Thermophysical properties of a deformable metal hydride bed

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Abstract:
A better understanding of the physicochemical phenomena of interaction between hydrogen and metal hydrides are necessary. Therefore, the determination of the properties physics that control transfers in metal hydrogen reactors, namely conductivity, absorption and desorption reaction kinetics, specific heat, permeability and porosity of the medium is of great interest. In this study, a mathematical model describing thermophysical properties of a deformable metal hydride bed has been developed, taking into account the expansion phenomen of the metal hydride bed during hydrogen absorption process.

Key words*: Metal hydride, thermophysical proprieties, deformable bed.*

1. INTRODUCTION

It is evident that "metal hydride" systems have become of extreme importance. Due to their thermodynamic properties, metal hydrides have been used to develop a large number of applications such as thermal and electrical energy storage units, hydrogen storage, heat systems, water pumps, heat engines, electric batteries, Ben Nasrallah et al. (1994) and Faouzi et al. (2009).

Recently, modeling and simulation studies of metal hydride reactors have been carried out in order to evaluate their performance Shahrzad et al. (2016). These studies assumed, for hydride beds, that the study medium is undeformable, but in reality the metal hydride tends to fragment into small particles which expand and contract upon absorption and desorption of hydrogen, respectively. For example, $LaNi_5$ undergoes a reversible volume expansion of around 25% Mellouli et al. (2016). This can cause strong metal hydride beds to form. packed, which can damage the container containing the metal hydride when they expand or swell, Gopal et al. (1995).

In a deformable hydride bed, the shear strain results from a change in granular volume, thus resulting a variation in physical properties (permeability, porosity, specific heat and thermal conductivity) of the metal hydride bed, Demircan et al. (2005).. In previous studies have been shown that the change in physical properties depends on the amount of absorbed hydrogen, which in turn varies with the volumetric strain, Mellouli et al. (2016). This study proves the anisotropy of physical properties induced by deformations in a deformable metal hydride bed.

Moreover, the physical properties of the deformable metal hydride bed such as porosity, effective conductivity, heat specific, and the particle diameter depend on the concentration of hydrogen. While there is no study that takes into account the influence of anisotropy on heat transfer within a hydride bed deformable.

In this paper we present a model which takes into account the swelling of the metal and its effect on the properties thermophysics of metal hydrides.

2. Expansion of the crystal lattice

2.1. *The Deformable volume*

Upon absorption of hydrogen the alloys underwent a reversible expansion of volume of around 25%. The penetration of the hydrogen atom in the interstices of the crystal lattice of the alloy causes a increase in particle size (Fig. 1).

This deformation depends on the quantity hydrogen atom penetrated, therefore mass fraction of hydrogen

It is assumed that the volume expansion is a linear relationship with the mass fraction of hydrogen, Mellouli et al. (2016).

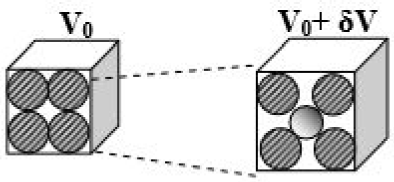
Therfore, the volume of the solid after absorption of hydrogen is:

$$vol(\tfrac{H}{M}) = vol\left(\left(\frac{H}{M}\right)_0\right) + \left(\frac{H}{M}\right)\delta_{vol} \tag{1}$$

During hydrogen absorption, the mesh of the crystal lattice increases by an equal volume ratio, Mellouli et al. (2016):

$$\delta_{vol} = \frac{V_{max} - V_{s0}}{\left(\frac{H}{M}\right)_{max}} \tag{2}$$

Figure.1 Crystal lattice expansion



Therfore the volume of solid after swelling is :

$$V(\tfrac{H}{M}) = V\left(\left(\frac{H}{M}\right)_0\right) + \left(\frac{H}{M}\right)\delta_{vol} = V\left(\left(\frac{H}{M}\right)_0\right) + \left(\frac{H}{M}\right)\frac{V_{max} - V_{s0}}{\left(\frac{H}{M}\right)_{max}} \tag{3}$$

Where,

$$V_s(\tfrac{H}{M}) = V_{s0}\left[1 + \left(\frac{V_{s\,max}}{V_{s0}} - 1\right)\frac{\left(\frac{H}{M}\right)}{\left(\frac{H}{M}\right)_{max}}\right] \tag{4}$$

2.2. *Evolution of the particle diameter :*

The particle diameter changes with the mass fraction of hydrogen according to the following relation, Gopal et al. (1995):

$$D(\tfrac{H}{M}) = D_{s0}\sqrt[3]{1 + \left(\frac{V_{s\,max}}{V_{s0}} - 1\right)\frac{\left(\frac{H}{M}\right)}{\left(\frac{H}{M}\right)_{max}}} \tag{5}$$

