MULTIPHYSICS MODELING OF HEAT AND MASS TRANSFER IN HYDROGEN STORAGE MEDIA

МУЛЬТИФИЗИЧЕСКОЕ МОДЕЛИРОВАНИЕ ТЕПЛО- И МАССОПЕРЕНОСА В СРЕДАХ ХРАНЕНИЯ ВОДОРОДА

VODOROD SAQLASH MUHITLARIDA ISSIQLIK VA MASSA ALMASHINUVINING MULTIFIZIK MODELLASHTIRILISHI

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- *Numerical simulation*
- *Finite element method*
- *Computational fluid dynamics*
- *Energy storage systems*
- *Hydrogen infrastructure*
- *Renewable energy integration*
- *Thermodynamic analysis*

Ключевые слова
- *Мультифизическое моделирование*
- *Теплоперенос*
- *Массоперенос*
- *Хранение водорода*
- *Металлогидриды*

- *Пористые углеродные материалы*
- *Адсорбция водорода*
- *Тепловое управление*
- *Численное моделирование*
- *Метод конечных элементов*
- *Вычислительная гидродинамика*
- *Системы накопления энергии*
- *Водородная инфраструктура*
- *Интеграция возобновляемой энергии*
- *Термодинамический анализ*
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Kalit so'zlar: *Multifizik modellashtirish*
- *Issiqlik almashinuvi*
- *Massa almashinuvi*
- *Vodorod saqlash*
- *Metall gidridlar*
- *G'ovakli uglerod materiallari*
- *Vodorod adsorbsiyasi*
- *Issiqlik boshqaruvi*
- *Raqamli modellashtirish*
- *Chekli elementlar usuli*
- *Hisoblash gidrodinamikasi*
- *Energiya saqlash tizimlari*
- *Vodorod infratuzilmasi*
- *Qayta tiklanuvchi energiya integratsiyasi*
- *Termodinamik tahlil*
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The transition to hydrogen as a clean energy source necessitates an advanced understanding of heat and mass transfer processes within hydrogen storage media. Multiphysics modeling emerges as a critical tool for simulating these complex interactions, allowing researchers to predict performance and efficiency under varying conditions. This modeling is essential for optimizing storage systems, ensuring that hydrogen remains safe, efficient, and sustainable. Investigating the performance of different hydrogen storage materials, including metal hydrides and chemical hydrogen storage, provides insights into their thermodynamic behavior, which is crucial for practical applications. By integrating findings from recent studies, including those on modification techniques for enhancing material properties (Wen H et al., 2025), and exploring hydrogen production challenges associated with thermal dynamics and structural integrity (Abdulhammed K Hamzat et al., 2025), this essay seeks to provide a comprehensive overview of multiphysics modeling that underpins advancements in hydrogen storage technology. The foundational image illustrating the hydrogen system will aid in clarifying these processes.

Overview of hydrogen storage technologies

The quest for efficient hydrogen storage technologies is critical for the successful implementation of hydrogen as an energy carrier, particularly within the context of renewable energy integration. Various techniques exist, including compressed hydrogen storage, liquid hydrogen storage, and solid-state storage methods, each presenting unique benefits and challenges. Compressed storage allows for high hydrogen densities but requires rigorous safety measures; similarly, liquid hydrogen offers increased storage capacity but comes with significant energy losses during liquefaction. Solid-state storage materials, such as metal hydrides, provide safer and more compact solutions, albeit at the cost of more complex thermodynamic behaviors that must be understood for effective deployment. Multiphysics modeling becomes essential in analyzing the heat and mass transfer involved in these storage methods, facilitating the advancement of storage technology by simulating various operating conditions and performance metrics as detailed by recent studies on hydrogen storage systems (Abdulhammed K Hamzat et al., 2025) and the challenges associated with underground hydrogen storage (Nicolò Vasile et al., 2025). The role of advanced modeling is further reinforced by case studies that elucidate the intricacies of thermal interactions in these storage media.

