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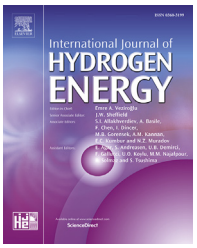

Mathematical modeling, numerical simulation and experimental comparison of the desorption process in a metal hydride hydrogen storage system

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 desorption reaction and its subsequent discharge in a metal hydride canister. Experimental tests are performed on an in-house fabricated setup. An extensive study on the effects of the metal properties and boundary conditions on discharging performance is carried out through non-destructive testing (NDT). Results show that the desorption process is more effective if the activation energy for desorption (E_d) and the reaction enthalpy (ΔH) decrease, and when the desorption rate coefficient (C_d) and the external convection heat transfer coefficient when the bottle is being heated (h) increase. Furthermore, porosity (ε) can be useful for the design of hydrogen storage systems, with a trade-off between charge/discharge time and storage capacity. Numerical and experimental results are compared achieving a good agreement. These results can be used to select metal hydride materials and also for the future evaluation of metal hydride degradation.

Introduction

In the last decades, the fossil fuel consumption has been steadily increasing and so, society, industry and governments have become aware of the necessities to invest in sustainable energies to reduce the carbon emissions. 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.

Hydrogen has been considered a good, carbon-free alternative to hydrocarbon fuels, as it is abundant in water and 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].

* *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 $[s^{-1}]$
C_d	Desorption rate constant $[s^{-1}]$
c_p	Heat capacity $[J\ kg^{-1}K^{-1}]$
E_a	Activation energy for absorption $[kJ\ mol^{-1}]$
E_d	Activation energy for desorption $[kJ\ mol^{-1}]$
f_L	Pressure loss coefficient $[kg\ m^{-4}s^{-1}]$
$\vec{g}$	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	Molecular weight $[kg\ mol^{-1}]$
$\vec{n}$	Normal vector
p	Pressure $[Pa]$
p_{eq}	Equilibrium pressure $[Pa]$
R	Universal gas constant $[J\ mol^{-1}K^{-1}]$
S_m	Mass source/sink term $[kg\ m^{-3}s^{-1}]$
S_T	Energy source/sink term $[W\ m^{-3}]$
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

a	Absorption
amb	Ambient
atm	Atmospheric
B	Bottom
d	Desorption
emp	Empty
h	Heater
ini	Initial
L	Lateral
ref	Reference
sat	Saturation

Superscripts

eff	Effective
g	Gas
m	Metal

Hydrogen storage techniques have been widely evaluated in recent years, and have been categorized in three main areas [5]:

1. High pressure gaseous hydrogen storage
2. Liquefaction of hydrogen gas and liquid-phase hydrogen storage
3. Material-based hydrogen storage, including: sorbents, chemical hydrogen storage materials and metal hydrides

Hydrogen stored as an absorbed element inside metal hydride materials offers certain advantages compared to high-pressure gaseous or cryogenic liquid storage systems in terms of compactness, storage at conditions close to ambient, energy required to store the hydrogen, 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 high energy density per unit of volume.

A lot of studies have been made regarding the modeling of hydrogen storage in metal hydride systems, but most of these studies are focused on hydrogen absorption reactions [2,6,8–20], and numerical studies of the hydrogen desorption process are relatively rare [3,14,19–27].

Prior studies show that reactions in metal beds can be effectively modeled as a two-dimensional problem. Jemni and Ben Nasrallah [12,22] developed two-dimensional heat and mass transfer models for hydrogen absorption and desorption respectively. 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. [28] experimentally determined the effective thermal conductivity, the equilibrium pressure and the reaction kinetics, as well as the temperature and the pressure over time. Then, they tested the validity of the theoretical model comparing it to the experimental results achieving a good agreement between all the data.

Regarding desorption, the main interest has been the enhancement of the reaction focusing on its thermal behavior. For this purpose, Chung et al. [14] developed a two-dimensional model and investigated the effects of heat convection on the charging/discharging performance. Both Darzi et al. [19] and Mellouli et al. [21], analyzed the cooling and heating of a cylindrical $LaNi_5$ metal hydride tank together with some kind of heat exchanger. The firsts ones, used an annular jacket filled with a phase change material (PCM), and the latter ones compared three different heat exchanger designs. They concluded that a properly designed heat exchanger can reduce the hydrogen charging/discharging times considerably. Moreover, Delavar et al. [24], numerically studied effects of parameters such as: heating fluid temperature around the tank, hydrogen outlet pressure, and heat transfer coefficient between heating fluid and the metal hydride storage tank during the hydrogen release. On the other hand, Wang et al. [29] studied two different scenarios during absorption, positioning the metal hydride bottle vertically or horizontally on the model. Unfortunately, neither Chung et al. [14], Darzi et al. [19], Mellouli et al. [21], Delavar et al. [24] nor Wang et al. [29] provided a comparison of the hydrogen desorption simulations with experiments.

Additionally, Kyoung at al [26]. developed a three-dimensional metal hydride model to be used for the design of industrial metal hydride storage vessels. The model was validated against the experimental data reported by Jemni et al. [28] achieving a good agreement. Mohammadshahi et al. [30] also focused on a practical application. They improved the metal hydride model to incorporate several features, such as: temperature variation of the cooling fluid or introduction of the non-ideal gas equation.

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