TEMPERATURE AND COMPOSITION DISTRIBUTIONS FOR $FeTiH_{1.6}$ AND Mg_2NiH_4 METAL HYDRIDES FOR TWO DIMENSIONAL HYDROGEN ENERGY CONDUCTION BED MODEL

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ABSTRACT

Hydrogen storage in the form of metal hydrides is receiving great attention for energy storage applications. The present study investigates the behaviour of the discharging process associated with $FeTiH_{1.6}$ and Mg_2NiH_4 metal hydrides through the conduction bed model. A computer code is applied to print out the temperature and metal hydride composition as well as the cumulative discharged hydrogen for different geometries and flow regimes.

1. INTRODUCTION

Hydrogen storage as metal hydrides is recommended for both stationary and ground transport applications from the view points of high volumetric hydrogen density as well as safe handling and long term stability without refrigeration requirements [1,2]. In a previous work [3], the problem of the discharging process associated with metal hydrides through the conduction bed model is solved analytically in space and time under certain simplifying assumptions encountered in the process of physical and mathematical simulation.In the computer code ' TOBAM ' [4], the energy and mass transfer rate associated with discharging process were solved numerically in two dimensions through the use of the alternating direction implicit (ADI) method [5]. The computer code has been carried out to solve the fluid energy equation and to allow for the variation of the fluid physical properties such as the thermal conductivity, specific heat and viscosity with the fluid operating temperature. The computer code gives as output the space - time temperature and metal hydride composition distributions as well as the cumulative discharged hydrogen associated with different bed geometries and flow regimes.

This paper presents the study of the space - time distributions of the temperature and composition of two specific metal hydrides; namely $FeTiH_{1.6}$ and Mg_2NiH_4 as well as the relevant accumulated discharged hydrogen.

2. REFERENCE MODEL

The reference conduction bed model is composed of a multiple of hollow cylindrical or rectangular plate cells. The code is applied to boundary condition alternatives (hereafter called CCTT) in which either convective boundary condition or insulated boundary condition is applied to the inner and outer surfaces of the bed according to the geometry and flow regime. In this alternative (CCTT) the lower surface is maintained at constant inlet fluid temperature while the upper surface is maintained at uniform temperature corresponding to the exit fluid temperature.

Table 1 shows different bed geometries and flow regimes applied in the computer code in order to have common bases for comparison between the cylindrical and the rectangular plate bed geometries. It is assumed

that the contained volume of the metal hydride bed is constant and is equivalent to the volume of a sphere of radius 10 cm. The inner and outer radii of cylindrical geometry were selected to be 1 and 11 cm respectively, and the thickness and height of the rectangular plate geometry were selected to be 20 and 10 cm respectively. The code adjusted the cylinder height and rectangular plate width to yield the constant volume.

The physical properties of $FeTiH_{1.6}$ and Mg_2NiH_4 metal hydrides are extracted from references [6,7]. Design and operating conditions are shown in Tables 2 and 3.

Table 1. Geometries and flow regimes allowed in the computer code.

Bed geometries and its alternative	Flow regime and boundary conditions
Rectangular Plate (P)	Fluid flows over the two opposite rectangular plate sides in the X-direction.
Cylinder (CI)	Fluid flows through a coaxial tube while the outer surface is insulated.
Cylinder (CO)	Fluid flows over the outer surface while the inner surface is insulated.
Cylinder (CIO)	Fluid flows through a coaxial tube also over the outer surface.

3. RESULTS AND CONCLUSIONS

The present results are corresponding to the use of water as the heat transfer fluid for $FeTiH_{1.6}$ metal hydride and the use of air for Mg_2NiH_4. Air is used instead of water for Mg_2NiH_4 , since the use of water will create problems of two phase flow as the equilibrium reaction temperature for this metal hydride is over 250 ° C.

Figure (1) and Figure (2) present the radial temperature distributions at different dimensionless axial distances and at certain discharging time associated with cylindrical geometry and CIO - flow regime for $FeTiH_{1.6}$ and Mg_2NiH_4 metal hydrides respectively. The concave shape of the temperature profiles is due to the endothermic dehydriding reaction. The maximum axial temperature profiles occur at the outer and inner surfaces of the bed (X=0 , X=1), where they are in a direct contact with the heating fluid. The radial temperature profiles are asymmetrical due to the heat transfer areas of the two surfaces perpendicular to the radius are not equal. It is noticed from Figures (2) and (1) that Mg_2NiH_4 has one reaction temperature plateau ' T_R' above which the dehydriding reaction occurs, while for $FeTiH_{1.6}$ there are four temperature plateaus corresponding to the four equilibrium reaction temperatures 17°C ,7°C, 3°C and 1°C. Thus for $FeTiH_{1.6}$ the reaction occurs sequentially from the lower plateau to the higher one. For Mg_2NiH_4 metal hydride, the inside radial locations of the axial temperature profiles 0.2, 0.3 and 0.5 are at the reaction temperature ' T_R' i.e, the dehydriding reaction has not finished yet due to the poor heat transfer properties of air as heating fluid.