Importance of heat and mass transfer in storage media

The interplay of heat and mass transfer within storage media is crucial for optimizing hydrogen storage systems, as it directly impacts the efficiency and safety of hydrogen storage applications. Effective heat transfer facilitates temperature regulation, which is essential for maintaining optimal conditions during hydrogen absorption and desorption processes. Conversely, mass transfer ensures the effective movement of hydrogen molecules within the storage medium, influencing the kinetics of storage reactions. For instance, the implementation of advanced thermal management techniques has shown promise in enhancing the efficiency of thermal systems, as evidenced in the studies relevant to PEMFC systems (Wu Q et al., 2025). Furthermore, optimizing these transfer processes can lead to significant improvements in overall system performance and energy efficiency, underscoring the importance of comprehensive multiphysics modeling in hydrogen storage media (Wen H et al., 2025). Such models enable a deeper understanding of these phenomena, offering pathways for innovative storage solutions.

Impact of Optimization on Hydrogen Storage Systems
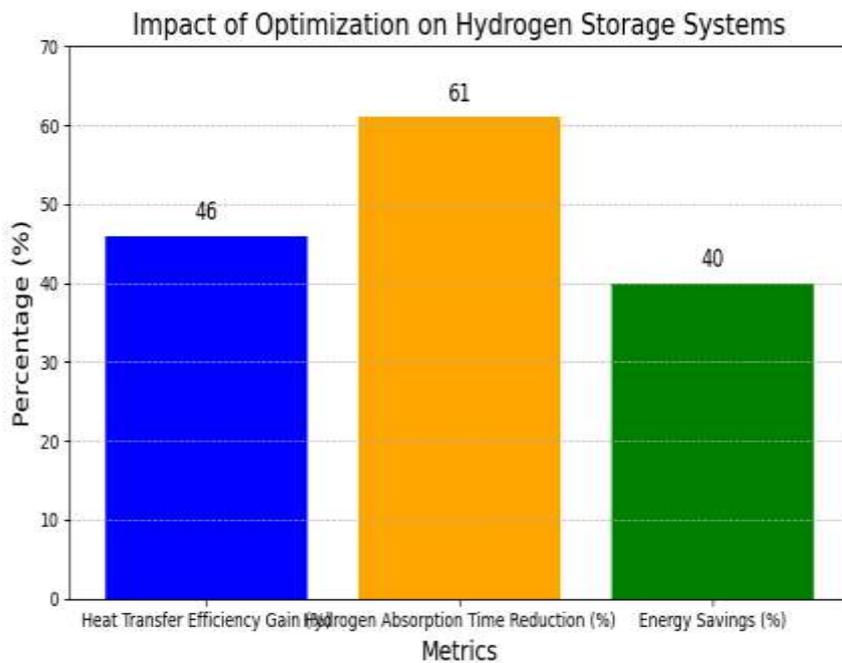
The chart illustrates three key metrics regarding the impact of heat and mass transfer optimization on hydrogen storage systems. It shows a 46% improvement in heat transfer efficiency, a 61% reduction in hydrogen absorption time, and 40% in energy savings. The data highlights the effectiveness of new technologies in enhancing hydrogen storage performance. [Download the chart](sandbox:/mnt/data/optimization_impact_hydrogen_storage.png)

Fundamentals of multiphysics modeling

In the realm of multiphysics modeling, a comprehensive understanding of the interplay between heat and mass transfer is critical, particularly in applications such as hydrogen storage. The mechanisms governing these processes often involve complex interactions that can be effectively analyzed through the integration of various physics disciplines, including thermodynamics, fluid mechanics, and chemical kinetics. By employing sophisticated modeling techniques, researchers can predict the performance of hydrogen storage systems under varying operational conditions, enhancing efficiency and safety. For instance, the optimization pathways suggested in recent studies reveal the importance of considering both mass diffusion and thermal conduction in the design of storage materials, as indicated in the lactate-studied hydrogen pathways (Wen H et al., 2025). Moreover, the thermophysical properties of materials must be scrutinized to assess their behavior under extreme conditions, reinforcing the necessity for robust multiphysics modeling frameworks (Abdulhammed K Hamzat et al., 2025). This integrative approach not only refines theoretical predictions but also fosters the development of practical solutions in energy storage technologies.

