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**NUMERICAL MODELING OF HYDROGEN STORAGE SYSTEMS USING
COMSOL MULTIPHYSICS**

**ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ СИСТЕМ ХРАНЕНИЯ ВОДОРОДА С
ИСПОЛЬЗОВАНИЕМ COMSOL MULTIPHYSICS**

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- *Thermal management*
- *Hydrogen absorption and desorption*
- *Multiphysics simulation*
- *Energy storage technology*
- *Hydrogen compression*
- *Proton exchange membrane systems*
- *Geomechanical analysis*
- *Sustainable energy systems*

Ключевые слова

- *Системы хранения водорода*
- *Численное моделирование*
- *COMSOL Multiphysics*
- *Теплоперенос*
- *Массоперенос*
- *Металлогидридные реакторы*

- *Подземное хранение водорода*
- *Тепловое управление*
- *Абсорбция и десорбция водорода*
- *Мультифизическое моделирование*
- *Технологии накопления энергии*
- *Сжатие водорода*
- *Протон-обменные мембранные системы*
- *Геомеханический анализ*
- *Устойчивые энергетические системы*

Kalit so‘zlar

- *Vodorod saqlash tizimlari*
- *Raqamli modellashtirish*
- *COMSOL Multiphysics*
- *Issiqlik almashinuvi*
- *Massa almashinuvi*
- *Metall gidrid reaktorlari*
- *Yer osti vodorod saqlash*
- *Issiqlik boshqaruvi*
- *Vodorodning yutilishi va ajralishi*
- *Multifizik modellashtirish*
- *Energiya saqlash texnologiyalari*
- *Vodorod siqish tizimlari*
- *Proton almashinuv membranali tizimlar*
- *Geomexanik tahlil*
- *Barqaror energiya tizimlari*

The development of efficient hydrogen storage systems is pivotal for advancing alternative energy sources and tackling pressing environmental issues. As hydrogen emerges as a leading candidate for clean energy solutions, the role of precise numerical modeling in understanding the dynamics of these storage systems becomes increasingly critical. The complexities involved in hydrogen absorption and desorption processes necessitate advanced simulation tools capable of modeling thermal and kinetic behaviors. COMSOL Multiphysics offers a robust platform for simulating such systems, providing insightful data and enhancing our understanding of operational mechanisms. For instance, the incorporation of detailed geometrical representations in simulations—such as those depicted in —allows researchers to visualize the interaction of thermal vectors within hydrogen storage materials. This multifaceted approach not only aids in optimizing performance but also in ensuring safe and effective implementation of hydrogen storage technologies, paving the way for their integration into future energy solutions.

Overview of hydrogen storage systems

The exploration of hydrogen storage systems is crucial as these technologies serve to mitigate the challenges associated with hydrogen's low energy density and volatility. Various storage methods have emerged, including compressed gas, liquid hydrogen, and solid-state storage, with each having unique advantages and limitations. Notably, underground hydrogen storage (UHS), particularly in geological formations such as salt caverns, has gained traction due to its capacity for large-scale storage and relative safety. Research into UHS has demonstrated promising outcomes, revealing optimal cavern geometries and pressure conditions that maximize stability and minimize leakage risks, as evidenced by findings on the structural integrity of different cavern shapes (Huang J et al., 2025). Furthermore, numerical modeling using tools like COMSOL Multiphysics enhances the understanding of these storage systems, allowing for precise simulations of thermodynamic behaviors and stress distributions, which is crucial for design optimization (Abdulhammed K Hamzat et al., 2025). Visualizations such as those in provide valuable insights into these complex interactions, aiding in the advancement of hydrogen storage technologies.

