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NUMERICAL TRANSIENT HEAT TRANSFER ANALYSIS OF REACTOR FOR MAGNESIUM BASED ALLOY FOR HYDROGEN STORAGE APPLICATION

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Abstract - Metal hydrides are potential hydrogen storage media. They release hydrogen at moderate temperatures and pressures. Magnesium hydride is a promising approach for stationary power system application, due to high hydrogen storage capacity by weight. Magnesium hydride based reactor design is more complex due to high thermal energy release and absorption during hydriding reaction and dehydriding reaction, respectively. In this study, results of a numerical modeling study are presented for a 1.5 kg Magnesium alloy based hydriding reactor. Temperature profile in the reactor is computed by FEM analysis using ANSYS software for hydriding and dehydriding reaction. FEM analysis indicates that the reactor temperature is raised from 200 °C to 422 ºC in 20 minutes during the hydriding process. Hence, a "cooling system" is required for maintaining temperature during the hydriding process. During the dehydriding process, maximum temperature drop occurs from 350 °C to 189 ºC in 20 minutes. Therefore, an external heat source of 2 kW is required for maintaining the temperature during dehydriding. Details are presented.

Keywords - *Hydrogen storage; Metal hydride; Hydriding reactor; Finite element analysis.*

I. INTRODUCTION

Hydrogen storage is one of the central technical barriers to the wide deployment of hydrogen energy, particularly for automotive applications (e.g. hydrogen fuel cell vehicles) [1, 2]. Current hydrogen storage methods including gas compression and liquefaction are not optimal due to the associated large quantity of energy consumption and safety issues. A promising alternative is solid metal hydride storage. Metal hydrides absorb / desorb hydrogen at relatively low pressures with a high volumetric density, which offers safety and cost advantage. A very promising approach is to use Magnesium based alloys. Magnesium based alloys are considered promising because of their hydrogen storage capacity, light weight, and low cost compared with alternative systems. The hydride, MgH_2 can store up to 7.6 % mass of hydrogen [3–5].

However, metal hydrides have relatively high heat of reaction and low thermal conductivity [6, 7]. Hence, the performance of metal hydride based reactor depends on the rate at which the amount of heat is supplied during dehydriding process or removed from the metal hydride during hydriding process. Coupled heat and mass transfer with chemical reaction takes place in such systems and therefore the dynamics of hydriding or dehydriding process are complicated. As a consequence, Finite Element Modeling (FEM) analysis of such a system is needed for accurate modeling of the reactor thermal dynamics. In this paper, modeling and transient thermal analysis using ANSYS software of Magnesium alloy based hydriding reactor is presented.

II. METHODOLOGY

The first and basic step is to establish axisymmetric model geometry in Pro/Engineer Wildfire. Geometrical model of metal hydride reactor is created in Pro/Engineer Wildfire and imported through IGES or STEP files into ANSYS software and then fine element mesh is generated. The FEM simulations are performed for various materials used in reactor, hydrogen, metal hydride and cerawool (as insulation). The analysis is based on transient thermal analysis of metal hydride reactor in which following parameters are considered: the operating temperature of the reactor, temperature of surrounding atmosphere of the reactor as well as free convection and radiation heat transfer on the external boundaries of the outer cylinder of the reactor. Transient thermal analysis determines temperature profile as a function of time.

III. RESULTS & DISCUSSIONS

A. Modeling

Modeling serves as a tool to optimize the reactor design. The physical model of the metal hydride reactor is illustrated in Fig. 1. The system consists of two concentric tubes. The inner tube of the reactor is a porous filter. It distributes the hydrogen gas uniformly throughout the reactor. A porous filter is used as the inner most tube of 50 mm diameter. Importance of the porous filter is to prevent the fine hydride particles from being carried away by the hydrogen gas during dehydriding reaction. Stainless steel mesh having 1 µm pore size is used as porous filter. The annular space between the porous filter and the outer tube is filled with the alloy (Mg based alloy

composition). This hydride stored reactor is designed for 1.5 kg capacity of metal hydride alloy. Fig. 2 shows the cross section view of physical components of the metal hydride reactor system.