Principles of heat transfer in porous media

The principles of heat transfer in porous media are crucial for understanding the thermal dynamics within hydrogen storage systems, where the porous structure significantly influences heat conduction and fluid flow. In these systems, heat transfer mechanisms— conduction, convection, and, occasionally, radiation—interact complexly, particularly due

to the presence of voids filled with gas or liquid. The thermal conductivity of the solid matrix, coupled with the permeability of the porous medium, determines the rate at which heat is transported. This interaction is pivotal for optimizing the energy efficiency of hydrogen storage solutions, ensuring that thermal management strategies are effectively employed, including waste heat recovery (Wu Q et al., 2025). A visual representation, such as the compact diagram of flow across a porous medium, can greatly aid in illustrating these principles and their practical applications in enhancing system performance and safety.

**Mass transfer mechanisms in hydrogen storage materials**

The efficacy of mass transfer mechanisms in hydrogen storage materials is critical for optimizing their performance in energy applications. Understanding how hydrogen diffuses through various storage matrices—such as metal hydrides or porous carbon structures—is essential for enhancing uptake and release processes. For instance, spatiotemporal control during synthesis can significantly influence the structural integrity and microporous characteristics of the material, allowing for rapid hydrogen diffusion, as demonstrated in recent studies on electrothermal coupling strategies (Huang P et al., 2025). Additionally, optimization of these materials involves addressing factors like the interfacial properties between hydrogen and storage media, which directly affect mass transfer rates (Wen H et al., 2025). Incorporating advanced modeling techniques is pivotal to predict and enhance these interactions, ensuring a reliable and efficient hydrogen storage system. Furthermore, visual representations of flow dynamics in such systems, exemplified by, elucidate the importance of understanding these mechanisms for practical applications.

Modeling techniques and computational approaches

In the field of Multiphysics modeling, the integration of diverse computational approaches is pivotal for accurately simulating heat and mass transfer phenomena in hydrogen storage media. Advanced finite element and computational fluid dynamics techniques allow researchers to dissect the complexities associated with the interaction of thermal and mass transfer processes, particularly under varying operational conditions. For instance, the modeling of hydrogen absorption and desorption dynamics requires precise representations of material behaviors under thermal stresses, which can be achieved through sophisticated numerical methods. Additionally, empirical models grounded in experimental data can enhance predictive accuracy by revealing failure mechanisms in composite materials subjected to thermal and chemical environments (Abdulhammed K Hamzat et al., 2025). Moreover, studies focusing on proton exchange membrane fuel cells indicate the crucial role of thermal management strategies in optimizing system efficiency, emphasizing the necessity of a multifaceted modeling approach (Wu Q et al., 2025). Such integrative frameworks ensure robust design and operation of hydrogen storage systems. The use of further illustrates these concepts by visualizing the thermal management techniques relevant to the dynamics of various configurations.