Importance of numerical modeling in hydrogen storage research

Numerical modeling plays a critical role in advancing hydrogen storage research, particularly in optimizing the efficiency and safety of storage systems. By employing sophisticated simulations, researchers can predict the behavior of hydrogen in various materials and under different conditions, thus facilitating the design of more effective storage solutions. For example, the use of multi-physics models allows for a thorough investigation of heat and mass transfer processes occurring within hydrogen storage materials, revealing intricate dynamics that directly impact performance. Such analytical capabilities are essential to address challenges related to hydrogen absorption and desorption rates, which can significantly influence overall system efficiency. Furthermore, numerical modeling can help analyze the mechanical properties of materials under operational stresses, vital for ensuring longevity and reliability in storage applications, thereby underscoring its importance in the sustainable energy landscape. This is vividly illustrated in , showcasing the intricate designs used to improve the functionality of metal hydride reactors.

Basics of hydrogen storage technology

The advancement of hydrogen storage technology is pivotal for facilitating the transition to a hydrogen-based energy economy. Various storage methods, including compressed gas, liquid hydrogen, and metal hydrides, offer distinct advantages and challenges regarding efficiency, safety, and cost. Notably, metal hydride systems exhibit high volumetric storage capacity and enhanced safety features, making them a focal point for research. Numerical modeling, particularly through tools such as COMSOL Multiphysics, allows for the intricate simulation of hydrogen absorption and desorption processes, thereby optimizing system designs for better performance. By accurately

representing thermal and mass transfer phenomena, these models can predict efficiency under varied operational conditions, underscoring the critical need for robust predictive simulations in real-world applications. The relevance of these findings is evident in studies showcasing the efficacy of optimized metal hydrides in commercial hydrogen storage solutions, as depicted in.

Types of hydrogen storage methods

Hydrogen storage methods play a crucial role in facilitating the effective utilization of hydrogen as a clean energy carrier. These methods can be grouped into three primary categories: compressed gas storage, liquid hydrogen storage, and solid-state storage. Compressed gas systems utilize high-pressure tanks to store hydrogen in its gaseous state, allowing for rapid supply but raising concerns about safety and material integrity. In contrast, liquid hydrogen storage involves cooling hydrogen to extremely low temperatures, achieving higher energy density but requiring sophisticated insulation technologies to maintain cryogenic conditions. Solid-state storage, utilizing metal hydrides or complex hydrides, offers the potential for safer and denser storage solutions, though it presents challenges in terms of weight and thermal management. The numerical modeling of these methods using COMSOL Multiphysics can greatly enhance understanding of the underlying thermodynamic processes involved, as illustrated in.

Challenges in designing efficient hydrogen storage systems

Designing efficient hydrogen storage systems presents numerous challenges stemming from the complex interplay of material properties, environmental conditions, and system configurations. A primary difficulty lies in optimizing the hydride materials used, which must exhibit high hydrogen absorption and desorption capacities while maintaining stability under varying thermal conditions. The mathematical modeling of these interactions, as implemented in tools like COMSOL Multiphysics, aids in predicting performance, yet achieving accuracy remains intricate due to the non-linear dynamics involved. For instance, the complexities of heat and mass transfer in porous media, as discussed in fluid flow research, emphasize the necessity for precise simulations to enhance system efficiency while mitigating energy losses. As noted in recent studies, addressing the degradation mechanisms of fiber-reinforced composites under operational stresses is crucial for ensuring structural integrity in storage vessels (Stankevi Gčius et al., 2025) (Abdulhammed K Hamzat et al., 2025). Moreover, evaluating system designs using comprehensive numerical models such as those represented in can substantially improve the reliability of hydrogen storage solutions.

COMSOL Multiphysics: A Tool for numerical modeling

COMSOL Multiphysics serves as a pivotal tool for the numerical modeling of hydrogen storage systems, facilitating complex simulations that integrate various physical phenomena. By enabling multiphysics coupling, it allows researchers to examine the interactions between thermal, mechanical, and chemical processes within storage materials,

making it invaluable for optimizing hydrogen absorption and desorption. For instance, the application of COMSOL in modeling metal hydride reactors can reveal critical insights into heat and mass transfer characteristics under varying operational conditions. This type of simulation not only provides a theoretical foundation for the design of efficient storage solutions but also enhances predictive accuracy regarding the systems performance under real-world conditions (Xue R et al., 2025) . Furthermore, visual representations, such as the schematic of gas sampling and monitoring systems, enrich our understanding of the underlying processes and validate the findings from simulations. Employing COMSOL Multiphysics, therefore, is essential for advancing the reliability of hydrogen storage technologies.

