Optimizing High-Performance Metal Hydride Tanks for Electrochemical Energy Storage

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Abstract

Electrochemical energy storage is a critical area of research in the development of sustainable energy technologies, including fuel cells and energy storage systems. Among the various storage solutions, metal hydrides have emerged as promising materials due to their high capacity for storing chemical fuels, safety, and potential for reversible electrochemical cycling. However, challenges related to **thermal management** and **mechanical integrity** significantly impact on their efficiency and long-term durability.

During absorption and desorption processes, metal hydrides undergo exothermic and endothermic reactions, generating significant temperature gradients that can hinder reaction kinetics and lead to localized overheating or cooling[1]–[6]. This necessitates the optimization of heat transfer mechanisms to maintain efficient energy storage and retrieval. Furthermore, repeated absorption/desorption cycles induce volume expansion and contraction in the metal hydride material, leading to **mechanical stress accumulation, fatigue failure, and potential structural degradation** of the storage tank.

This study focuses on the **multi-physics modeling and optimization** of a metal hydride-based electrochemical storage system using **COMSOL Multiphysics**. The modeling will aim to enhance thermal management and mechanical stability over time through **time-dependent simulations**. Using numerical simulations with **finite element methods (FEM)**, the research will investigate **heat and mass transfer** within the metal hydride bed, the effects of **thermally induced stresses**, and the role of **topological lattice structures** in mitigating mechanical failure. The findings will contribute to the development of **next-generation chemical fuel storage tanks** with improved energy efficiency, higher durability, and enhanced safety over both short and long-term cycles.

Introduction

The growing demand for **sustainable and high-efficiency energy storage systems** has led to extensive research on electrochemical technologies, including solid-state storage solutions. Chemical fuel storage plays a key role in the **transition to renewable energy**, offering an alternative to fossil fuels in applications ranging from fuel cells to grid energy storage. However, the low volumetric energy density of conventional gaseous fuels presents a major challenge, requiring innovative storage solutions such as **high-pressure tanks, cryogenic liquid storage, and solid-state storage in metal hydrides**.

Among these, **metal hydrides** are of particular interest due to their ability to **store gaseous fuels at moderate pressures and temperatures** while offering a compact and safe solution compared to conventional storage methods[1], [7]. Despite these advantages, metal hydride storage systems suffer from two major limitations:

1. **Thermal Management Challenges :**
    - The absorption of stored gas in metal hydrides is an **exothermic reaction**, generating heat that can reduce reaction rates and cause localized overheating.
    - The desorption process is **endothermic**, requiring efficient heat input to sustain continuous operation.
    - Poor heat dissipation within the hydride bed can lead to **reaction inhomogeneity**, reducing overall storage performance.
2. **Mechanical Degradation and Structural Failure:**
    - Repeated **gas absorption and desorption cycles** induce **volume expansion and contraction**, leading to material fatigue and cracking.
    - Thermal cycling generates **internal stress**, which can weaken the structural integrity of the storage tank over time.
    - Sudden mechanical loads, such as **impacts, shocks, or drops**, pose safety risks that must be addressed through optimized structural design.

To overcome these challenges, **advanced multi-physics modeling** is required to study and optimize the thermomechanical behavior of metal hydride storage systems. This research will focus on :

- **heat and mass transfer simulations** using **COMSOL Multiphysics** to design efficient thermal management strategies that account for real-time changes during absorption and desorption processes.
- **Finite element analysis (FEA)** to evaluate mechanical stresses and develop fatigue-resistant storage tanks over multiple **time cycles**.
- **Topological optimization** of lattice structures to improve impact resistance, energy absorption, and overall system reliability.

By integrating **numerical modeling with experimental validation**, this study aims to contribute to the development of **next-generation electrochemical energy storage solutions**, ensuring **higher efficiency, durability, and safety** for future energy applications, with a clear focus on both **short-term performance** and **long-term sustainability**.

Methodology

The methodology for this study involves a combination of **numerical simulations**, **finite element analysis (FEA)**, and **experimental validation** to achieve optimal thermal management and mechanical stability in metal hydride-based electrochemical storage systems. The key steps of the methodology are as follows:

1. **Multi-Physics Modeling (COMSOL Multiphysics):**
    - **Heat Transfer Simulation:** Implement **time-dependent simulations** to model the heat generation, dissipation, and transfer within the metal hydride bed during hydrogen absorption and desorption.

- **Mass Transfer Simulation:** Model the movement and distribution of the stored gas within the hydride material during charge/discharge cycles.
- **Mechanical Stress Analysis:** Use FEA to analyze the stresses generated by thermal expansion and contraction of the material during absorption/desorption, as well as the mechanical impact of external forces such as shock or vibration.

2. **Finite Element Analysis (FEA):**
    - Evaluate the structural integrity of the storage tank by simulating mechanical stresses and identifying critical areas of failure due to **thermal cycling** and **repeated loading**.
    - Model **topological optimization** to enhance the lattice structure of the tank and improve its mechanical performance under dynamic conditions.
3. **Experimental Validation :**
    - Develop a small-scale prototype of the metal hydride storage tank for experimental testing.
    - Validate the numerical models by comparing the simulated thermal and mechanical behavior with the experimental data obtained from the prototype.
4. **Optimization :**
    - Perform **parametric studies** to optimize tank geometry, material properties, and thermal management systems.
    - Refine the design based on simulation results and experimental feedback to achieve the highest possible performance and safety levels.

Innovation

This study presents several **innovative aspects**:

1. **Coupled Multi-Physics Modeling:** The integration of **thermal, mechanical, and mass transfer simulations** into a unified model offers a comprehensive approach to optimizing electrochemical storage tanks. This is one of the first studies to combine **time-dependent thermal behavior** with **finite element stress analysis** in the context of metal hydride storage systems.
2. **Topological Optimization:** The **lattice structure optimization** of the storage tank is a novel approach aimed at improving energy absorption during impact and enhancing **mechanical resilience** under thermal and mechanical stresses.
3. **Experimental Validation of Advanced Models:** The combination of numerical modeling with experimental testing in real-world conditions ensures that the proposed solutions are not only theoretically sound but also practically applicable.

Scientific Challenges

The project addresses several **scientific challenges**:

1. **Thermal Non-Uniformities:** Accurately modeling **heat distribution** and managing temperature gradients in metal hydride beds during hydrogen absorption/desorption cycles.

2. **Mechanical Stress Accumulation:** Understanding how repeated cycles of **expansion and contraction** under thermal loading lead to **fatigue failure** and cracking in storage materials.
3. **Impact of External Loads:** Modeling the **response of the tank to external shocks and mechanical stress** under real-life conditions, ensuring the safety and durability of the storage system.

Work Plan

1. **Phase 1: Literature Review and Preliminary Research (Month 0-6)**
   - Conduct a comprehensive review of existing metal hydride storage systems and multi-physics modeling techniques.
   - Identify key challenges and gaps in current research.
2. **Phase 2: Model Development (Month 6-18)**
   - Set up **COMSOL Multiphysics** simulations for heat transfer, mass transfer, and mechanical stress.
   - Implement **time-dependent simulations** for the absorption/desorption cycles.
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3. **Phase 3: Optimization and Analysis (Month 18-30)**
   - Perform parametric studies and **topological optimization** on the tank's design.
   - Refine the model and design based on experimental feedback.
4. **Phase 4: Final Report and Dissemination (Month 30-36)**
   - Prepare a detailed final report on the findings.
   - Present the results at relevant scientific conferences and in peer-reviewed journals.

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