

INVESTIGATION OF METAL HYDRIDE BASED THERMOCHEMICAL ENERGY STORAGE SYSTEM FOR HIGH TEMPERATURE APPLICATIONS

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INDIAN INSTITUTE OF TECHNOLOGY DELHI
FEBRUARY 2025**

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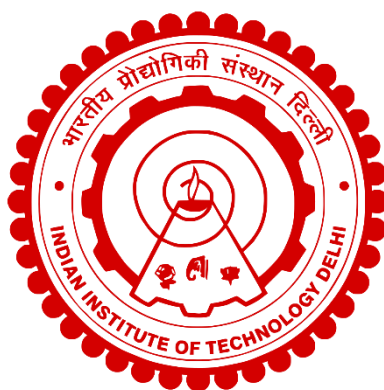
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Submitted

in fulfilment of the requirement of degree of Doctor of Philosophy

to the



Indian Institute of Technology Delhi

February 2025

Dedicated

to

My Grandparents...

Certificate

This is to certify that this thesis entitled **“Investigation of Metal Hydride based Thermochemical Energy Storage System for High Temperature Applications”** being submitted by Mr. Sumeet Kumar Dubey (Entry No.: 2018ESZ8054) to Indian Institute of Technology Delhi in fulfilment of the requirements for the award of the degree of **Doctor of Philosophy** is a record of bonafide research work performed by him under my guidance and supervision at **Department of Energy Science and Engineering, Indian Institute of Technology Delhi, New Delhi, India.**

The results obtained herein have not been submitted in part or in full to any other university or institute for the award of any degree to the best of my knowledge.

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Acknowledgements

At the outset, I express my heartfelt gratitude to the almighty for bestowing upon me abundant blessings and instilling in me the determination to bring this work toward finality. I hardly know where to start expressing my gratitude, but for sure gratitude goes to all those who have supported and helped in completing this work. It is impossible to list all the names, but several people deserve my sincere and special thanks.

I want to convey my profound gratitude, respect, and appreciation to my PhD supervisor, Dr. K. Ravi Kumar, for his insightful guidance, which has been a cornerstone of my doctoral journey. His encouragement and recognition during various stages of this work have helped me to navigate this journey as a novice.

I would like to express my gratefulness to the members of my research committee, Prof. Tara Chandra Kandpal, Prof. M. R. Ravi, and Dr. Kaushik Saha, for their constructive guidance and priceless feedback during the different evaluation phases of my endeavour, which improved the quality of my research work. I am also thankful to the Head of the Department for providing the necessary facilities to complete this research work. I am also thankful to Prof. Satheesh A from VIT Vellore and Dr. Vinod Kumar Sharma from NIT Calicut for their opinion and support at several stages of the work. A special thanks to Prof. S V Karra from Department of Material Science and Engineering, IIT Delhi for providing supports regarding the physical characterisation of metal hydride sample.

I would also like to acknowledge the Science and Engineering Research Board (SERB), Department of Science and Technology (DST), Government of India, and Confederation of Indian Industry (CII) for awarding “Prime Minister Fellowship for Doctoral Research” in collaboration with Indian Oil Corporation Limited, Research and Development Centre as an

industry partner. The guidance provided by Dr. Vinay Tiwari (Industry mentor) and Dr. Umish Srivastva (Industry Head of the Department) has helped me to improve the quality of the work. I want to thank all my colleagues in the institute (especially Dr. Anish Malan, Dr. Ram Kumar Pal, Dr. Alok Kumar Ray, Dr. Shubham Jain, Mr. Rajeev Awasthi, Mr. Naveen T K, Mr. Shantanu Kumar, Mr. Shubha Deep Paul, Mr. Gaurav Arora, Mr. Mallayya Swami, Mr. Tarun Goel, Mr. Ajay Kumar Udayraj Yadav, and Mr. Yash Prakash Mishra) for their support and encouragement during the completion of the work. I am also thankful to the Industrial Research and Development (IRD) unit of the institute for awarding me research excellence travel award to present my research work in the conference “2024 The 8th International Conference on Green Energy and Applications” held at NTU Singapore.

I want to thank my parents (Mr. P. N. Dubey and Mrs. Saroj Dubey), Sisters, and brothers-in-law for their constant support, encouragement, and belief in my abilities, which helped me overcome the challenges during my Ph.D. I am also grateful to my lifetime partner, Mrs. Shivani Mishra, for her constant motivation and support during the tough time of this journey. Her encouragement and belief in my abilities have been a constant source of strength and her sacrifices and patience have enabled me to focus on my work. I would also like to thank my father-in-law and mother-in-law for constantly encouraging me for the best.

