3D Modeling of Hydrogen Absorption in Metal Hydride Hydrogen Storage Bottles

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Introduction

The highly increasing energy demand and reduction of available fossil energy sources have made it important to develop new techniques for energy storage, being hydrogen a good alternative for the future. That is the reason why the storage of hydrogen as an absorbed element in metal hydride bottles has been studied.

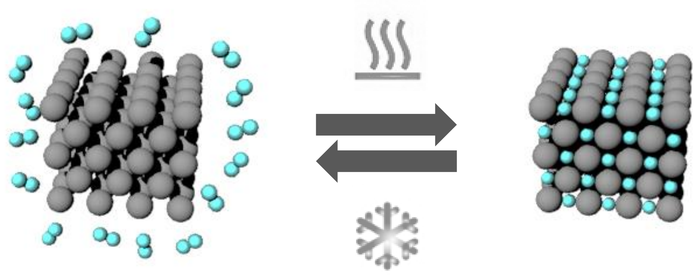

Figure 1. Reaction of H_2 molecule with a storage material

The objective is to study the hydrogen charge process both experimentally and numerically in order to understand how it works and which parameters can be modified to obtain the desired metal hydride behavior.

Computational Methods

Hydrogen flows through the pores of the metal (Brinkman equations), then it is absorbed into the metal through an exothermic reaction (Heat Transfer in Fluids). Consequently the metal hydride density increases due to the addition of hydrogen (Domain ODE and DAE).

$$\varepsilon \frac{\partial \rho^g}{\partial t} + \nabla \cdot (\rho^g \vec{u}) = -S_m$$

$$\frac{\rho^g}{\varepsilon}\frac{\partial \vec{u}}{\partial t} = -\nabla p + \nabla \cdot \tau - \frac{\mu}{K}\vec{u} - \frac{S_m}{\varepsilon^2}\vec{u} + \rho^g \vec{g}$$

$$\frac{\partial \overline{\rho c_p} T}{\partial t} + \nabla \cdot \left(\rho^g c_p^g \vec{u} T\right) = \nabla \cdot \left(k^{eff} \nabla T\right) + S_T$$

A 2D-axisymmetrical and time dependent model has been implemented.

- Initial thermodynamic equilibrium and absence of hydrogen in the bottle.
- Walls are impermeable and convection is applied between them and surrounding air.
- Inlet has a specified temperature and pressure.

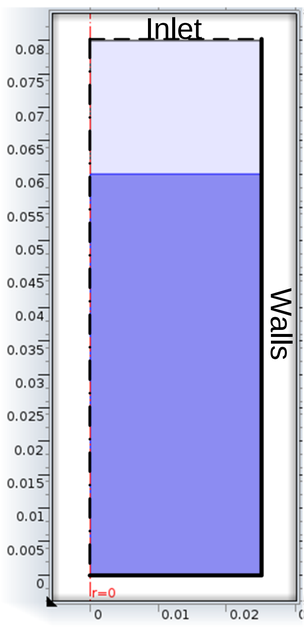

Figure 2. Geometry and boundary conditions

Results and validation

The generated heat is extracted applying a heat transfer coefficient between the walls of the bottle and the surrounding air, which will force the temperature to decrease in the wall region (Figure 3). The effect of the cooling level has great impact on the charging process as the hydrogen absorption rate depends on the bottle temperature. The cooler the bottle is, the higher the absorption rate and the faster the bottle will be filled (Figure 4).