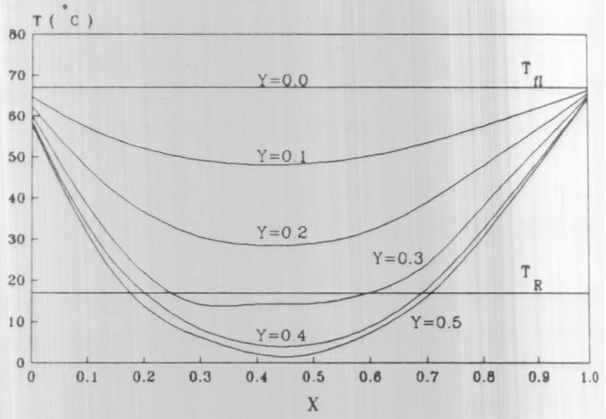

Figure 1. Radial temperature profiles at 60 minutes the discharging time and at different dimensionle axial distances for $FeTiH_{1.6}$.

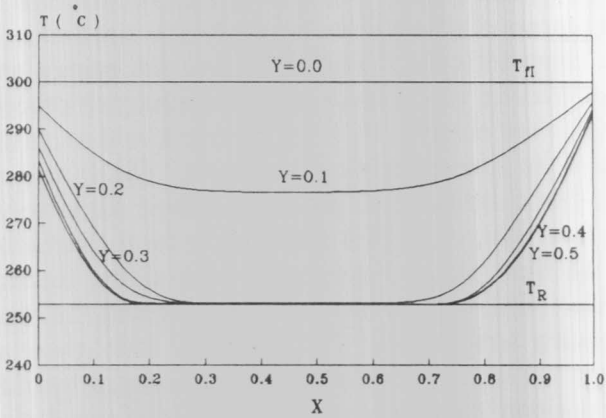

Figure 2. Radial temperature profiles at 180 minut of the discharging time and at different dimensionle axial distances for Mg_2NiH_4.

Table 2. Physical and operating conditions of $FeTiH_{1.6}$.

Parameter	Value
Bed effective thermal conductivity, Cal./cm.sec°C	0.004134
Solid heat capacity, Cal./gm °C	0.15
Solid density, gm/cm^3	5.88
Heat of reaction per unit mass of hydrogen, Cal./gm H_2	
For $FeTiH_x$ with $0.1 \leq x \leq 1.04$	3361.0
For $FeTiH_x$ with $1.04 < x \leq 1.2$	3700.0
For $FeTiH_x$ with $1.2 < x \leq 1.4$	3980.0
For $FeTiH_x$ with $1.4 < x \leq 1.6$	4030.0
Molecular weight, gm /gm mole	105.6
Bed void fraction	0.4
Bed hydrogen pressure, atm.	3.0
Initial hydrogen-to-metal atom ratio	0.8
Final hydrogen-to-metal atom ratio	0.05
Water mass flux, gm/cm^2. sec	10.0
Inlet fluid temperature, T_{fl}, excess the equilibrium reaction temperature of FeTiH, °C	50.0

Table 3. Physical and operating conditions of Mg_2NiH_4

Parameter	Value
Bed effective thermal conductivity, Cal./cm.sec°C	0.0012402
Solid heat capacity, Cal./gm °C	0.25
Solid density, gm/cm^3	2.563
Heat of reaction per unit mass of hydrogen, Cal./gm H_2	7722.22
Molecular weight, gm /gm mole	112.0
Bed void fraction	0.4
Bed hydrogen pressure, atm.	1.0
Initial hydrogen-to-metal atom ratio	1.2
Final hydrogen-to-metal atom ratio	0.1
Air mass flux, gm/cm^2. sec	0.6
Inlet fluid temperature, T_{fl}, excess the equilibrium reaction temperature, °C	50.0

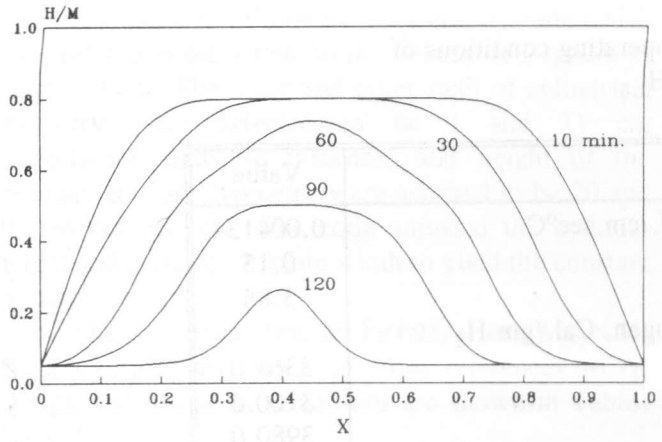

Figure 3. The dimensionless radial behaviour of hydrogen-to-metal atom ratio (H/M) at mid axial plane (Y=0.5) and at different discharging time for $FeTiH_{1.6}$.

