A Study of Thermo-Fluid Behaviour in Tubular Metal Hydride Beds in the Hydriding Process

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Abstract

Hydrogen, the most abundant element in the universe, has great potential as an energy source, and can be generated from renewable energy sources. It is also produces more energy per unit weight than any other fuel. However, low density hydrogen exposes several storage problems such as high pressure and large volume requirements. Storing hydrogen efficiently in metal hydride compounds appears to be the storage method of the future due to high volumetric storage, capacity, compaction, safety, environmental friendly [1-5]. An accurate mathematical modeling is required to optimize the design and operating parameters of such storage systems, to make up for the weak points of experimental studies and to understand fully the hydrogen reaction and heat transfer mechanisms. This approach is made by COMSOL Multiphysics, in where some partial differential equations are numerically solved. We used this software for the solution of the energy, mass and momentum balance equations that describe the hydrogen absorption and desorption procedure. Thermodynamic or engineering properties like the reaction enthalpy ΔH , entropy ΔS , metal's porosity and the tank dimensions were changed in order to affect the hydrogenation/dehydrogenation procedure. Reducing the enthalpy to -37,600 J/mol the process was not possible while the optimum value was found to be close to -32,600 J/mol. Considering that the porosity is up to 0.75 the reaction is more intensive but it becomes slower after about 130 s. By increasing the dimensions of the tank, the reaction becomes barely strong but slower while by reducing the size of the tank, the reaction becomes faster but the heat exchange becomes lower. In Figure 1 and Figure 2 we present the results of the metal hydride tanks by using the same and different properties. In the present study, we have examined the effect of changing thermodynamic and engineering parameters on the absorption of hydrogen by using different values that were determined experimentally. The change of ΔH and ΔS can significantly affect the reaction because they affect the equilibrium pressure, according to Van't Hoff's law. The increase of porosity could change the reaction due to the fact that the volumetric storage area becomes larger. Finally, the dimensions of the reactor seems to play a major role in the reaction and it seems that as the volume of the reactor increases the hydrogen has more space to move so the mean free path increases. The Knudsen number increases affecting

significantly the permeability. As the absorption of hydrogen is a very complex process, with a wide number of variables it is critical the knowledge of the macroscopic and microscopic values in the process in order to control and optimize the metal hydride tank.

Reference

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Figures used in the abstract

Figure 1: Figure 1. The first reactor left in Figure 1a and inner in Figure 1b, has $\Delta H = -32,600$ J/mol, while the second has $\Delta H = -22,200$ J/mol.



Figure 2: Figure 2. Hydriding process for three different reaction enthalpies (Figure 2a), and three different reaction entropies (Figure 2b).