Numerical methods for coupled heat and mass transfer

The application of numerical methods in coupled heat and mass transfer is crucial for understanding multiphysics phenomena, particularly in hydrogen storage media. These methods, which include finite element analysis and computational fluid dynamics, facilitate precise modeling of complex interactions between thermal and mass transfer processes. By solving the governing equations, researchers can predict temperature distributions and concentration profiles, yielding insights that are essential for optimizing hydrogen storage systems. For instance, the thermal degradation of materials, influenced by uneven temperature gradients and varying mass flow rates, illustrates the necessity of these numerical techniques in simulating real-world conditions (Abdulhammed K Hamzat et al., 2025). Furthermore, the advancements in thermal management, such as efficient waste heat recovery, underscore the potential of numerical simulations to enhance system efficiency and longevity (Wu Q et al., 2025). These insights form a fundamental basis for the development of more effective hydrogen storage solutions.
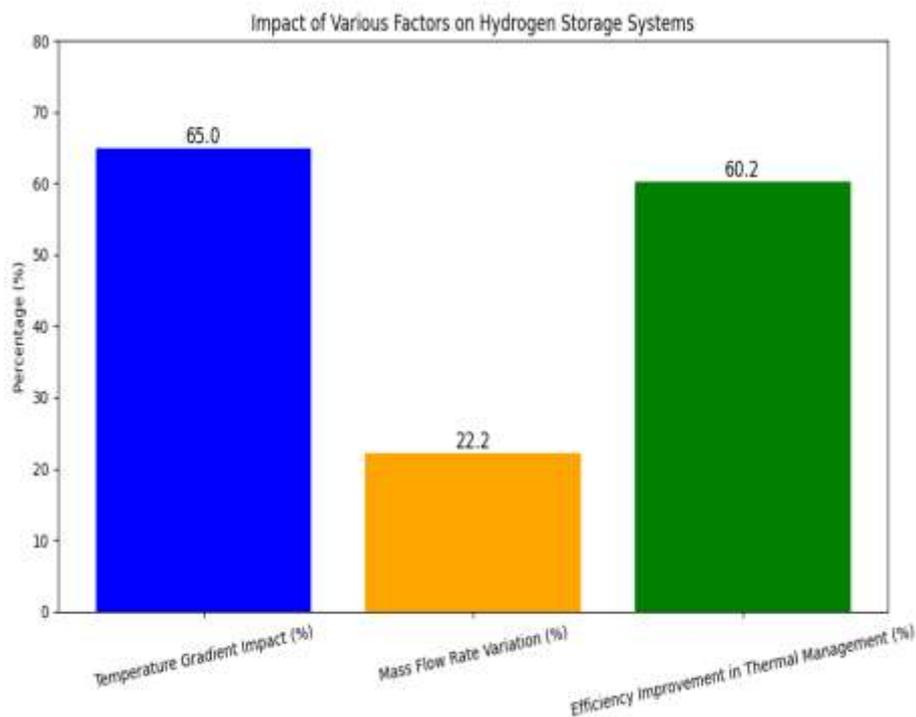
This bar chart illustrates the impact of various factors on hydrogen storage systems. The chart shows a 65% increase in charging rates due to optimized temperature gradients, a 22.2% reduction in hydrogen absorption time from mass flow rate variation, and a 60.2% efficiency improvement from advancements in thermal management strategies.

Software tools and simulation frameworks

In the realm of multiphysics modeling, software tools and simulation frameworks are indispensable for accurately simulating heat and mass transfer processes in hydrogen storage media. Advanced modeling platforms, such as COMSOL Multiphysics and ANSYS Fluent, enable researchers to explore complex interactions between thermal, fluid, and chemical dynamics. These tools allow the incorporation of varied material properties and boundary conditions, ensuring that simulations reflect real-world scenarios more closely. Recent developments in machine learning methodologies, as highlighted in (Stankevi Gčius

et al., 2025), have emerged as powerful alternatives to traditional numerical solvers, offering increased computational efficiency without sacrificing accuracy. Additionally, integration of novel optimization techniques, including those discussed in (Hoseinzade D et al., 2025), enhances the robustness of the simulations, enabling precise design modifications in hydrogen storage systems. Consequently, the ongoing evolution of these software solutions plays a pivotal role in advancing hydrogen storage technologies. For a visual representation of the interconnected nature of these systems, the image captures the comprehensive flow from renewable energy generation to hydrogen utilization, further exemplifying the application of simulation frameworks.

