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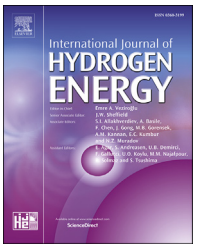

Effect of metal hydride properties in hydrogen absorption through 2D-axisymmetric modeling and experimental testing in storage canisters

Raquel Busqué [a,*], *Ricardo Torres* [b], *Joan Grau* [b], *Vicente Roda* [a], *Attila Husar* [a]

[a] *Institut de Robòtica i Informàtica Industrial, CSIC-UPC, Llorens i Artigas 4-6, 08028, Barcelona, Spain*
[b] *Fluid Mechanics Department, EEBE UPC – Barcelona Tech, C/ Eduard Maristany, 10-14, 08019, Barcelona, Spain*

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ABSTRACT

A two-dimensional axisymmetric model is developed to study the hydrogen absorption reaction and resultant mass and heat transport phenomena inside a metal hydride canister. The model is compared against published literature and experimental data. Experimental tests are performed on an in-house fabricated setup using different cooling scenarios. An extensive study on the effects of the metal properties on charging performance is carried out through non-destructive testing (NDT). Results show that the properties that most influence the charging performance are: absorption rate constant (C_a), activation energy (E_a) and thermal conductivity (k^m). A Higher porosity (ε) reduces charging time and amount of hydrogen stored while a higher cooling level produces a faster charging process. These results can be used to select metal hydride materials but also to estimate the metal hydride internal state and the process can be used for future evaluation of metal hydride degradation.

Introduction

As energy consumption increases, society, industry and governments have become aware of the necessities to invest in sustainable energies that can decrease the problems associated with the use of fossil fuels and other non-renewable sources. Recent studies [1] show that the use of hydrogen as an energy vector can aid to satisfy the present and future energy demands without additional carbon emissions.

Due to its calorific value and being environmentally friendly, hydrogen energy has become a possible replacement for fossil fuels, depending on how it is produced. As hydrogen is abundant in water and in various hydrocarbons, it could be easily produced using renewable energy sources. Hence, it can facilitate the transition from the present fossil fuel energy economy to a future hydrogen based economy [2,3].

A major concern that needs to be addressed to make hydrogen technology economically feasible is the safe storage of hydrogen in vessels with the desirable weight, volume and cost. The future of hydrogen as an energy vector will strongly depend on these technologies [4].

Hydrogen has the particularity of having a very low energy density per unit of volume, so it requires a lot of volume to

* *Corresponding author.*
E-mail addresses: rbusque@iri.upc.edu (R. Busqué), ricardo.torres@upc.edu (R. Torres), joan.grau@upc.edu (J. Grau), vroda@iri.upc.edu (V. Roda), ahusar@iri.upc.edu (A. Husar).
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Nomenclature

C_a	Absorption rate constant $[s^{-1}]$
E_a	Activation Energy $[kJ\ mol^{-1}]$
$\vec{g}$	Gravity $[m\ s^{-2}]$
h	Convection coefficient $[W\ m^{-2}K^{-1}]$
H/M	Hydrogen to metal ratio
k	Thermal conductivity $[W\ m^{-1}K^{-1}]$
K	Permeability $[m^2]$
m	Mass $[kg]$
M	Molecular weight $[kg\ mol^{-1}]$
n	Number of moles $[mol]$
$\vec{n}$	Normal vector
p	Pressure $[Pa]$
R	Universal gas constant $[J\ mol^{-1}K^{-1}]$
S	Source term
t	Time $[s]$
T	Temperature $[K]$
$\vec{u}$	Velocity field$[m\ s^{-1}]$

Greeks

ΔH	Reaction enthalpy$[kJ\ mol^{-1}]$
ΔS	Entropy $[J\ mol^{-1}K^{-1}]$
ε	Porosity
θ	Absorbed hydrogen fraction
μ	Dynamic viscosity$[kg\ m^{-1}s^{-1}]$
ρ	Density $[kg\ m^{-3}]$

Subscripts

0	Initial
emp	Empty
eq	Equilibrium
m	Mass (source term)
sat	Saturation
T	Energy (source term)
in	Inlet
atm	Atmospheric
amb	Ambient

Superscripts

eff	Effective
g	Gas
m	Metal
ref	Reference

store a large amount of energy in gaseous state. This is a problem when there is a limited amount of storage space available, for example in automotive applications.

Hydrogen can be stored in many ways, for example as a compressed gas inside high-pressure tanks. In order to satisfy space limitations and energy requirements depending on the application, pressures are typically around 70 MPa. These levels of pressure cause safety concerns and a high energy cost when pressurizing the tanks.

Liquid storage in cryogenic tanks constitutes another possible alternative. The problem is that it would require extremely low temperatures and also a cooling system that would have high energy costs as well.

Hydrogen can also be stored as an absorbed element in solid porous materials (metal hydride) [5]. Metal hydride based hydrogen storage offers certain advantages compared to high-pressure gaseous or cryogenic liquid storage systems in terms of compactness, storage at conditions close to ambient, possibility of tailoring metal hydrides to suit different temperature-pressure requirements, as well as being inherently safe because hydrogen is stored at low pressure [6–8]. The disadvantage is that it offers low energetic density per unit of mass due to the weight of the metal itself. But on the contrary, it offers a high energy density per unit of volume.

A primary application of hydrogen storage is proton exchange membrane fuel cells (PEMFCs), which use pure hydrogen as their fuel [9].

Prior studies show that reactions in metal beds can be effectively modeled as a two-dimensional problem. Jemni and Ben Nasrallah developed two-dimensional heat and mass transfer models for hydrogen absorption and desorption respectively [10,11]. Their results show that the difference between the solid and hydrogen temperatures is negligible, except for some limited areas close to the gas outlet and tank wall, so the local thermal equilibrium hypothesis can be used. In a subsequent study, Jemni et al. [12] conducted an experimental test to determine the effective thermal conductivity, the equilibrium pressure, and reaction kinetics to validate the theoretical model. A good agreement between measured and theoretical results was obtained.

Muthukumar et al. [13,14] numerically investigated the performance of a metal hydride storage device at different supply pressures, cooling fluid temperatures, overall heat transfer coefficients and bed thicknesses using a two-dimensional heat and mass transfer model. An analysis of the performance of a storage system with embedded cooling tubes during the absorption of hydrogen was also carried out. Different container geometries, depending upon the number and arrangement of cooling tubes inside the hydride bed were simulated.

Also Jiao et al. [15] studied the effects of cooling level and charging pressure in a two-dimensional axisymmetric model. They concluded that increasing the heat transfer coefficient (cooling the bottle) and charging pressure improves the hydrogen absorption.

Nam et al. [16] developed a three-dimensional model to study the hydrogen absorption reaction, heat and mass transport phenomena in a metal hydride hydrogen storage tank. A parametric study was carried out for various designs and hydrogen feed pressures. The simulation results demonstrate that the external surface to volume ratio is one of the key factors to determine the hydrogen absorption performance, and that the use of a higher hydrogen supply pressure leads to not only rapid hydrogen charging performance but also a reduction in the cooling burden of the tank.

Chung et al. [17] investigated the influences of buffer area and heat convection. The hydrogen storage canister comprises of a cylindrical metal bed and a void buffer area above the metal. The buffer area is considered as a domain of pure hydrogen gas. Simulation results show the buffer area reduces the reaction rates by increasing thermal resistance to the heat transfer from the outside cooling/heating bath.

Regarding experimental results, Dhaou et al. [18] empirically studied hydriding/dehydriding rates and the pressure–concentration isotherms for different metal

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