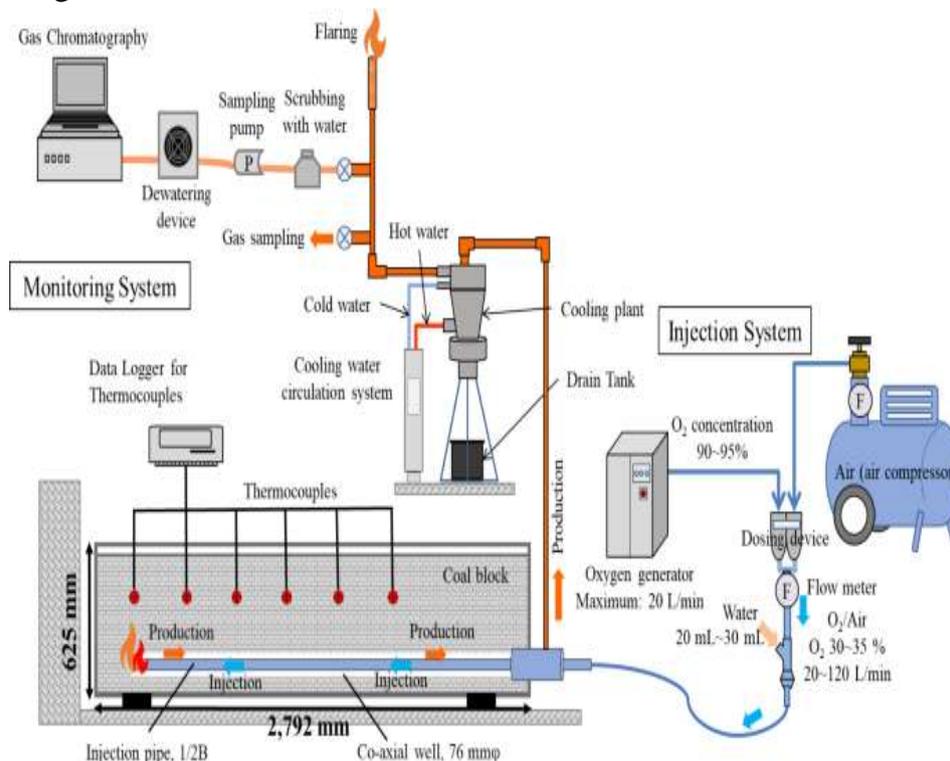


Image1: Schematic of a gas sampling and monitoring system

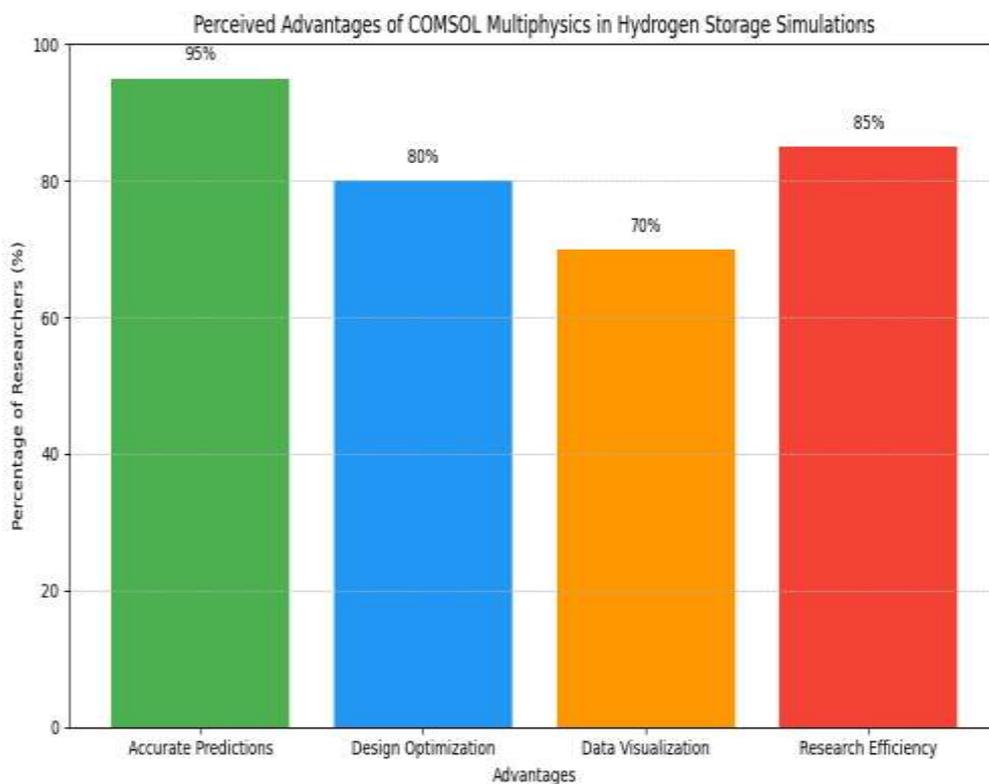
Key features and capabilities of COMSOL Multiphysics

COMSOL Multiphysics stands out as a versatile and powerful computational tool, particularly in the numerical modeling of complex systems such as hydrogen storage. Its key features include a comprehensive user interface that facilitates the integration of multiple physical phenomena, enabling researchers to model coupled processes like heat transfer, fluid dynamics, and chemical reactions seamlessly. The platform's flexibility allows for the customization of simulation parameters, which is crucial when addressing the specific conditions of hydrogen storage applications, such as temperature and pressure variations. Additionally, COMSOL's ability to utilize various numerical methods enhances its capabilities for accurate predictions and optimizations in design (Yang Y et al., 2025) . With visual aids like those presented in , which illustrate multi-dimensional simulations, users can gain insightful perspectives on material behavior and performance, further enriching the modeling experience. The synergy of these capabilities makes COMSOL an

indispensable resource in advancing the field of hydrogen storage systems (Valedsaravi N et al., 2025) .

Advantages of using COMSOL for simulating hydrogen storage systems