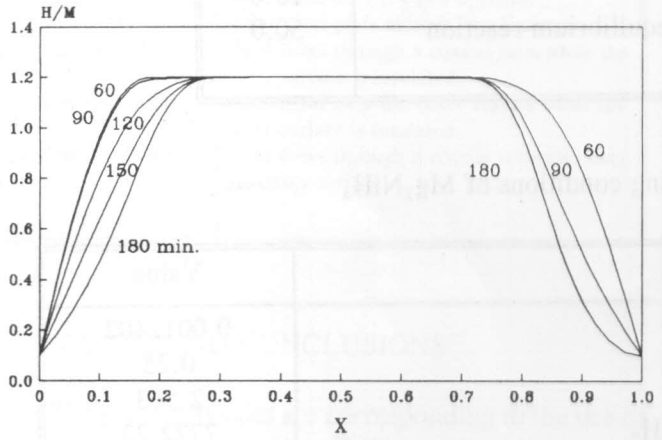

Figure 4. The dimensionless radial behaviour of hydrogen-to-metal atom ratio (H/M) at mid axial plane (Y=0.5) and at different discharging time for Mg_2NiH_4.

Figure (3) and Figure (4) show the radial behaviour of hydrogen - to - metal atom ratio (H/M) for $FeTiH_{1.6}$ and Mg_2NiH_4 respectively at mid axial plane (Y=0.5) and at different discharging time associated with cylindrical geometry and CIO - flow regime. The inner and outer surfaces of the bed (X=0 , X=1) are the most effective locations to liberate hydrogen since they are in direct contact with the heating fluid. From Figure (3), it is obvious that $FeTiH_x$ has four composition plateaus corresponding to the four values of x, *1.6, 1.4, 1.2 and 1.04. Each composition* plateau is characterized by certain equilibrium reaction temperature as mentioned before. The hydrogen is discharged sequentially from the higher composition plateau to the lower one. Thus, there are more than one reaction zone which discharges hydrogen at the same discharging time. The composition (H/M) profile at 60 minutes matches well with the temperature profile at mid axial plane (Y=0.5), since hydrogen discharges from the four composition plateaus. In Figure (4) it is obvious that the dehydriding reaction is still occurring and not all hydrogen has been discharged yet. This behaviour matches well with the temperature distribution which is shown in Figure (2).

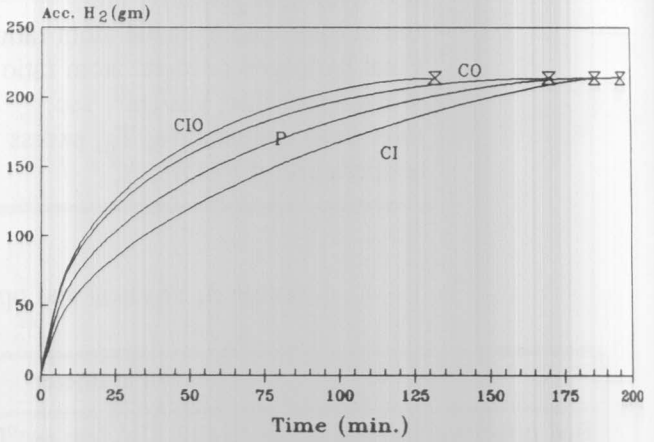

Figure 5. Time behaviour of the accumulated hydrogen in grams for different geometries and flow regimes for $FeTiH_{1.6}$.

Figure (5) and Figure (6) show the time behaviour of the cumulative hydrogen discharged from $FeTiH_{1.6}$ and Mg_2NiH_4 metal hydride storage beds respectively for different geometries and flow regimes. Results have shown that hydrogen discharge rate of $FeTiH_{1.6}$ metal hydride is higher than that of Mg_2NiH_4 metal hydride for all the studied flow regimes. For both the two metal hydrides, it can be shown that for the same volume of metal hydride, the hydrogen discharging rate is the highest for the CIO-flow regime alternative while it is the lowest for the CI-flow regime alternative.

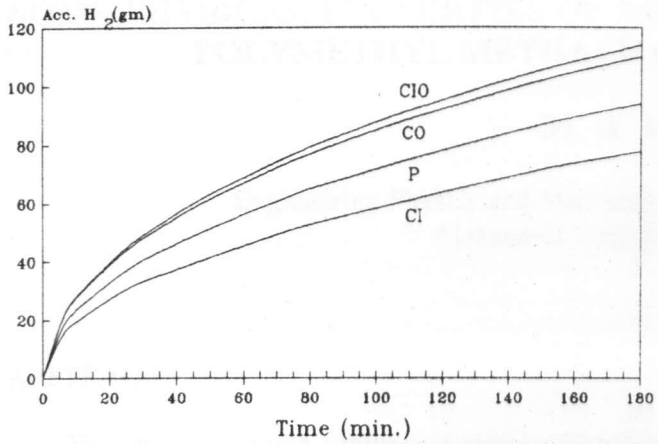

Figure 6. Time behaviour of the accumulated hydrogen in grams for different geometries and flow regimes for Mg_2NiH_4.

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