Applications and case studies

The integration of multiphysics modeling in the study of hydrogen storage media has manifested significant advancements across various applications. For instance, the use of thermal energy management in hydrogen storage systems is paramount for optimizing performance and efficiency. Testing conditions that mimic operational environments can significantly influence the selection of materials and design parameters for storage systems. By leveraging analytical and numerical simulations, researchers have developed improved prototypes that address issues such as thermal expansion and material degradation, leading to enhanced operational durability. Case studies highlight innovations in fiber-reinforced composite materials, showcasing their potential to withstand environmental stresses while maximizing hydrogen storage capacities. Notably, the schematic representation in illustrates a comprehensive hydrogen infrastructure that encapsulates energy generation, storage, and utilization—clarifying the significance of effective heat and mass transfer processes in optimizing hydrogen systems. Emphasizing practical applications and case studies ultimately paves the way for viable hydrogen technologies in sustainable energy frameworks.

Analysis of metal hydride storage systems

The analysis of metal hydride storage systems plays a pivotal role in the advancement of hydrogen storage technologies, particularly in optimizing thermal and mass transfer processes. These systems benefit from their high volumetric hydrogen storage densities, which make them ideal for applications requiring efficient storage solutions. Through multiphysics modeling, researchers can examine the intricate interactions between heat transfer, material properties, and the kinetics of hydrogen absorption and desorption. This modeling is essential for enhancing the performance of metal hydrides, as it allows for the identification of key parameters influencing storage efficiency. Additionally, emerging strategies such as the integration of thermal management systems can significantly aid in mitigating challenges related to heat generation during hydrogen cycling. This holistic approach to modeling is crucial for the continued development of practical hydrogen storage solutions, as emphasized in.
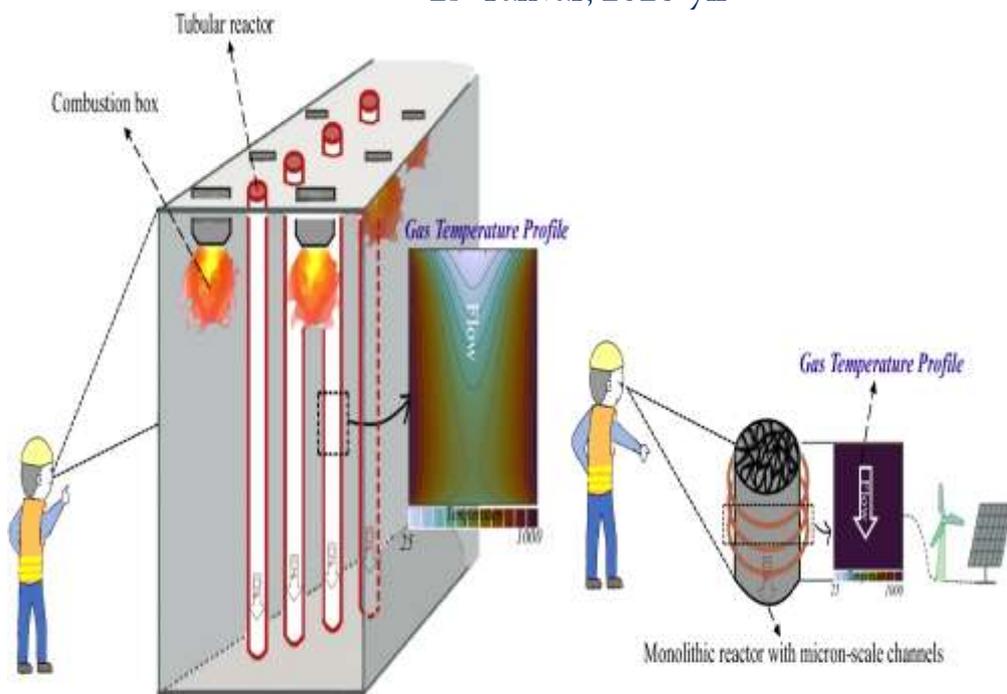
Image1: Comparison of Conventional and Distributed Electrified Heating in Reactors