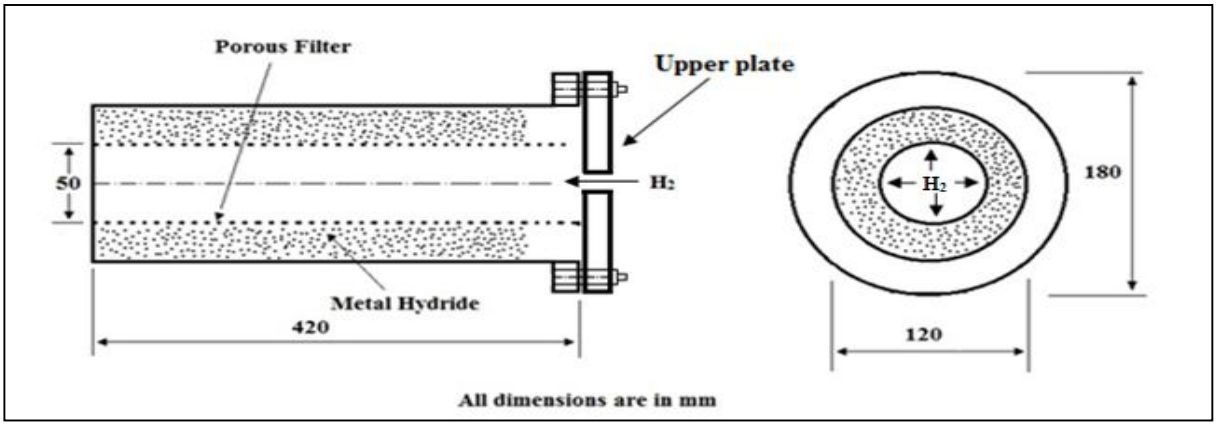

Fig. 1 : Schematic diagram of coaxially cylindrical metal hydride reactor

B. Mesh generation

Mesh generation is one of the most critical aspects of engineering simulation. Too many mesh cells may result in long solver runs, and too few may lead to inaccurate results. ANSYS meshing technology provides a means to optimize the mesh size and geometry. It has been built on the strengths of stand-alone class meshing tools. Fig. 3 shows the fine meshing of the metal hydride system. Total number of elements used are 92,374 and the number of nodes are 1,94,099.

C. FEM analysis

The performance of metal hydride reactor system depends on the metal hydride alloys used. In this analysis, we have used a Magnesium alloy composition. The fine meshed model of reactor is generated by ANSYS software for FEM analysis. For the transient thermal analysis of reactor, standard technical parameters
are considered, which are reported in literature (see Table 1). The following assumptions are made for simplifying the transient thermal analysis:

- The porous metal hydride is considered as a solid.
- Heat transfer and absorption by hydrogen is neglected.
- Heat transfer through the metal hydride bed is assumed uniform.
- The formation enthalpy, density, thermal conductivity and specific heat of MgH_2 are independent of concentration and hydrogen pressure.
- Strength of heat source during hydriding reaction is constant. Similarly, during dehydriding, the heat sink is assumed to be a constant.

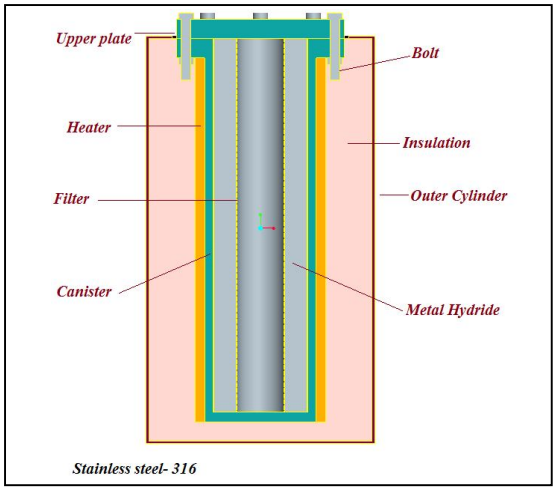

Fig. 2 : Cross-section view of metal hydride reactor;

