Heat and mass transfer analysis on metal hydrogenreactor filled with $MmNi_{4.6}Al_{0.4}$using a lumped model

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Abstract— **In this paper, a lumped parameter model applied to simulate charge–discharge cycle of the hydrogen storage device filled with MmNi4.6Al0.4using MATLAB. In this study, a simplified lumped model employs general mass and energy balance equations is developed and validated by comparing the simulations to the experimental data available in the literature. The numerical results show that the predicted hydrogen storage for several parameters such as pressure and temperature is in a good agreement with the experimental data.**

Keywords— Hydrogen storage, Metal hydride, Heat and mass transfer.

I. INTRODUCTION

Hydrogen is the most common element in the universe and is an ideal candidate as fuel source (its molecule has the highest energy content per unit weight of any known fuel). Hydrogen can be stored as (i) compressed gas, (ii) cryogenic liquid, (iii) solid fuel as chemical or physical combination with materials, such as metal hydrides, complex hydrides and carbon materials.

Metal hydride based hydrogen storage systems offer higher volumetric density and better safety compared to conventional methods such as compression or liquefaction of hydrogen. Metal hydride is used to supply hydrogen to the fuel cell in many applications. However, on-board hydrogen storage is one of the major issues that need to be resolved.Experimental investigation to determinethe reaction kinetics, equilibrium pressure, and thermal conductivity of hydride bed during both absorption and desorption processes have been performed [1].The basic phenomena which underlie hydrogen absorption and desorption in metal hydrides have long been studied [2], with special focus on their kinetic characteristics, which have been thoroughly analyzed by means of experimental investigations and numerical models.Hydrogen storage has been the subject of intensive research for many years, according to the previous studies. [4-11] developed a 2D and 3D mathematical model for heat and mass transfer in compact cylindrical reactors.

Complicated reactor geometries have been considered, such as an annular metal hydride bed surrounded on both sides by cooling fluid [12], or two concentric annular beds both surrounded by cooling fluid [13], or multiple heat transfer tubes and filters embedded in the metal hydride bed in a cylindrical container [14], in order to provide more insight into absorption kinetics by approaching the working conditions of a real metal hydride storage system.

In a classical lumped model equations describing mass en heat transfer are ordinary differential equations (ODEs) rather than partial differential equations (PDEs). The dependent variables, such as mass absorbed and temperature, are function of time alone and independent of the position (x,y,z) in the reactor. Therefore, in this study, a lumpedmodel is applied to investigate the effects of various parameters on the hydrogen absorption de alloy fills the space between the filter (inner wall of hydride bed) and the inner concentric tube of the reactor. Hydrogen is supplied into the bed radially through a porous filter. as shown in figure 1.

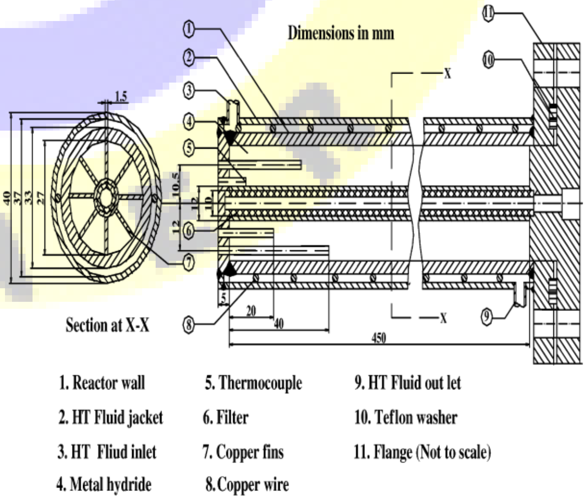


Fig. 1. Original scheme of the storage system, taken from [1].

Nomenclature

A	cell geometric area, m^2
C_a	constant rate for $LaNi_5$, 1/s
C_p	specific heat, J/kg K
D_p	metal hydride particle diameter, m
E_a	activation energy, J/mol H_2
R	universal gas constant, J/mol K
h	heat transfer coefficient, W/m^2 K
k	thermal conductivity, W/m K
K	permeability (m^2)
M	metal hydride
P	gas pressure, bar
P_{eq}	equilibrium pressure, bar
t	time, s
T	temperature, K
$\vec{u}$	

Greekletters

ΔH°	reaction heat of formation, J/kg
ε	porosity
μ	dynamic viscosity, kg/m s
ρ	metal or gas density, kg/m^3
φ	heat transfer rate, W/m^2
ρ	