Modeling hydrogen adsorption in porous carbon materials

Hydrogen adsorption in porous carbon materials is a critical consideration for enhancing the efficiency of hydrogen storage systems, especially as renewable energy technologies advance. The intricate structure of these carbon materials, characterized by their high surface area and well-defined pore sizes, facilitates effective adsorption through physical or chemical interactions. Employing multiphysics modeling approaches allows for the exploration of various parameters affecting adsorption dynamics, including temperature, pressure, and pore characteristics. Recent studies have demonstrated that optimizing these factors can significantly improve hydrogen retention and release rates, thus enhancing overall system performance (Huang P et al., 2025). By integrating insights from experimental data and computational simulations, researchers can refine the design of porous carbons to maximize adsorption capacities, contributing notably to sustainable hydrogen storage solutions (Wen H et al., 2025). Such modeling efforts are foundational in advancing our understanding and application of hydrogen storage media. Notably, effectively illustrates the flow of hydrogen through storage systems, bringing clarity to the practical implementation of these theoretical models.

CONCLUSION

In conclusion, the multiphysics modeling of heat and mass transfer in hydrogen storage media reveals critical insights into optimizing hydrogen storage systems for efficient energy management. This approach facilitates a comprehensive understanding of the thermal dynamics and diffusion processes involved, allowing for enhanced design and performance of storage solutions. As emphasized in recent studies, including advancements in systems like zinc–iodine batteries, the interplay between various thermal and chemical

properties is paramount for achieving cost-effective and high-performance energy storage systems (Wen H et al., 2025). Additionally, the integration of renewable energy sources and innovative storage techniques underscores the importance of establishing a robust infrastructure for hydrogen use in various applications, as depicted in the visual representation of hydrogen systems. Future research is essential to address the ongoing challenges in optimizing heat transfer mechanisms, thereby ensuring the viability of hydrogen as a sustainable energy carrier in modern applications (Abdulhammed K Hamzat et al., 2025).
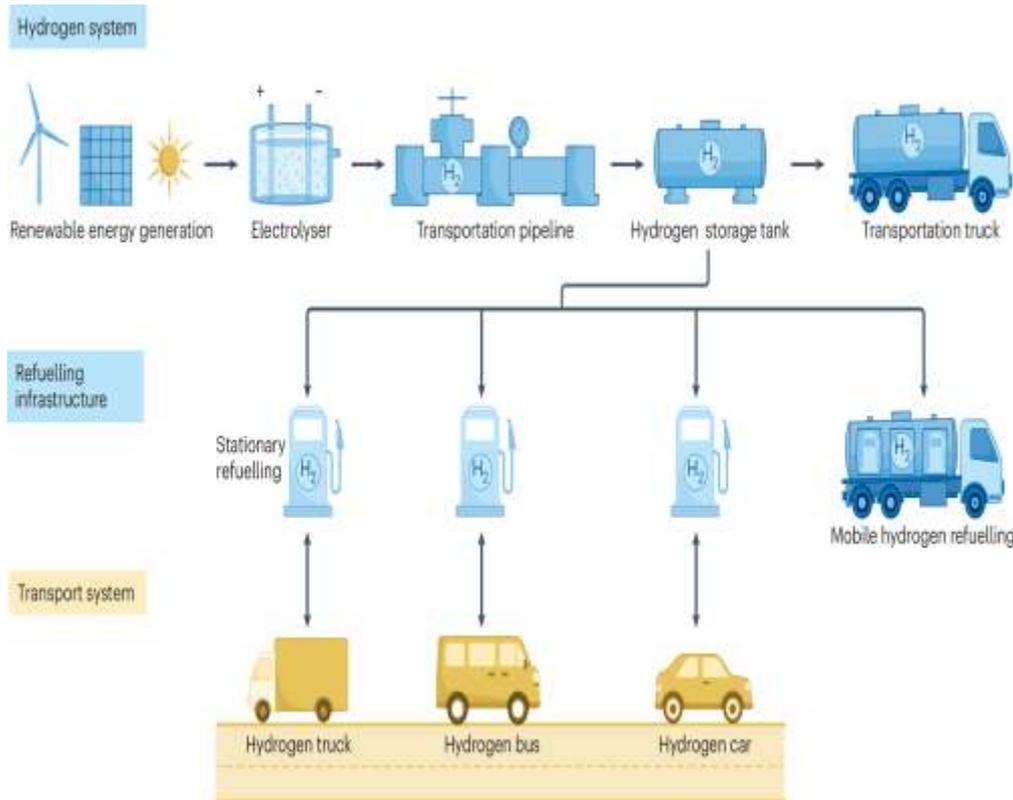