(Sumeet Kumar Dubey)

Abstract

Thermal energy storage is considered as one of the viable solutions for intermittency and diurnal variation of solar energy. Utilization of thermal energy storage helps to improve the capacity utilization factor and dispatchability of solar thermal power plants. Thermochemical energy storage has higher energy storage capacity and lower heat losses, implying higher energy storage efficiency as compared to sensible and latent heat storage. In this thesis, investigation of a metal hydride based thermochemical energy storage system is proposed for high temperature (500°C) applications. As metal hydride based thermochemical energy storage has high thermal stability, longer cyclic life, and better reversibility as compared to other thermochemical energy storage systems. Therefore, it can be an appropriate solution for high temperature energy storage applications.

A dual metal hydride system uses two metal hydrides, namely high temperature and low temperature metal hydride. Energy storage takes place in high temperature metal hydride and therefore, it is also known as energy storage media. The hydrogen released from high temperature metal hydride is stored in low temperature metal hydride. In this work, NaMgH₂F is used as energy storage media, while Mg₂NiH₄ is used as low temperature metal hydride for hydrogen storage.

An experimental test facility is developed to characterize the metal hydride sample up to an operating temperature of 300°C. Physical characterization of the Magnesium Nickel (Mg-Ni) alloy sample is performed using X-ray diffraction (XRD) and scanning electron microscope (SEM) analysis, followed by development of pressure composition isotherm of Mg-Ni alloy at 250°C, 275°C, and 300°C. The Mg-Ni alloy sample has shown relatively lower plateau pressure at the above mentioned temperature as compared to other complex metal hydrides. The absorption plateau for 250°C, 275°C, and 300°C starts around 1.4 bar, 1.8 bar, and 3.8 bar,

respectively. The maximum hydrogen storage density of 3.31 wt% is observed, which is approximately 90% of the theoretical hydrogen storage density reported in the literature.

The numerical study performed in this work investigates the heat transfer and performance analysis, such as energy absorption, desorption, and storage efficiency, of individual metal hydrides with variations in geometries and heat transfer flow arrangements. The identification of adequate heat transfer fluid tubes and the effect of aspect ratio (diameter to height ratio) on the energy storage and heat transfer phenomenon in Mg_2NiH_4 is performed. The outcome of this analysis concluded that the reactor geometry with less aspect ratio has shown better heat transfer in the cross sectional domain. It also concluded that heat transfer fluid tubes embedded in metal hydride reactor needs nearly 18% of the metal hydride cross sectional area (area cross section ratio) for effective heat exchange between the metal hydride and heat transfer fluid. The adequate heat transfer fluid tubes are identified in this analysis for aspect ratios 0.5, 1, and 2 are 32, 48, and 54, respectively. A maximum and minimum energy storage efficiency of 93.27% and 91% is observed for aspect ratios 2 and 0.5, respectively.

The outcome of the study performed on Mg_2NiH_4 is used while modelling NaMgH_2F for energy storage characteristics. The analysis performed on NaMgH_2F investigated the effect of variation of initial metal hydride reactor temperature and different heat transfer fluid flow configurations on heat transfer and performance characteristics of metal hydride system. The heat transfer fluid flow configuration 1 has axial heat transfer fluid tubes distributed radially in the cross section, while configuration 2 has circumferential heat transfer fluid arrangement along with axial heat transfer fluid tubes distributed radially in the cross section. The study concluded that higher initial temperature of metal hydride reactor results in higher thermal energy storage efficiency. The metal hydride reactor with circumferential heat transfer fluid flow arrangement (configuration 2) has shown better heat transfer characteristics. A maximum

thermal energy storage efficiency of 96.4% is obtained for the metal hydride reactor at 823 K with circumferential heat transfer fluid flow arrangement.

A dual metal hydride bed system is developed by utilizing the outcomes of the analysis performed on individual metal hydrides. The dual metal hydride bed system is studied for the heat transfer and performance characteristics with different thermal conductivities of energy storage media. The energy storage efficiency of the dual metal hydride system improved marginally from 94.44% to 95.11% when the thermal conductivity of high temperature metal hydride is increased from 0.5 W/(m.K) to 4 W/(m.K). In addition, the single metal hydride system and dual metal hydride bed system are compared for the thermal and energy storage characteristics. The maximum energy storage efficiency is found to be higher for dual metal hydride system as compared to single metal hydride system. The maximum average temperature variation of energy storage media was 33 K and 4 K for single and dual metal hydride based thermal energy storage system, respectively.