Subscripts

eff	effective
eq	equilibrium
g	gas phase (hydrogen)
Ss	saturation
S	solide
f	fluide cooling

II. MATHEMATICAL MODELLING

The system is consisted of a cylindrical tank filled with porous $MmNi_{4.6}Al_{0.4}$ and with a cooling (heating) system during absorption (desorption), water was chosen as the heat transfer fluid. A mathematical model was developed to evaluate the transient heat and mass transfer in a cylindrical metal hydride tank and predict the time-varying temperature field and mass of hydrogen stored, as a function of the thermal conductivity of the enhanced hydride material, and thermal boundary conditions. In order to simplify the model, some assumptions have been made. The assumptions made in the present model are as follows: (1) temperature is uniform in the tank; (2) hydrogen is regarded as an ideal gas; (3) local thermal equilibrium is assumed between the solid metal and hydrogen gas; (4) the effect of pressure variation in the tank is negligible; and (5) thermal and physical properties are considered independent of bed temperature and concentration.

II.1. Mass balance for hydrogen

The balance of mass equation for hydrogen may be written as follow:

For absorption:

$$\frac{dm_{H_2}}{dt} = -SC.m_{MH}\cdot\frac{MW_{H_2}}{MW_{MH}}\frac{dx}{dt} + \dot{m}_{in} \quad (1)$$

For desorption:

$$\frac{dm_{H_2}}{dt} = -SC.m_{MH}\cdot\frac{MW_{H_2}}{MW_{MH}}\frac{dx}{dt} - \dot{m}_{out} \quad (2)$$

II.2. Mass balance for metal hydride

The balance of mass equation for metal hydride for absorption or desorption may be written as follow:

$$\frac{dm_{MH}}{dt} = m_{MH}\frac{dx}{dt} \quad (3)$$

II.3. Kinetic reaction

The amount of hydrogen that is absorbed by the metal with time is given by the reaction rate, which is expressed as:

For absorption:

$$\frac{dx}{dt} = C_a\exp\left(-\frac{E_a}{RT}\right)\ln\left(\frac{P_a}{P_{eq}}\right)\left(1-\frac{m_{MH}}{m_s}\right) \quad (4)$$

For desorption:

$$\frac{dx}{dt} = C_d \exp\left(-\frac{E_d}{RT}\right) \ln\left(\frac{P_d - P_{eq}}{P_{eq}}\right)\left(\frac{m_{MH}}{m_s}\right)$$
(5)

II.4. Equilibrium pressure

For absorption:

$$P_{eq} = \left[\frac{\Delta S_a}{R} - \frac{\Delta H_a}{RT} + (\varphi_s + \varphi_0)\tan\left(\pi\left(\frac{x}{x_m} - \frac{1}{2}\right)\right) + \frac{\varphi}{2}\right] 10^5 \quad (6)$$

For desorption:

$$P_{eq} = \left[\frac{\Delta S_d}{R} - \frac{\Delta H_d}{RT} + (\varphi_s - \varphi_0)\tan\left(\pi\left(\frac{x}{x_m} - \frac{1}{2}\right)\right) - \frac{\varphi}{2}\right]$$
(7)

II.5. Energy equation

The energy equation could be expressed as follow:

For absorption:

$$\left(m_{H_2}C_{pH_2} + m_s C_{ps}\right)\frac{dT}{dt} = \dot{m}_{in} C_{pH_2}(T_{in} - T) + AU(T \ldots - \frac{\Delta H_d S C m_s}{MW_{MH}}\frac{dx}{dt} \quad (8)$$

For desorption:

$$\left(m_{H_2}C_{pH_2} + m_s C_{ps}\right)\frac{dT}{dt} = AU(T_{wd} - T) + \frac{\Delta H_d S C m_s}{MW_{MH}} \frac{d\ldots}{d\ldots}$$
(9)

II.6. Initial conditions

Initially, at absorption cycle the temperature, pressure, and the metal hydride mass in the tank are assumed to be constant:

$$T_{in} = T_{wa} \;;\; P_s = P_0 \;\text{ and }\; m_s = m_{s0} \qquad (10)$$

In adsorption cycle the temperature of the reactor is equal to the heating water temperature $T_d = T_{wd}$

III. RESULTS AND DISCUSSION

The present analysis is carried out using a cylindrical reactor of having 27mm internal diameter with 3mm wall thickness and450mm length [1].

Thermo-physical properties of thehydridingalloy and various constants used in the mathematical modeling arelisted in Table 1.

