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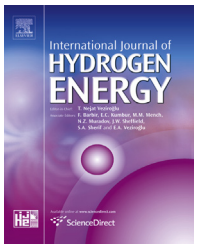

A case study of a hydride container performance applying non dimensional parameters

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ABSTRACT

Many efforts have been done so far to understand sorption dynamics of hydride containers for hydrogen storage. Particularly, there are many articles in literature where experimental results for different hydride systems and container set-ups were successfully simulated using basically the same group of models. This fact is the base of a previous work where we defined a series of non dimensional parameters which may be used to estimate absorption time of hydride containers.

In this work we compare estimated absorption times with experimental outcomes for a prototype hydride container. We performed non dimensional analysis of our finned container prototype at two scales, i.e.: overall or macroscopic container scale and pore or microscopic scale. We discuss about this simplified model approach that allows estimating, with few parameters, the reaction time of a complex-geometry prototype.

The prototype container was designed according to the results of a numerical optimization that maximized the amount of hydrogen absorbed for a 3 min charging period. Experimental results indicate good agreement between estimated and experimental absorption time, making the non dimensional method a useful tool at preliminary stages of hydride container design.

Introduction

Hydrogen as energy carrier has some technical limitations that need to be addressed to promote its massive use. One major issue is hydrogen storage, owing to its low density and high chemical reactivity. Storage by means of hydrides is a feasible option, especially when considering stationary applications. Hydride systems might be less expensive than high pressure or cryogenic storage that need a large amount of energy for compressing or liquefying the hydrogen. This results in hydride systems having lower operational cost [1].

Hydride containers are complex systems. Sorption reactions involve considerable reaction heat while the effective thermal conductivity of hydride powder is quite low. This causes important temperature changes that limit the sorption

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Nomenclature

1D	one dimensional
$\widehat{C}$	pressure drop parameter, bar
C_{sg}	hydride capacity, kg H_g/kg hydride, –
ΔH	molar entalpy of reaction, J mol^{-1}
E	activation energy, J mol^{-1}
ε	hydride porosity, –
F	heat conductive material fraction, –
k	thermal conductivity, W m^{-1} K^{-1}
$\widehat{k}$	kinetics constant, s^{-1}
K	pressure drop coefficient
L	characteristic length, m
m	mass, kg
$\dot{m}$	mass flow rate, kg s^{-1}
n	pressure drop exponent, –
M	molecular weight, kg mol^{-1}
NDC	non dimensional conductance, –
NDFT	non dimensional fill time, –
NDK	non dimensional kinetics, –
P	pressure, bar
R	ideal gas constant, 8.315 J mol^{-1} K^{-1}
SS	stainless steel
δ	density, kg m^{-3}
t	time, s
τ	characteristic decay time, s
T	temperature, K
V	volume, m^3

Subindex

0	fitting parameter
1	fitting parameter
90%	at 90% of total capacity
abs	absorption
cont	container
d	heat conductive material
des	desired (reaction time)
e	equilibrium
eff	effective
ext	external
g	hydrogen gas
kin	kinetics
line	hydrogen line
max	maximum
MH	metal hydride and interstitial hydrogen mixture
pore	pore
s	hydride or solid
supply	hydrogen supply to hydride container
tank	hydrogen tank

reaction. When analyzing hydride containers both thermal and chemical issues have to be assessed simultaneously obtaining temperature and hydrogen concentration profiles, usually by numerical tools ([2–5] also see Table 1 in the work of Melnichuk et al. [6]). These profiles depend on the absorbing material, the container geometry and conductivity, pressure and temperature conditions and hydrogen flow through the metal hydride bulk [7]. Furthermore, in some cases the reaction kinetics of the absorbing material cannot be disregarded.

In addition to these phenomena, which were modeled and predicted by many authors, we observe an appreciable degree of uncertainty in some parameters such as porosity and thermal conductivity of the metal hydride. Both parameters also vary during sorption reaction, for reasons such as the volume change of the particles during hydration [8]. According to sensitivity analysis, thermal conductivity of the hydride could have a significant effect on the global reaction time [9].

Table 1 – Parameters for non dimensional calculations.

Parameter	Value	Reference
T_{max} (°C)	60.9 (P_g = 30 bar)	This work
ΔH_{Abs} (J mol_g^{-1})	27,020	This work
C_{sg} (kg_g/kg_{MH})	1.15×10^{-2}	This work
k_d (W m^{-1} K^{-1})	138	[12]
ρ_s (kg m^{-3})	8.3×10^3	[13]
ε	0.5	[13]
κ_{abs} (s^{-1})	59.2	[14]
E_{abs} (J mol_g^{-1})	21,170	[14]
P_e (bar)	3.4 (T_{ext} = 0 °C)	This work
	7.7 (T_{ext} = 20 °C)	This work

Therefore, considering the complexity of the physical system and the uncertainties introduced by some parameters, a simplified model providing an estimated reaction time, could be useful and even desirable in comparison to more complex models.

In this work we analyze the reaction time of a prototype hydride container using non dimensional parameters that were presented in a previous work [6]. The objective of this work is to compare the estimated absorption time obtained by non dimensional analysis with experimental results, and to certain extent to validate these theoretical predictions. The container was designed based on the results of a numerical optimization that maximized the amount of hydrogen absorbed for a 3 min charging period [10]. Therefore it is expected that most of the absorption would occur during that time.

Non dimensional parameter analysis

Outline

In a previous work we developed a series of non dimensional parameters that provide an approximate measure of the relative importance of the different factors on the absorption process of a hydride container [6]. It is worth noting the same concepts can easily be applied to desorption dynamics. This work was based on the non dimensional conductance (NDC) defined by Visaria et al. [9], which can be regarded as the approximate ratio between the thermal evolution time and the desired charging time.