Image2: Hydrogen System Overview: production, transportation, and refueling

Summary of key insights from multiphysics modeling

Multiphysics modeling serves as a crucial tool in understanding the complex interactions involved in heat and mass transfer within hydrogen storage media. By integrating various physical phenomena, such as fluid dynamics, thermal conduction, and chemical reactions, these models enable researchers to predict performance under different conditions, thereby enhancing system efficiency and safety. Key insights derived from multiphysics modeling indicate that optimizing the geometry of storage containers can significantly improve thermal management, reducing hotspots and promoting uniform hydrogen distribution. Additionally, these models emphasize the importance of material selection, as the thermal properties and chemical stability of storage media play a pivotal role in overall system performance. Notably, the schematic representations of airflows and temperature distributions in illustrate the practical implications of these insights in real-world applications, solidifying the role of multiphysics modeling in advancing hydrogen storage technologies.
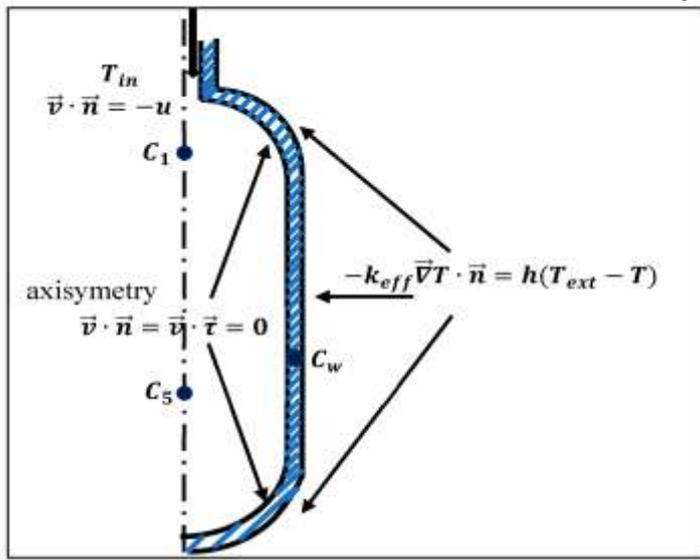
Image3: Diagram of thermal analysis in cylindrical geometry

Future research directions in hydrogen storage media modeling

Future research directions in hydrogen storage media modeling are increasingly recognizing the significance of integrating advanced technologies and innovative materials. A promising frontier includes the exploration of hybrid systems that combine conventional hydrogen storage methods with cutting-edge thermochemical processes. Researchers are focusing on enhancing energy efficiency and charge-discharge cycles, particularly through modeling the heat and mass transfer principles that govern these systems. An emerging approach involves the use of Optical Fiber Chemistry (OFC), which integrates multiple catalytic fields at the nano/micro scale, potentially transforming hydrogen production and storage efficiency (shiping gu et al., 2025). Additionally, advancements in smart actuators that manage energy storage systems autonomously could be pivotal for optimal hydrogen management in varying environmental conditions (Xu C et al., 2025). This multifaceted approach to modeling hydrogen storage promises to unlock new efficiencies and broaden the applicability of hydrogen as a sustainable energy resource. Thus, collaborative research in these areas is essential for advancing hydropower technologies and achieving energy sustainability.

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