In summary, the study presents a detailed heat transfer and performance analysis of a dual metal hydride bed system. The study compares the heat transfer and performance characteristics of single and dual metal hydride bed systems. The outcomes of the analysis will facilitate the designing of a metal hydride based thermal energy storage system with effective heat transfer and enhanced energy storage characteristics for high temperature applications.

सारांश

तापीय ऊर्जा भंडारण को सौर ऊर्जा के दैनिक परिवर्तन और अनियमित स्वभाव के लिए एक उचित समाधान माना जाता है। तापीय ऊर्जा भंडारण का प्रयोग, सौर तापीय बिजली संयंत्रों के क्षमता उपयोग अनुपात और प्रेषण क्षमता के संवर्धन में सहायक होता है। ऊष्मा-रासायनिक ऊर्जा भंडारण में उच्च ऊर्जा भंडारण क्षमता और निम्न ऊष्मा हानि होती है, जो संवेदनशील और गुप्त ऊष्मा भंडारण प्रणाली की तुलना में उच्च ऊर्जा भंडारण घनत्व को दर्शाता है। इस शोध में उच्च तापीय (500°C) अनुप्रयोगों के लिए धातु हाइड्राइड आधारित ऊष्मा-रासायनिक ऊर्जा भंडारण प्रणाली की जांच प्रस्तावित है। अन्य ऊष्मा-रासायनिक ऊर्जा भंडारण प्रणालियों की तुलना में धातु हाइड्राइड आधारित ऊष्मा-रासायनिक ऊर्जा भंडारण प्रणाली में उच्च तापीय स्थिरता, लंबा जीवन चक्र और बेहतर उत्क्रमणीयता होती है। इसलिए, यह उच्च तापीय ऊर्जा भंडारण अनुप्रयोगों के लिए एक उपयुक्त समाधान हो सकता है।

एक द्विधातु हाइड्राइड प्रणाली दो धातुओं का उपयोग करती है जिनको उच्च तापीय और निम्न तापीय धातु हाइड्राइड के नाम से जाना जाता है। ऊर्जा भंडारण उच्च तापीय धातु हाइड्राइड में होता है और इसलिए इसे ऊर्जा भंडारण पदार्थ के रूप में भी जाना जाता है। उच्च तापीय धातु हाइड्राइड से निकलने वाले हाइड्रोजन को निम्न तापीय धातु हाइड्राइड में संग्रहित किया जाता है। इस कार्य में, NaMgH_2F का उपयोग ऊर्जा भंडारण पदार्थ के रूप में और Mg_2NiH_4 का उपयोग हाइड्रोजन भंडारण के लिए निम्न तापीय धातु हाइड्राइड के रूप में किया गया है।

इस अध्ययन में 300°C के परिचालन तापमान तक धातु हाइड्राइड के नमूने के अभिलक्षणन के लिए एक प्रयोगात्मक परीक्षण संयंत्र विकसित किया गया है। मैग्नीशियम निकेल (Mg-Ni) मिश्र धातु के नमूने के भौतिक गुणों का अभिलक्षणन एक्स-रे विवर्तन (XRD) और स्कैनिंग इलेक्ट्रॉन माइक्रोस्कोप (SEM) यन्त्र का उपयोग करके किया गया है, इसके बाद 250°C , 275°C और 300°C पर Mg-Ni मिश्र धातु का प्रेशर कम्पोजीशन आइसोथर्म रेखित किया गया है। Mg-Ni मिश्र धातु के नमूने ने अन्य जटिल धातु हाइड्राइडों की तुलना में उपर्युक्त तापमान पर अपेक्षाकृत कम दाब पर हाइड्रोजन अवशोषण दिखाया है। 250°C ,

275°C और 300°C के लिए अवशोषण दाब क्रमशः 1.4 बार, 1.8 बार और 3.8 बार के निकट शुरू होता है। अधिकतम हाइड्रोजन भंडारण घनत्व 3.31 wt% देखा गया है, जो वैज्ञानिक साहित्य में बताए गए सैद्धांतिक हाइड्रोजन भंडारण घनत्व का लगभग 90% है।