3. *Thermophysical proprieties of the Metal hydride:*

3.1. *Prosity :*

The porosity varies with the size of the particles which in turn varies depending on the hydrogen concentration, Mellouli et al. (2016):

$$\varepsilon(\tfrac{H}{M}) = \frac{V_{Pore}}{V_{tot}} = \frac{V_{tot} - V_s\left(\frac{H}{M}\right)}{V_{tot}} \quad (6)$$

Therfore the porosity is expressed by the following relation:

$$\varepsilon(\tfrac{H}{M}) = 1 - \frac{V_{s0}}{V_{tot}}\left[1 + \left(\frac{V_{s\max}}{V_{s0}} - 1\right)\frac{\left(\frac{H}{M}\right)}{\left(\frac{H}{M}\right)_{\max}}\right] \quad (7)$$

The figure. 2 shows the change in porosity as a function of the mass fraction of hydrogen.

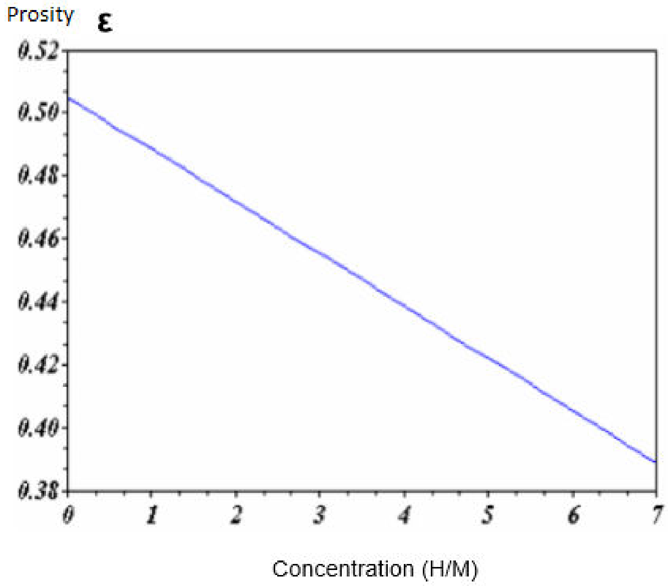


Figure 2. Variation of the hydride bed porosity as a function of the mass fraction

The porosity decreases when the mass fraction of hydrogen increases, this is explained by the increase in the volume of solid and consequently in the total volume of the metal hydride bed.
The similar study of experimental investigation of the swelling/shrinkage of hydride bed have been presented by Masahiro et al. (2013) and Benoit et al. (2012) and they found the similar results in which the porosity changes only due to the particle expansion and contraction.

3.2. *Permeability :*

Permeability characterizes the suitability of the environment porous to allow the fluid contained in pores. The model for estimating the permeability, depending on the average diameter of grains assumed to be spherical is that Kozeny-Carman:

$$k(\tfrac{H}{M}) = V_{s0}\frac{\varphi_s D^2 \varepsilon\left(\frac{H}{M}\right)^3}{150\left(1 - \varepsilon\left(\frac{H}{M}\right)\right)^2} \quad (8)$$

Particles are spheres $\varphi_s = 1$

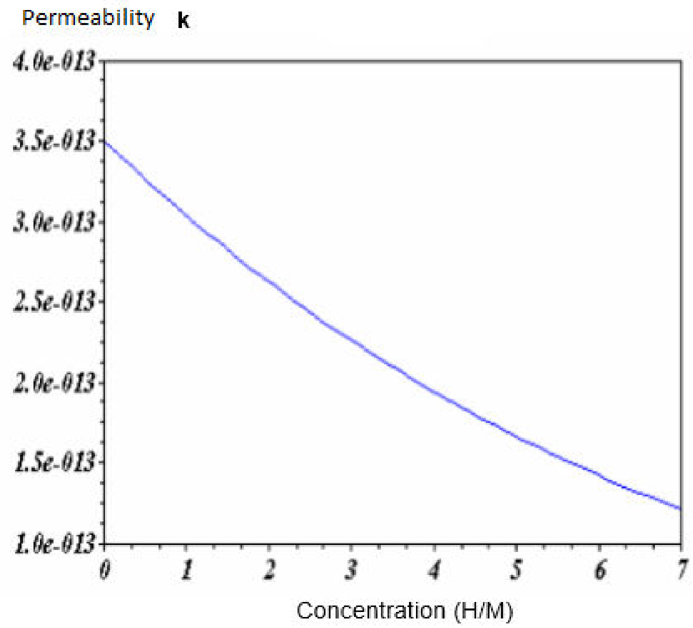


Figure 3. Variation of the permeability as a function of the mass fraction

The figure. 3 shows the change in permeability as a function of the mass fraction of hydrogen. The permeability decreases with the increase in the amount of hydrogen absorbed by the metal as the pore size decreases.