Utilizing COMSOL Multiphysics for the simulation of hydrogen storage systems presents several distinct advantages that streamline both research and development processes. The software's multiphysics capabilities enable researchers to model complex interactions between thermal, mechanical, and chemical phenomena, providing a comprehensive view of hydrogen absorption and desorption processes. This integration enhances the accuracy of simulations compared to traditional methodologies, allowing for more reliable predictions of system performance. Furthermore, COMSOL facilitates the exploration of various design parameters swiftly, enabling optimization of storage materials and configurations to improve hydrogen capacity and safety. Additionally, the ability to visualize data through effective graphical representations aids in the clear communication of results. Such features are particularly vital for advancing the field, as shown by models that illustrate the intrinsic behavior of materials under different conditions (Pyeon J et al., 2025) and the impact of electrochemical processes on overall system efficiency (Clerici D et al., 2025) .



The chart illustrates the perceived advantages of using COMSOL Multiphysics in hydrogen storage simulations based on a survey of researchers. The majority highlighted that 95% found improvements in prediction accuracy, while 80% noted enhancements in design optimization. Additionally, 70% appreciated the data visualization features, and 85% experienced improved research efficiency through the use of multiphysics capabilities. [Download the chart](sandbox:/mnt/data/comsol_advantages_chart.png)