इस कार्य में किया गया संख्यात्मक अध्ययन ज्यामिति और ऊष्मा स्थानांतरण प्रवाह प्रबंध में बदलाव के साथ अलग-अलग धातु हाइड्राइडों के ऊष्मा स्थानांतरण और प्रदर्शन विश्लेषण, जैसे अवशोषण, विशोषण और भंडारण दक्षता का अन्वेषण प्रस्तुत करता है। इसके साथ ही Mg_2NiH_4 में ऊर्जा भंडारण और ऊष्मा स्थानांतरण पर पर्याप्त तरल ट्यूबों की गणना और स्वरूप अनुपात (व्यास से ऊंचाई अनुपात) के प्रभाव की जांच प्रस्तुत की गयी है। इस विश्लेषण के नतीजे से यह निष्कर्ष पाया गया कि कम स्वरूप अनुपात वाले संयंत्र ने अनुप्रस्थ काट क्षेत्र में बेहतर ऊष्मा स्थानांतरण प्रस्तुत किया। यह भी निष्कर्ष निकाला गया कि धातु हाइड्राइड और ऊष्मा स्थानांतरण तरल के बीच प्रभावी ऊष्मा विनिमय के लिए अंतःस्थापित ऊष्मा स्थानांतरण तरल ट्यूबों को धातु हाइड्राइड अनुप्रस्थ काट क्षेत्र (क्षेत्र क्रॉस सेक्शन अनुपात) के लगभग 18% क्षेत्रफल की आवश्यकता होती है। इस विश्लेषण में स्वरूप अनुपात 0.5, 1, और 2 के लिए पर्याप्त ऊष्मा स्थानांतरण तरल ट्यूबों की संख्या क्रमशः 32, 48, और 54 प्राप्त हुई। स्वरूप अनुपात 2 और 0.5 के लिए अधिकतम और न्यूनतम ऊर्जा भंडारण घनत्व क्रमशः 93.27% और 91% देखा गया है।

Mg_2NiH_4 पर किए गए अध्ययन के परिणामों का उपयोग $NaMgH_2F$ मॉडलिंग में ऊर्जा भंडारण विशेषताओं के अध्ययन के लिए किया गया है। $NaMgH_2F$ पर किए गए विश्लेषण में धातु हाइड्राइड संयंत्र की ऊष्मा स्थानांतरण प्रणाली और प्रदर्शन विशेषताओं पर प्रारंभिक तापमान में बदलाव और विभिन्न ऊष्मा स्थानांतरण तरल प्रवाह विन्यासों के प्रभाव की जांच की गई है। ऊष्मा स्थानांतरण तरल प्रवाह विन्यास 1 में अक्षीय ऊष्मा स्थानांतरण तरल ट्यूब अनुप्रस्थ काट क्षेत्र में त्रिज्यीय दिशा में वितरित हैं, जबकि विन्यास 2 में अनुप्रस्थ काट क्षेत्र में त्रिज्यीय दिशा में वितरित अक्षीय ऊष्मा स्थानांतरण तरल ट्यूब के साथ परिधीय ऊष्मा स्थानांतरण तरल व्यवस्था भी है। इस अध्ययन से यह निष्कर्ष निकला कि उच्च

प्रारंभिक तापमान वाले धातु हाइड्राइड संयंत्र में अधिक ऊर्जा भंडारण दक्षता प्राप्त हुई है। परिधीय ऊष्मा स्थानांतरण तरल प्रवाह व्यवस्था (configuration 2) के साथ धातु हाइड्राइड संयंत्र ने बेहतर ऊष्मा स्थानांतरण के लक्षणों को दिखाया है। परिधीय ऊष्मा स्थानांतरण तरल प्रवाह व्यवस्था के साथ 823 K पर धातु हाइड्राइड संयंत्र के लिए 96.4% की अधिकतम तापीय ऊर्जा भंडारण दक्षता प्राप्त की गई है।

अलग अलग धातु हाइड्राइडों पर किए गए विश्लेषणों के परिणामों का उपयोग करके एक द्विधातु हाइड्राइड प्रणाली विकसित की गई है। ऊर्जा भंडारण पदार्थ की विभिन्न ऊष्मा चालकताओं के साथ ऊष्मा स्थानांतरण और प्रदर्शन की विशेषताओं के लिए द्विधातु हाइड्राइड प्रणाली का अध्ययन भी किया गया है। जब उच्च तापीय धातु हाइड्राइड की ऊष्मा चालकता 0.5 W/(m.K) से बढ़ाकर 4 W/(m.K) कर दी जाती है, तो द्विधातु हाइड्राइड प्रणाली की ऊर्जा भंडारण दक्षता 94.44% से बढ़कर 95.11% हो जाती है। इसके अलावा, ऊष्मीय और ऊर्जा भंडारण की विशेषताओं को ज्ञात करने के लिए एकल धातु हाइड्राइड प्रणाली और द्विधातु हाइड्राइड प्रणाली की तुलना की गयी है। एकल धातु हाइड्राइड प्रणाली की तुलना में द्विधातु हाइड्राइड प्रणाली की अधिकतम ऊर्जा भंडारण दक्षता अधिक पाई गई है। एकल और द्विधातु हाइड्राइड आधारित ऊष्मीय ऊर्जा भंडारण प्रणाली के लिए ऊर्जा भंडारण पदार्थ के अधिकतम औसत तापमान में वृद्धि क्रमशः 33 K और 4 K पाई गई।

