Modeling and Optimization of a Mg-Metal Hydride Rectangular Tank in the Hydriding Process

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Abstract

Using a metal hydride as a material for hydrogen storage is a novel, alternative way for energy application. The metal hydride has the absolute hydrogen quantity which can bear at the material temperature condition and has the property of the chemical reaction which can absorb and desorb the hydrogen according to the mutual relations with the surrounding hydrogen pressure. The temperature and supplied pressure can be easily controlled during the cycling process of hydrogenation and dehydrogenation and the fully understanding of the reaction mechanisms is very important for the proper design of relevant hydrogen storage units. It is difficult to predict accurately the physical phenomena occurring in the bed only by using the experimental approaching method. Thus, a numerically approaching method is necessary to make up for the weak points of experimental study and to fully understand the hydrogen reaction and heat, mass and momentum transfer mechanisms in the metal hydride bed. So the differential equations which describe energy, mass and momentum must be solved. This is performed by using the COMSOL Multiphysics software. The aim of such simulations is to understand how different reactor configurations and operating characteristics affect the absorption process. In the present study we considered two different reactor configurations: the first reactor (BED-1) is a rectangular metal hydride bed containing powdered Mg, while the second tank (BED-2) has holes perpendicular to its large surface, also containing Mg. These holes were organized in the geometry in order to simulate the flux of ambient air through the reactor, which subsequently affects the heat transfer and indirectly the mass transfer of hydrogen atoms through the metal. The hydriding reaction between Mg and hydrogen occurs in the temperature range of 250-3200 degC and has very endothermic characteristics. The comparison of the hydriding kinetics in two different metal hydride beds (BED-1, BED-2) is studying, aiming to find out the best conditions of hydrogen absorption by Mg. In Figure 1, there is a simultaneous change in temperature with time. The presence of holes, seems to reduce the maximum exothermic temperature, but the reaction rate seems to be the same, with maximum absorption rate at 230-240 s. As seen in Figure 2 the pressure decreases faster in the case of the BED-1, which lead us to consider that the reaction is more violent in that case. This is confirmed from the Figure 3, where the concentration at BED-1 approaches the maximum value (6

mol/m^3) faster than BED-2. The total heat fluxes for both beds is seen in Figure 4, where the flux for the BED-2 has a maximum at 420 W/m^2 , which indicates the great heat flux for both the external cooling fluid and between the holes and the bulk. Concluding, the presence of holes seems to affect the absorption of hydrogen and make it less violent, but the reaction for both beds, is very significant.

Reference

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Figures used in the abstract

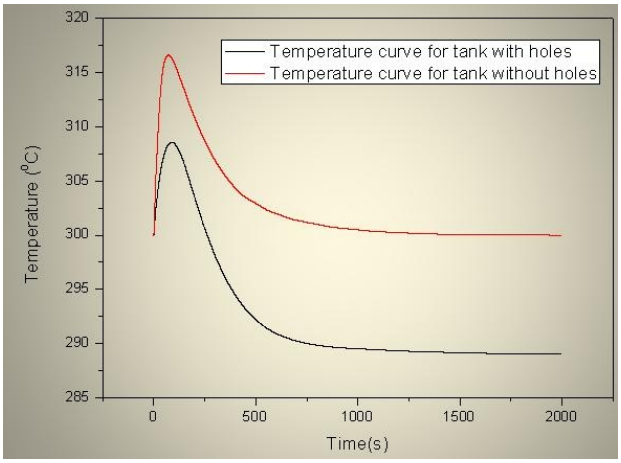

Figure 1: Temperature evolution for BED-1 and BED-2.

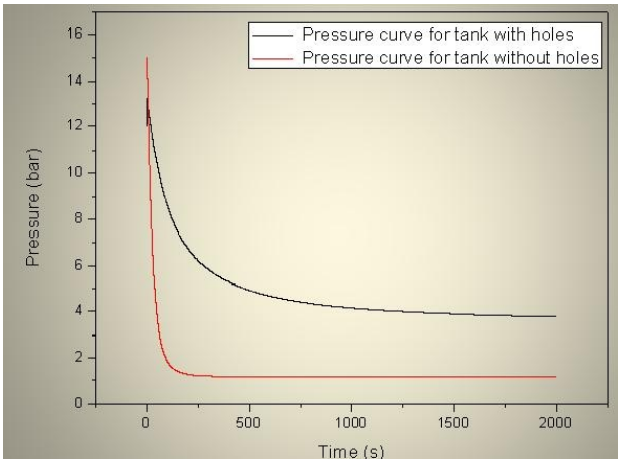

Figure 2: Pressure change for the two beds.

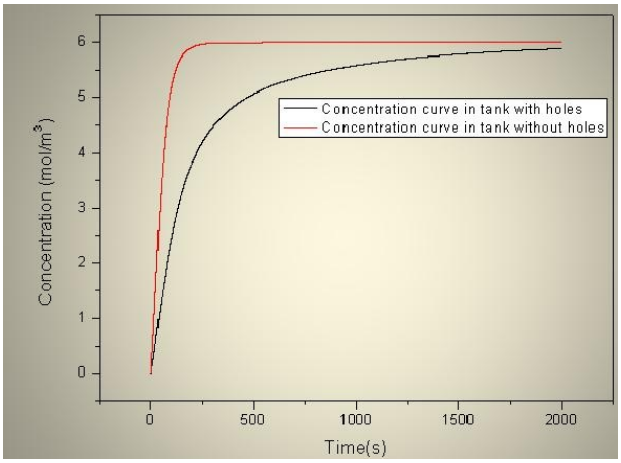

Figure 3: Absorption response for the two hydride bed configurations.

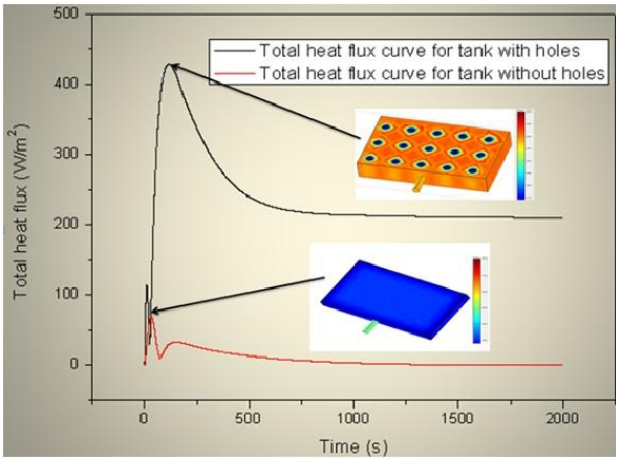

Figure 4: Total heat flux evolution for BED-1 and BED-2 respectively (BED-1 down and BED-2 up are shown).