Table 1 shows the thermo-physical properties of metal hydrides, properties of hydrogen and constants used in the analysis [1].

Table1 – List of parameters used in the analysis [1]

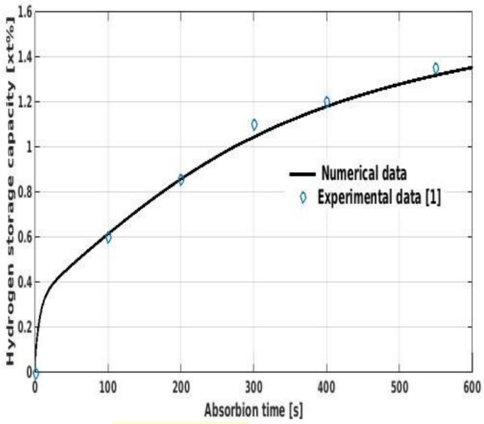
Quantity	Value
Reactor geometry	
Length of the cylinder (mm)	475
Inner radius of inner cylinder (mm)	4.5
Inner radius of outer cylinder (mm)	12
Thickness of cylinder wall (mm)	3
Properties	
Initial and inlet temperature, T_0& T_{in} (°C)	20
Pressures, *P* (bar)	10.0
Porosity of the hydride bed, ε	0.5
Permeability of the hydride bed K (m^{-2})	10^{-8}
Thermal conductivity of the bed, ke (W/m.K)	1.6
Specific heat capacities, C_p (J/kg.K)	419
Activation energy,E_a (J/mol)	21170
Density of the hydride, ρ (kg/m^3)	8400
Reaction constant, C_a (1/s)	100
Properties of hydrogen	
Thermal conductivity of hydrogen, (W/m K)	0.1272
Specific heat of hydrogen, (J/kg K)	14500
Density of hydrogen, (kg/m3)	0.0838
Constants	
Universal gas constant (J/mol K)	8.314
Slope factor(φ_s)	0.35
Constant (φ_0)	0.15

φ

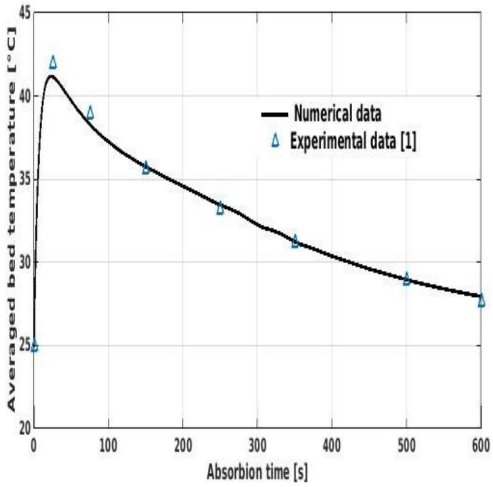
Figs. 3 and 4 showed that the numerically predicted averagebed temperature profile and hydrogen storage capacity at a constant supply pressure of 35 bar, and water inlet temperature of 25 °C are in good agreement with the experimentalresults reported by Muthukumar et al. [1].

Figs. 2 illustrate the effect of supply pressure on hydrogen storage capacity and averaged bed temperature, a lower supply pressures determine lower amounts of absorbed hydrogen,due to thehydriding reaction kinetics. Lower temperatures are alsoreached.

(**A**)

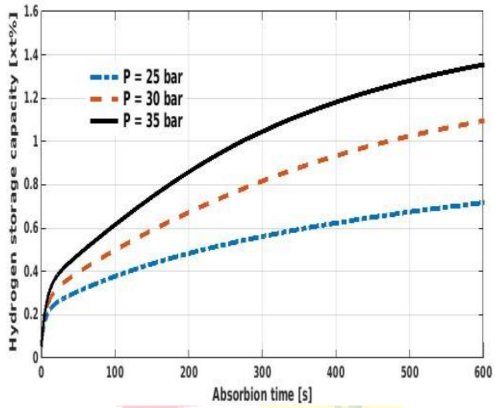


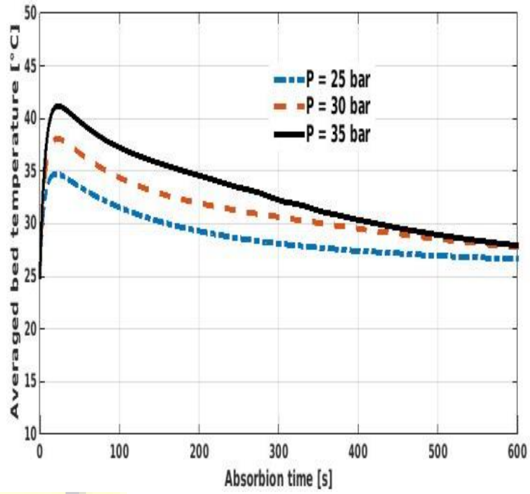
(B)



Figs. 2 – Comparison between experimental data [1] and numerical results of absorption at constant supply pressure (35 bars) on hydrogen storage capacity (A) and averaged bed temperature (B).

