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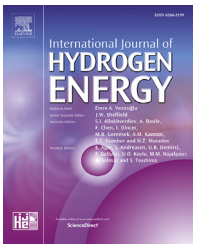

Computational analysis of hydrogen storage capacity using process parameters for three different metal hydride materials

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ABSTRACT

In this study, hydrogen storage capacity were analyzed by considering hydrogen absorption test rig depending on some reactor design parameters such as metal hydride particle size, having fins at the tank, hydrogen inlet pressure, inlet radius of the tank, coolant temperature, general convective heat transfer coefficient and wall thickness of the tank. In the specified design parameters of the hydrogen storage system we put these in COMSOL Multiphysics 5.1 software to obtain some approaches in the large scale. All parameters were analyzed using three different metal hydrides of the $MmNi_{4,6}Al_{0,4}$, $LaNi_{4.75}Al_{0.25}$ and $LaNi_5$. Some parameters like temperature distribution inside the tank, amount of the hydrogen mass to be stored in the tank, the time durations of them and the variations of the equilibrium pressure of the system were optimized.

Introduction

The most significant feature of hydrogen is its ability to be stored. There are numerous methods being used for the storage of hydrogen, like in the form of gas as being compressed, in the form of liquid as being cooled at low temperatures or physically storage within carbon nano tubes. Among the storage methods, it has been indicated that the most effective storage method was the storage in the form of metal hydride due to high storage capacity, suitable operation conditions. Both the hydrogen gas motion and the physical properties of the metal hydride complicate the problem. Therefore several experimental and numerical works exist on different aspects of the designing paramemeters of the storage tanks [1–5]. Some attempts were done by authors in literature about analytical method and numerical simulation. Some others were performed the assessment of metal hydride-based hydrogen storage systems depending on metal alloys, mass flow of hydrogen, process temperature and pressure [6–15].

Jiao et al. [16] studied the effects of various operating conditions on the hydrogen absorption processes in a metal hydride tank. They simulated and reported the relevant equations and formulations by Fluent software. Ye et al. [17] performed the numerical analysis of heat and mass transfer during absorption of hydrogen in metal hydride storage tanks by using HWT 5800 ($Ti_{0.98}Zr_{0.02}V_{0.43}Fe_{0.09}Cr_{0.05}Mn_{1.5}$) metal

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hydride material and reported the hydriding reaction results in 2D mathematical modelling.

Muthukumar et al. [18] studied the parametric aspects of a metal hydride based hydrogen storage device. They concluded that at the supply condition of 30 bar and 298 K, $MmNi_{4.6}Al_{0.4}$ stores about 13.1 g of hydrogen per kg of alloy and that any increment in overall heat transfer coefficient beyond 1250 W/m^2K is not beneficial. In another study, Muthukumar et al. [19] studied the parametric aspects and the numerical analysis of the coupled heat and mass transfer in metal hydride-based hydrogen storage reactor. They concluded that the maximum absorption time difference of about 300 s is obtained for the bed thickness of 17.5 mm at 20 bar supply pressure. Additionally some authors were busy on the computational models and simulations in metal hydride hydrogen storage vessels [20–23].

It is evident from the literature that both the rates of absorption and desorption are controlled by heat and mass transfer characteristics of hydride bed. Further it is clearly observed from the literature that the most relevant parameters for the optimization design of the metal hydrides tank are the hydrogen charge pressure, the permeability and the thermal conductivity of the metal hydride absorbent bed. In view of the above, one can conclude that there is a lack of rigorous heat and mass studies on metal hydride based hydrogen storage device at different operating conditions. Further they have not studied the effects of various operating parameters such as supply pressure, absorption temperature, vessel inner radius, cooling fluid temperature, etc. on the hydrogen storage performance of the reactor. Additionally, the comparison of the effects of using different kind of metal hydrides on the reactor performance has not been studied yet. The present study not only aims to predict the optimum temperature distribution and the maximum amount of hydrogen to be stored in the tank, but also makes easy to understand the comparison among three different metal hydrides of the $MmNi_{4,6}Al_{0,4}$, $LaNi_{4.75}Al_{0.25}$ and $LaNi_5$.

Mathematical model

The mathematical model is developed by COMSOL Multiphysics 5.1 software by using a cylindrical metal hydride storage tank. The hydrogen gas is supplied in order to study the effects of storage tank geometry and different operating parameters. COMSOL software is specialized in solving the coupled heat and mass transfer problems in porous media. The physics are added in the model including energy balance, hydride mass balance, momentum balance and kinetic equations. The geometry of the hydrogen storage tank modelled for the analysis and the parametric dimension variations are given in Table 1. The parameters used as the fixed values for each of $MmNi_{4.6}Al_{0,4}$, $LaNi_{4.75}Al_{0.25}$ and $LaNi_5$ metal hydride materials in the FEM study are shown in Table 2.

Problem formulation

The modelling of the absorption and desorption processes of hydrogen with metal hydride requires a fairly complex modelling approach. Multiple physical equations have to be solved in a such a way that the real situation should be achieved and the generated model should be suited well with the experimental data [24–26]. In addition, these equations should be correctly modelled with each other as well as with the Solver algorithm.

Basically the approaches to be applied are as follows:

a) Free flow of hydrogen is to be modelled by Navier-Stokes momentum equations,
b) The flow in the porous structure of hydrogen to be modelled by Darcy equation,

Table 1 – The geometry of the hydrogen storage tank modelled for the analysis and the variation of its values.

Parameter	Value
Radius	10 mm
Height including metal hydride material	83.6 mm
Free height	27.9 mm
Inlet radius	0.95 mm
Inlet height	8.5 mm
Length of fins	5 mm
Width of fins	1.6 mm
Step for fins	4.6 mm
Number of fins	25
Wall thickness	1.0 mm
Degree of angle of fins	0 deg

Table 2 – The parameters used as the fixed values in the analysis.

Parameter	Metal hydride powder		
	$MmNi_{4.6}Al_{0.4}$	$LaNi_{4.75}Al_{0.25}$	$LaNi_5$
Porosity	0.5	0.5	0.5
Diffusion coefficient (H_2) m^2/s	50×10^{-9}	50×10^{-9}	50×10^{-9}
H_2 initial concentration, g	0	0	0
Initial pressure for the storage tank, Bar	1	1	1
Reaction rate constant (Absorption), 1/s	59.187	59	59.187
Reaction rate constant (Desorption), 1/s	9,57	9.57	9.57
Activation energy – Absorption, J/mol	21179.6	21000	21179.6
Activation energy – Desorption, J/mol	16420	16420	15473
Reaction enthalpy, J/mol	28000	32000	30800
Reaction entropy, J/mol	104.5	100	104.5
Hysteresis factor	0.2	0.2	0.2
Saturation density of metal hydride, kg/m^3	8400	4400	8394
Thermal conductivity of metal hydride, W/mK	1.6	10	1.32
Specific heat value of metal hydride, J/kgK	419	2800	419
Density of metal, kg/m^3	7800	7800	7800
Vessel material heat conduction, W/mK	80	80	80
Specific heat of metal, J/kgK	2000	2000	2000
Time step, S	5	5	5
Total simulation time, S	650	650	650

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