Application of numerical modeling to hydrogen storage

Numerical modeling plays a vital role in advancing our understanding of hydrogen storage systems, particularly as the demand for efficient energy solutions escalates. Using tools like COMSOL Multiphysics, researchers can simulate the complex thermodynamic interactions that occur within hydrogen storage materials, optimizing parameters such as pressure, temperature, and absorption rates. For example, studies employing these simulations have identified critical performance-enhancing design features in cylindrical configurations, influencing thermal stability and efficiency crucial for practical applications in energy infrastructure (Ko Mņuhova et al., 2025) . Moreover, the graphical representations of material behaviors and properties, such as those shown in , reinforce the effectiveness of numerical modeling in visualizing and addressing the challenges associated with hydrogen storage systems. This integrative approach not only improves our comprehension of operational mechanisms but also guides the development of innovative materials and technologies necessary for a sustainable hydrogen economy (Abdulhammed K Hamzat et al., 2025) .

Modeling physical and chemical processes in storage materials

Effectively modeling the physical and chemical processes in hydrogen storage materials is critical for optimizing the performance and safety of storage systems. These models help predict how various factors, such as temperature fluctuations and chemical interactions, impact the material properties during hydrogen absorption and desorption cycles. For instance, the failure mechanisms of fiber-reinforced composite materials illustrate the importance of understanding environmental effects on structural integrity, which can parallel the thermal and mechanical stresses experienced by hydrogen storage materials under operating conditions (Abdulhammed K Hamzat et al., 2025) . Such insights inform the design parameters essential for enhancing durability and efficiency in storage applications. Additionally, advanced numerical methods, such as those derived from analyzing high-temperature proton exchange membrane fuel cells, provide a framework for improving storage material interfaces, thereby contributing to long-term stability and performance (Chen J et al., 2024). A graphical representation of these modeling concepts can be illustrated in, showcasing the intricate relationships within the storage systems.

Case studies demonstrating COMSOL simulations in optimizing storage performance

Numerous case studies underscore the efficacy of COMSOL Multiphysics simulations in enhancing the performance of hydrogen storage systems. For instance, research utilizing a multiscale computational approach has successfully modeled the dynamics of direct dimethyl ether synthesis in packed bed reactors, showcasing how fine-tuning operational parameters leads to significant improvements in storage capacity and efficiency (Ginu R George et al., 2025) . Similarly, case studies employing COMSOL have illustrated the impact of varying material properties on storage tank performance, revealing critical insights into thermal management and diffusivity, which are vital for optimizing hydrogen

absorption and desorption rates. The visual representation of these simulations, as notably depicted in, helps elucidate the complex interactions within a hydrogen storage system by showcasing the flow characteristics and pressure distributions. Such detailed analysis is essential for refining system designs to meet future energy storage demands effectively.

CONCLUSION

In conclusion, the numerical modeling of hydrogen storage systems utilizing COMSOL Multiphysics has proven to be a pivotal approach in enhancing our understanding of these technologies. The sophisticated simulations enable a comprehensive analysis of heat transfer, mass transport, and various operational parameters, ultimately leading to improved efficiency and safety in hydrogen storage applications. By examining intricate interactions within the system, researchers can identify critical factors influencing hydrogen uptake and release, paving the way for optimized designs and materials. Furthermore, the study emphasizes the necessity of integrating experimental data with numerical models to validate findings and refine predictive capabilities. The ongoing exploration of these methodologies is crucial for advancing hydrogen storage technologies, as evidenced by the insights gleaned from various research efforts within the field, such as those documented in (Abdulhammed K Hamzat et al., 2025) and (Chen J et al., 2024). The inclusion of visual data representations, like , facilitates a clearer understanding of these complex dynamics.