(**A**)



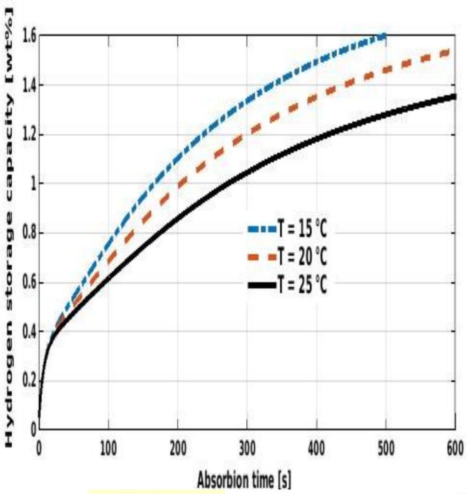


(B)

Figs. 3 – Effect of supply pressure on hydrogen storage capacity (A)and averaged bed temperature (B).

Figs. 3 present theeffect of cooling fluid temperature at constantsupply pressure on hydrogen storage capacity and averaged bed temperature, it is clear to observe from equation (6) that the bed temperature influences the hydride equilibrium pressure. Hence, for a lower temperature allowfor higher amounts of hydrogen to beabsorbed.

(A)



(B)

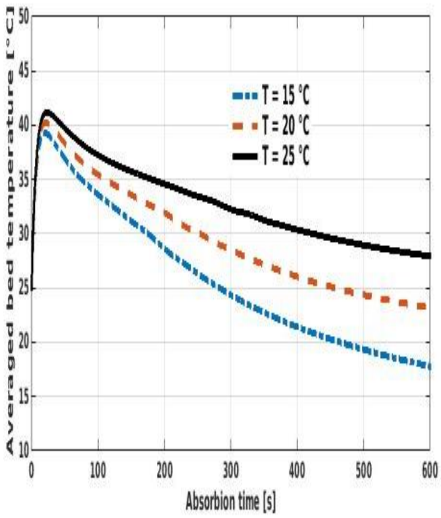


Fig. 4 – Effect of cooling fluid temperature on hydrogen storage capacity (A) and averaged bed temperature (B).

Fig. 5show that the predicted average bed temperatureprofiles during desorption processmatchclosely with the experimental data reported by Muthukumaret al. [1]. Due to the poor thermal conductivity of the metal hydride,the necessary amount of heat is not transferred to the metalhydride bed. Hence, the hydride bed takes the heat from the beditself and starts to desorb the hydrogen.

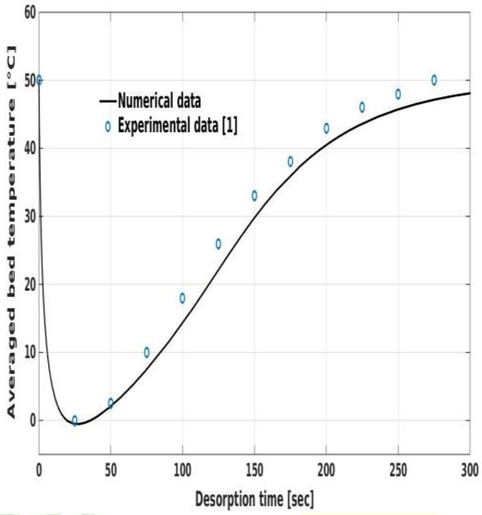


Fig. 5 – Comparison between experimental data [1] and numerical results of desorption at constant supply pressure (1 bar) on hydrogen storage capacity.

The results obtainedfor MmNi4.6Fe0.4 hydride beds during the desorptionprocess are presented in fig. 6 at different hot fluid temperatures varyingfrom 30 to 50 °C.