3.3. *Specific heat :*

The specific heat of alloys varies with the ammount of the absorbed hydrogen Gopal et al. (1992). Therefore, it's far vital to take thinking about this change. This observe carried out Neumann Kopp's rule which proves that molar specific heat is about same to the sum of heats of the atoms that make up the alloy.

We carried out Dulong Petit's rule for the molar specific heat of La and Ni. The molar specific heat of hydrogen is taken 10.04 J mol^{-1} K^{-1}. Therfore the specific heat of the hydride bed is expressed as fellow:

$$C_{ps}\left(\tfrac{H}{M}\right) = \frac{\left(3.1R + 10.04\left(\frac{H}{M}\right)\right)\times 6}{M_{alloy} + 6\left(\frac{H}{M}\right)} \times 1000 \qquad (9)$$

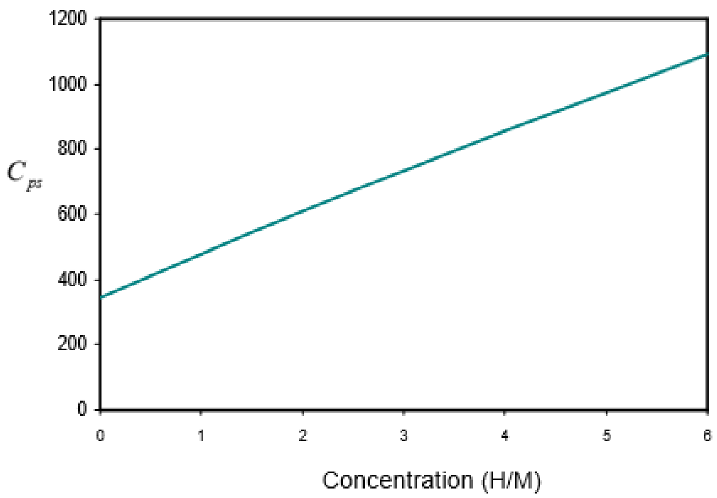


Figure 4. Variation of the specific heat of $LaNi_5$ depending on the mass fraction

The change in the specific heat Cps given in Figure 4 above increases linearly with the increase in the mass fraction of hydrogen.

3.4. *Effective Thermal Conductivity :*

The metal hydride bed thermal conductivity increases with absorbd quantity of hydrogen, Muthukumar et al. (1994) and Choi et al. (1990). This can occur due to changes of thermophysical properties of the alloy and the swelling phenomen of the bed.The correlation was used in this study and its expressed as following:

$$\lambda_{eff} = 0.06 + 0.4 \frac{\left(\frac{H}{M}\right)}{\left(\frac{H}{M}\right)_{\max}} \tag{10}$$

The evolution of thermal conductivity effective given by figure 4 below increases linearly with increasing the mass fraction of hydrogen because the absorption reaction is exothermic.

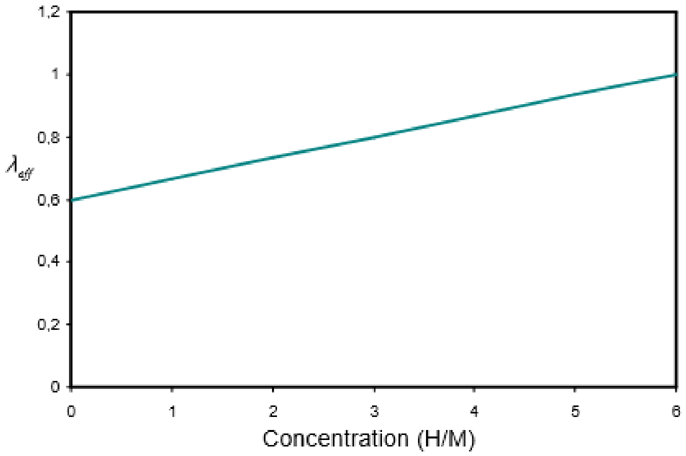


Figure 5. Change in effective thermal conductivity of $LaNi_5$ depending on the mass fraction

Conclusion:

In this article, the formulas of the thermophysical properties of a deformable metal hydride bed was developed. The thermophysical properties was expressed as a function of the reacted hydrogen fraction at absorption process.

This study showed that the thermophysics properties of the metal hydride bed: the porosity, the thermal conductivity, the specific heat, and the permeability depend on the reacted hydrogen fraction absorbed by the alloy. The formulas of the thermophysical properties are expected to prove useful for mathematical modelisation and numerical simulations of metal hydride packed beds that take into account the phenomen of the swelling/shrinkage of hydride beds.

Nomenclature

C_p	Specific heat
D	Diameter
$\frac{H}{M}$	Hydrogen Concentration
k	Permeability

V	Volume
ε	Porosity
Subscript	
Eff	Effevtive
Max	Maximum
0	Initial
S	Solid
Tot	Total
Vol	Volume

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