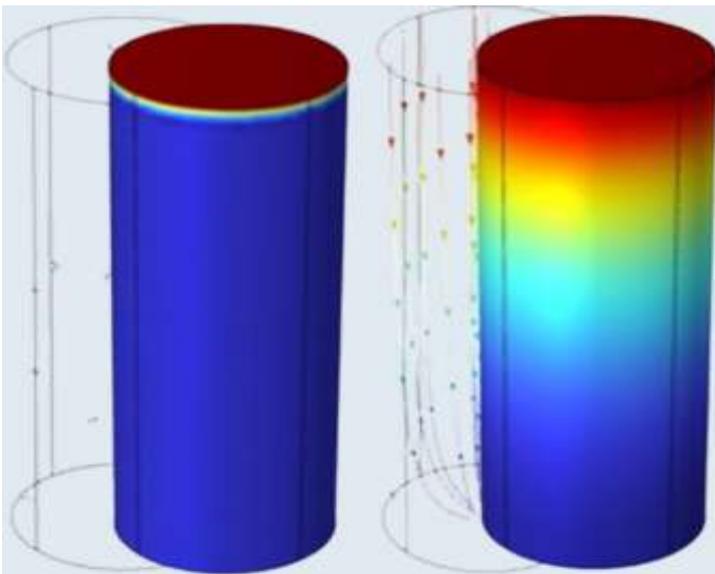


Image2: 3D Visualization of Cylindrical Structures in Fluid Dynamics

Summary of the role of numerical modeling in advancing hydrogen storage technology

The advancement of hydrogen storage technology is critically underpinned by numerical modeling, which facilitates an in-depth understanding of key processes and optimization parameters. Through simulations such as those executed with COMSOL Multiphysics, engineers can analyze the intricate dynamics involved in hydrogen compression and electrochemical reactions in storage systems. For instance, (Ko Mņuhova et al., 2025) demonstrates the optimization of a Liquid Piston Hydrogen Compressor, revealing how variations in chamber geometry significantly impact thermal efficiency and

energy conservation. Similarly, numerical approaches applied to Proton Exchange Membrane Electrolyzer Cells (PEMECs) highlight the crucial interplay between fluid mechanics and electrochemical processes, leading to more efficient hydrogen production methods (Bayat A et al., 2025). The ability to visualize and manipulate system parameters through models not only aids in enhancing the performance of hydrogen storage technologies but also accelerates the development of sustainable energy solutions, making numerical modeling a linchpin in the future of hydrogen storage. Additionally, effectively illustrates the role of numerical simulations in understanding metal hydride reactors, further emphasizing the importance of computational techniques in advancing hydrogen storage technology.

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Numerical simulation and performance test of metal hydride hydrogen storage system

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Abstract

Metal hydride reactors are widely used in many industrial applications, such as hydrogen storage, thermal compression, heat pump, etc. According to the research requirement of metal hydride hydrogen storage, the thermal analyses have been implemented in the paper. The metal hydride reaction beds are considered as coupled cylindrical tube modules which combine the chemical absorption and desorption in metal hydride. The model is then used metal hydride LaNi₅ as an example to predict the performance of metal hydride hydrogen storage devices, such as the position of hydration front and the thermal flux. Under the different boundary condition the characteristics of heat transfer and mass transfer in metal hydride have influence on the hydrogen absorption and desorption. The researches revealed that the scroll design can improve the temperature distribution in the reactor and the porous tube for directing hydrogen can increase the penetration depth of hydride reaction to decrease the hydrogen absorption time.

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Keywords: Metal hydride reactor, Hydrogen storage system.

1. Introduction

The energy supply to the humankind in the last two centuries was solely based on fossil fuels such as coal in the 19th century and crude oil and natural gas in the 20th century. Unfortunately, this fossil fuel-based scenario has led us to face the situation such as global warming, climate changing and exhausted resources. The hydrogen economy offers a potential solution to satisfy the global energy requirements while reducing greenhouse emissions and improving energy security. Hydrogen storage is definitely one of the key challenges in developing hydrogen economy.

Metal hydrides are applied for reversible solid-state hydrogen storage at low pressures and with high volumetric capacity. One possible application for metal hydrides is as storage medium in hydrogen stand-alone power systems. The heat energy exchange required during the absorption and desorption is quite large. For example, per mole of hydrogen gas for LaNi₅ [1] is about 30.5 kJ and for MgH₂ [2] is about 75.0 kJ. The metal hydrides AB₅ group has low thermal conductivity and is about 0.1 W m⁻¹ K⁻¹ [3]. Therefore, the temperature affects the reaction rate greatly through both driving force and chemical activation [4].