संक्षेप में, यह अध्ययन द्विधातु हाइड्राइड प्रणाली के ऊष्मा स्थानांतरण और प्रदर्शन का विस्तृत विश्लेषण प्रस्तुत करता है। इस अध्ययन में एकल धातु हाइड्राइड प्रणाली और द्विधातु हाइड्राइड प्रणाली के ऊष्मा स्थानांतरण और प्रदर्शन की विशेषताओं की तुलना की गई है। इस विश्लेषण के परिणाम उच्च तापीय अनुप्रयोगों के लिए प्रभावी ऊष्मा स्थानांतरण और ऊर्जा भंडारण की विशेषताओं में वृद्धि के साथ धातु हाइड्राइड आधारित ऊष्मीय ऊर्जा भंडारण प्रणाली के रूपांकन की सुविधा प्रदान करेंगे।

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Nomenclature

Symbol

A	Constant $\{\Delta s/R\}$
B	Constant $\{\Delta s/R\}$ (K)
C	Rate constant (1/s)
c	Specific heat capacity (J/kg.K)
D	Diameter of MH bed (mm)
d	Diameter of HTF tubes (mm)
dT	Temperature difference (K)
E	Activation energy (J/mol)
g	Gram
h	Heat transfer coefficient (W/m ² K)
hp	Horsepower
l	Length (mm)
lpm	Litre per minute
m	Mass (g or kg)
mA	Milliampere
mbar	Millibar
msec	Milli second
M	Molar mass (g/mol)
p	Pressure (bar)
Q	Energy (J)
R	Universal gas constant (J/mol.K)
T	Temperature (K)

t	Time (s or min)
u	Velocity (m/s)
v	Volume (m ³)
wt%	Weight density (%)

Greek symbols

Δh	Enthalpy of reaction (J/mol)
Δs	Entropy of reaction (J/mol.K)
ε	Porosity
μ	Dynamic viscosity (Pa.s)
μm	Micrometer
ρ	Density (kg/m ³)
K	Permeability (m ²)
λ	Thermal conductivity (W/(m.K))
η	Efficiency (%)

Chemical element symbols

Al	Aluminum
Ar	Argon
Ce	Cerium
Co	Cobalt
Cr	Chromium
Cu	Copper
Fe	Iron
H ₂	Hydrogen gas
La	Lanthanum

Mg	Magnesium
Mg-Ni	Magnesium nickel
Mn	Manganese
Ni	Nickel
Sc	Scandium
Ti	Titanium
V	Vanadium
Y	Yttrium
Zr	Zirconium

Subscripts

a/abs	Absorption
b	Bottom
d/des	Desorption
emp	Empty
eq	Equilibrium
h	Hydrogen
HTF	Heat transfer fluid
ini	Initial
l	Length
MH	Metal hydride
r	Radius
rec	Received
rel	Released
sat	Saturated

s	Solid (metal hydride)
sto	Stored
sup	Supplied
t	Top

Abbreviations

A	Ampere
AC	Alternating current
ACR	Area cross section ratio
AR	Aspect ratio
bcc	Body centered cube
CSP	Concentrated solar power
CSTP	Concentrated solar thermal power
DoE	Department of energy
DC	Direct current
ENG	Expanded natural graphite
hcp	Hexagonal closed pack
HTF	Heat transfer fluid
HTMH	High temperature metal hydride
IEA	International energy agency
IRENA	International Renewable Energy Agency
LCoE	Levelized cost of electricity
LES	Latent energy storage
LTMH	Low temperature metal hydride
MH	Metal hydride

NV	Needle valve
PCI	Pressure composition isotherm
PCM	Phase change material
PV	Photovoltaic
rpm	Revolution per second
SES	Sensible energy storage
SEM	Scanning electron microscope
SS	Stainless steel
STPP	Solar thermal power plant
TCES	Thermochemical energy storage
TES	Thermal energy storage
V	Volt
WEC	World energy congress
XRD	X-ray diffraction
2-D	Two dimension
3-D	Three dimension