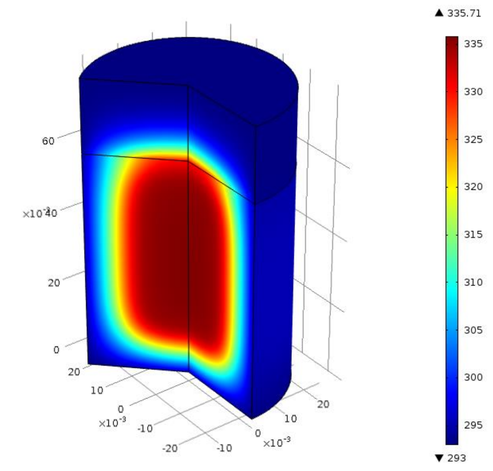

Figure 3. Temperature Distribution inside the bottle. Time=250s and h=1652 W m^{-2} K^{-1}

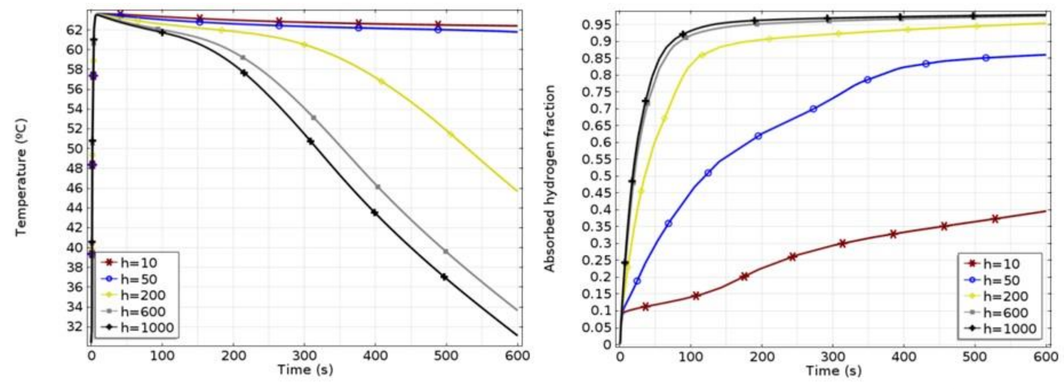

Figure 4. Effect of heat transfer coefficient on the evolution of temperature (left) and absorbed hydrogen fraction (right)

Besides analyzing the effect of the cooling level, a lot of parametric studies regarding metal properties have been carried out in order to discover their influence on the process.

The model has been experimentally validated showing a good agreement in different operating conditions.

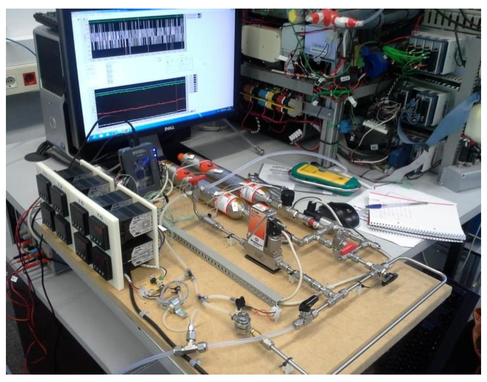

Figure 5. Experimental setup (perspective)

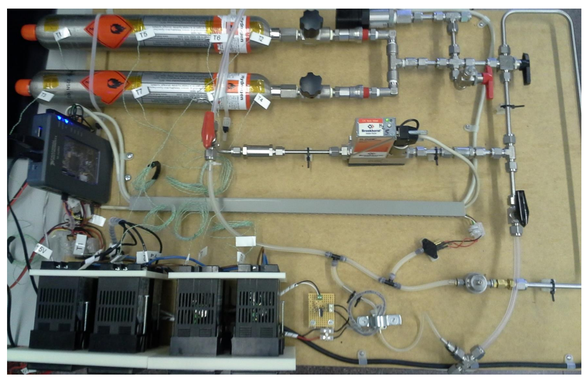

Figure 6. Experimental setup (top)

Conclusions

A three-dimensional metal hydride storage model has been implemented to simulate hydrogen absorption. The validity of this model has been tested experimentally and the calculated results agree well with the experimental data and demonstrate that the model successfully captures key experimental trends. This model has been used to analyze how the different charging variables and the cooling level affect the hydrogen absorption process for different scenarios as well as serving as a base to develop a metal hydride state of charge estimator in the future.

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