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Numerical simulation of the parametric influence on the wall strain distribution of vertically placed metal hydride based hydrogen storage container

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ABSTRACT

Metal hydride hydrogen storage alloys show significant thermal variations and dimensional non-homogeneity during their charge–discharge cycles. Pulverization, settling and agglomeration of these alloys and the consequent densification influence the rate of hydrogenation and wall strains on storage containers. In this study, numerical simulation of the wall strain distribution of a vertically placed hydrogen storage device is conducted with LaNi₅ as the hydrogen storage alloy. The influence of salient parameters such as bed thickness, hydrogen supply pressure and coolant temperature on wall strains is studied with its already known effect on sorption performance. Effect of the densification of hydride particles during hydriding is also studied.

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Introduction

Safe and effective means for storage of hydrogen is the major bottleneck in the realization of hydrogen economy. Solid state hydrogen storage devices using metal hydride alloys offer significant advantages over compressed and liquefied forms of hydrogen in terms of volume as well as energy requirements. However factors such as system weight, durability, operability and container compatibility need improvement to make it commercially viable.

Heat transfer is the major sorption rate controlling factor for metal hydrides with fast sorption kinetics. Hydriding of

these alloys also causes significant increase in lattice volume which can lead to fragmentation of hydride particles. Particles pulverized during charge–discharge cycles descend to the bottom of the container and finally agglomerate. This expansion, pulverization and subsequent agglomeration under high temperature cause strains on container walls. These strains can cause significant deformation or even failure of the container.

Most heat and mass transfer studies in hydride beds deal with 1D, 2D or 3D formulation of conservation equations in cylindrical coordinates. Early investigations [1,2] reported in literature deal with the radial variation of concentration and temperature. Existence of local thermal equilibrium between

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Nomenclature

b	bed thickness, m
B	shape factor
C_p	specific heat, $\text{J kg}^{-1} \text{K}^{-1}$
D	diffusivity, $\text{m}^2 \text{s}^{-1}$
E	activation energy, J mol^{-1}
F	reacted fraction
h	heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
h_b	bed height, mm
H_a	activation enthalpy, J
M	molecular weight, kg kmol^{-1}
\dot{m}	rate of hydrogen absorbed, $\text{kg m}^{-3} \text{s}^{-1}$
p	pressure, Pa
r	radial coordinate, m
R	universal gas constant, $\text{J K}^{-1} \text{mol}^{-1}$
t	time, s
T	temperature, K
Y	Young's modulus, N m^{-2}
z	axial coordinate, m

Greek letters

ΔH^0	heat of formation, J kg^{-1}
κ	permeability, m^2
λ	thermal conductivity, $\text{W m}^{-1} \text{K}^{-1}$
μ	dynamic viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
ϕ	porosity
θ	polar coordinate, radian
ρ	density, kg m^{-3}

Subscripts

a	absorption
d	desorption
e	effective
eq	equilibrium
f	fluid
H	hydrogen
s	solid
sat	saturated
0	initial condition

the solid and gas phases is assumed in these formulations. Their studies established heat transfer as the single most important factor that influences the sorption rate.

Majority of the work reported on the numerical study of heat and mass transfer in hydride bed deals with 2D conservation equations in differential form. In the more generalized version of this equation, investigators [3,4] reported separate mass and energy equations for these two phases. Even though thermo-physical properties are kept constant in several studies, more accurate models consider these properties as appropriate functions of hydrogen concentration, temperature and porosity. A discussion on thermal design and heat and mass transfer aspects of practical metal hydride based hydrogen storage devices have been made by the author [5,6]. These studies identified bed thickness, hydrogen supply pressure and coolant temperature as the salient parameters affecting hydrogenation performance.

A few experimental studies which examine the mechanical behavior of hydride container have also been reported in

literature. Experiments by Okumura et al. [7] showed that hydride particles get pulverized and fine particles settle gradually towards the bottom, causing very low porosity in these regions. McKillip et al. [8] and Nasako et al. [9] demonstrated the occurrence of high strains near the container bottom and attributed them to the reduced porosity in those regions. Ao et al. [10] found that these wall strains vary with hydrogen loading and cycle number.

Even though geometric parameters such as bed thickness and operating parameters such as hydrogen supply pressure and coolant temperature affect the hydrogenation performance of the storage device, their effect on the wall strains is not reported. The present paper deals with the effect of these parameters on the wall strains of a cylindrical, vertically oriented metal hydride based hydrogen storage container. The effect of hydride densification is also studied.

The physical model

Fig. 1 shows the schematic of vertically placed hydrogen storage container with central filter and outer cooling jacket. The device is filled with alloy particles to the given height. Hydrogen inducted at the given supply pressure to the container is distributed through the centrally located filter. Length of this filter tube is equal to the container length to avoid pressure variation in the bed.

During hydriding, storage intermetallics release sorption heat to the coolant circulated through the jacket. As heat transfer at the outer boundary of the storage bed is higher

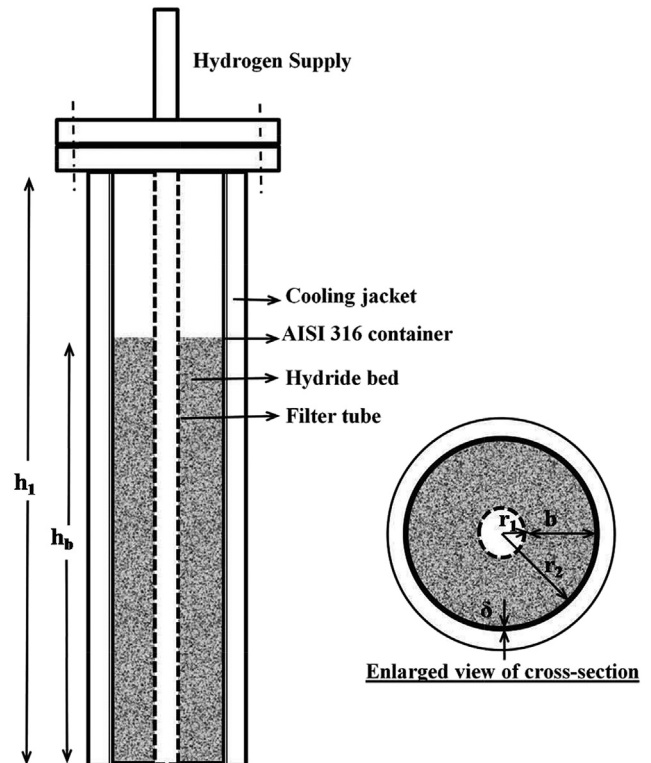


Fig. 1 – Schematic of metal hydride hydrogen storage container with central filter and annular cooling jacket.

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