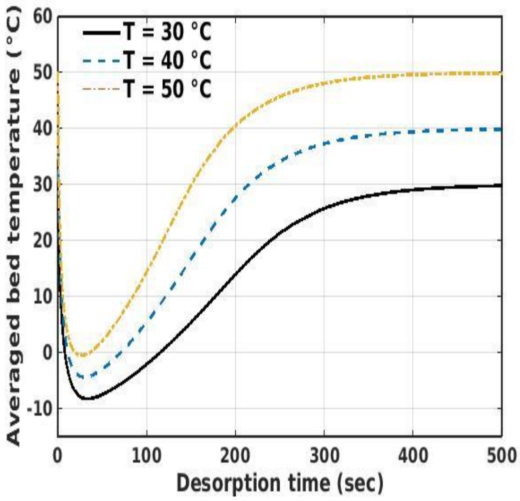


Fig. 6 - Desorption at constant discharge pressure (1 bar), comparison between experimentaldata [1] and numerical results.

VI. Conclusion

In this study, a lumpedmodel of a metal hydridehydrogenstorage system has been developed,to simulate the hydrogen storage system at different supply pressures,cooling fluid temperatures,containing the alloy $MmNi_{4,6}Fe_{0,4}$. The temperature and concentration profiles are reported.The numerical results showed good agreementwith the experimental data reported in the literature.

References

[1] Muthukumar P, Prakash Maiya M, Srinivasa Murthy S. Experiments on a metal hydride-based hydrogen storage device. Int J Hydrogen Energy 2005;30(15):1569–81.

[2] Zu¨ttel A. Materials for hydrogen storage. Mater Today 2003; 6(9):24–33.

[3] M. Gambini, M. Manno, and M. Vellini, \Numerical analysis and performance assessment of metal hydride-based hydrogen storage systems," Int J Hydrogen Energy,vol. 33, no. 21, pp. 6178{87, 2008.

[4] Jemni A, Ben Nasrallah S. Study of two-dimensional heat and mass transfer during adsorption in a metal-hydrogen reactor. Int J Hydrogen Energy 1995;20(1):43–52.

[5] Jemni A, Ben Nasrallah S. Study of two-dimensional heat and mass transfer during desorption in a metal-hydrogen reactor. Int J Hydrogen Energy 1995;20(11):881–91.

[6] Ben Nasrallah S, Jemni A. Heat and mass transfer models in metal-hydrogen reactor. Int J Hydrogen Energy 1997;22(1):67–76.

[7] Jemni A, Ben Nasrallah S, Lamloumi J. Experimental and theoretical study of a metal-hydrogen reactor. Int J Hydrogen Energy 1999;24(7):631–44.

[8] Askri F, Jemni A, Ben Nasrallah S. Study of two-dimensional and dynamic heat and mass transfer in a metal-hydrogen reactor. Int J Hydrogen Energy 2003;28(5):537–57.

[9] Askri F, Jemni A, Ben Nasrallah S. Prediction of transient heat and mass transfer in a closed metal-hydrogen reactor. Int J Hydrogen Energy 2004;29(2):195–208.

[10] Askri F, Jemni A, Ben Nasrallah S. Dynamic behavior of metal-hydrogen reactor during hydriding process. Int J Hydrogen Energy 2004;29(6):635–47.

[11] Mat MD, Kaplan Y. Numerical study of hydrogen absorption in an Lm–Ni 5 hydride reactor. Int J Hydrogen Energy 2001; 26(9):957–63.

[12] Demircan A, Demiralp M, Kaplan Y, Mat MD, Veziroglu TN.Experimental and theoretical analysis of hydrogen absorption in LaNi5 –H 2 reactors. Int J Hydrogen Energy 2005; 30(13–14):1437–46.

[13] Kikkinides ES, Georgiadis MC, Stubos AK. On the optimization of hydrogen storage in metal hydride beds. Int J Hydrogen Energy 2006;31(6):737–51.

[14] Mohan G, Prakash Maiya M, Srinivasa Murthy S. Performance simulation of metal hydride hydrogen storage device with embedded filters and heat exchanger tubes. Int J Hydrogen Energy 2007;32(18):4978–87.

[15] Gambini M. Performances of metal hydride heat pumps operating under dynamic conditions. Int J Hydrogen Energy 1989;14(11):821–30.

[16] Gambini M. Metal hydride energy systems performance evaluation. Part A: dynamic analysis model of heat and mass transfer. Int J Hydrogen Energy 1994;19(1):67–80.

[17] Gambini M. Metal hydride energy systems performance evaluation. Part B: performance analysis model of dual metal hydride energy systems. Int J Hydrogen Energy 1994;19(1): 81–97.