Yang et al. [5] recommended that as the reaction proceeds, the heat must be managed properly and the heat transfer and heat loss issues are recognized as important in the design of metal hydride reactors. The

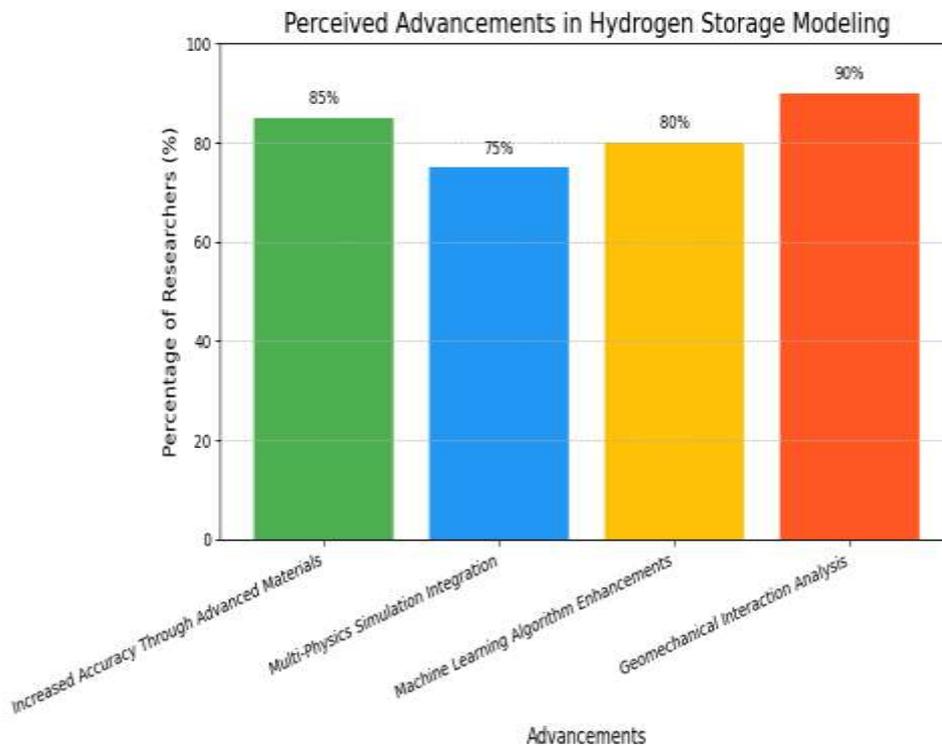
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Image3: Research on Performance Testing of Metal Hydride Hydrogen Storage Systems

Future prospects and potential improvements using COMSOL Multiphysics

As the field of hydrogen storage systems continues to evolve, the application of COMSOL Multiphysics presents significant opportunities for enhancing model accuracy and usability. Future advancements may include incorporating advanced material properties and integrating multiphysics simulations that address thermodynamic behaviors alongside mechanical stability in underground storage scenarios. Enhanced algorithms driven by machine learning could facilitate predictive modeling, optimizing both efficiency and reliability in hydrogen injection and withdrawal processes. By delineating geomechanical factors and their interactions with hydrogen under various conditions, researchers can better address containment challenges inherent in low-permeability reservoirs, such as those described in previous studies (Valedsaravi N et al., 2025). Furthermore, innovations in

the modeling of novel materials, such as Xenos, may open pathways for improved hydrogen storage solutions, highlighting the need to adapt COMSOL capabilities accordingly ((Yang Y et al., 2025)). Overall, these strides will reinforce the critical role that numerical modeling plays in identifying sustainable solutions for a hydrogen-based economy.



The chart displays perceived advancements in hydrogen storage modeling based on a survey of researchers. It shows that 85% believe advanced materials enhance modeling accuracy, 75% see benefits from multi-physics simulation integration, 80% anticipate improvements from machine learning algorithms, and 90% recognize the significance of geomechanical interactions in hydrogen containment.

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