition between failure modes (rupture to leakage) based on internal pressure and heating rate. Addressing the risks of fire propagation, Tamura et al. [167] found that the ignition of neighboring gasoline vehicles was caused by the burning of the originating vehicle's materials, not the hydrogen flame released by the TPRD, emphasizing the need for early detection and rapid extinguishing strategies, especially in confined spaces. Furthermore, Dadashzadeh et al. [89] showed that thermally unprotected tanks present a fatality risk significantly above acceptable levels, stressing the importance of increasing fire resistance time.

Advanced safety technologies, such as the validated "microleaks-no-burst" (mLNB) concept, represent a shift in mitigation strategy. This technology allows tanks without a TPRD to safely release hydrogen in a controlled manner through microleaks even under extreme fire conditions, completely eliminating the risk of explosion and fragment projection [168]. In conclusion, the body of literature demonstrates significant progress in understanding the thermal and structural failure mechanisms. The findings underscore the importance of designing tanks with optimized TPRD performance and thermal protection, which dramatically reduce risk to acceptable levels. The integration of experimental data with advanced numerical tools, such as CFD and robust failure models, allows for accurate prediction of failure modes and supports the development of technical standards and safer hydrogen storage systems.

7 Conclusion

The growing demand for sustainable energy solutions positions hydrogen as a strategic vector in the transition to a low-carbon economy. However, its large-scale adoption directly depends on the safety and efficiency of storage systems, especially high-pressure cylinders of types III and IV. This literature review highlighted that the modes of failure in these cylinders are multifactorial, involving manufacturing defects such as voids and bubbles, as well as complex mechanisms like hydrogen embrittlement, delamination, and thermal failures in fire scenarios.

The integrated analysis between numerical modeling, finite element simulations, and experimental validations proved essential for understanding the evolution of damage and proposing mitigation strategies. Failure criteria such as Hashin, Tsai-Wu, Puck, and GISSMO were widely used to predict the structural integrity of the vessels, while opti-

zation techniques—such as Netting Theory, evolutionary algorithms, and neural networks—showed great potential in improving mechanical performance and reducing costs.

Moreover, advances in safety technologies, such as thermal pressure relief systems (TPRD) and controlled micro-leakage strategies (mLNB), reinforce the importance of multidisciplinary approaches to ensure the reliability of cylinders in extreme conditions. The review also highlighted the relevance of integrating structural design and manufacturing processes, such as filament winding and automated fiber deposition, to minimize defects and maximize the durability of the tanks.

Therefore, the development of safer, lighter, and more efficient cylinders requires not only the improvement of materials and manufacturing methods but also the rigorous application of predictive models and robust failure criteria. This integrated approach is essential to enable the safe use of hydrogen as a clean energy source, promoting its acceptance in vehicular, industrial, and space applications.

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Declarations

Competing Interests The authors declare no competing interests.

Ethical Approval This study did not involve human participants or animals. All analyses were performed in accordance with accepted principles of scientific integrity and research ethics.

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