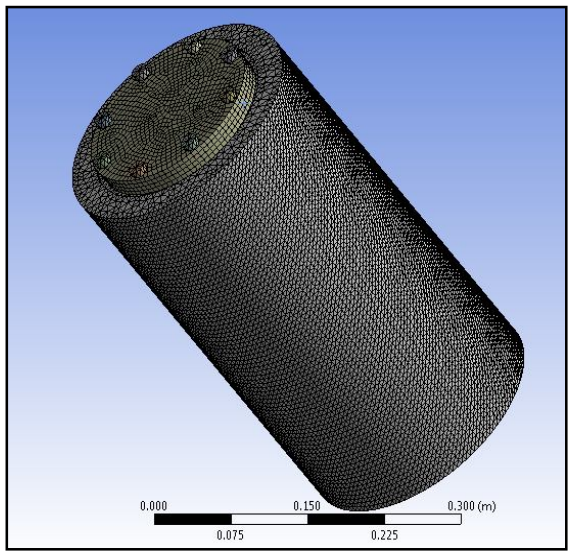

Fig. 3 : Meshed model

TABLE I : A COMPILATION OF VARIOUS THERMO-PHYSICAL PROPERTIES USED FOR FEM ANALYSIS

Parameter	Value
Properties of Hydrogen	
Thermal conductivity	0.1272 W/m·K
Specific heat	14.283 kJ/kg·K
Density	0.0838 kg/m3
Molecular mass of hydrogen	2.01588 g/mol
Properties of MgH2	
Thermal conductivity	5 W/m·K
Specific heat	1013 kJ/kg·K
Apparent density	981 kg/m3
ΔH (formation enthalpy)	75 kJ/mol H_2
ΔS (entropy of reaction)	120 J/mol H_2·K
Properties reactor (SS-316 type)	
Thermal conductivity	21.4 W/m·K
Specific heat	550 kJ/kg·K
Density	8.027 kg/m3
Emissivity	0.6
Properties of cerawool insulation	
Thermal conductivity	0.04 W/m·K
Specific heat	0.67 kJ/kg·K
Density	64 kg/m3
Universal gas constant (R)	8.314 J/mol·K

1) Hydriding process:

For the hydriding reaction, hydrogen is supplied to Mg alloy bed through the porous filter. This reaction is an exothermic chemical reaction. Hence, it absorbs hydrogen by releasing heat (75 kJ per mole of hydrogen).

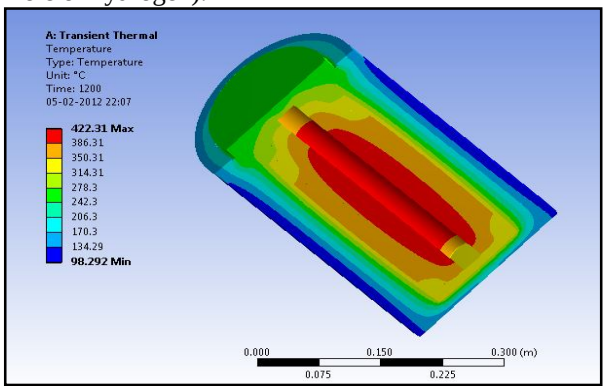

Fig. 4 : Temperature distribution during hydriding process at time, t=1200 sec, after initiation of hydriding

Therefore, temperature increases during hydriding process. This reaction occurs at a temperature of 200 ºC and a pressure of 30 bar. Maximum 80 to 90 % moles of hydrogen is absorbed within the first 20 minutes. Hence, for transient thermal analysis, we consider 1200 sec for hydriding reaction time. Absorbed total number of moles of hydrogen is 37.5 moles. Therefore, total released heat is 2.34 kW during hydriding reaction. Therefore, for transient thermal analysis, initial boundary conditions are formulated as below:

- Initial temperature of reactor is 200 ºC.
- Heat generation rate in metal hydride bed is 2.34 kW.
- Hydriding reaction time is 1200 sec.
- Free convection and radiation heat transfer boundary condition on outer cylinder are assumed. For simplicity, we use heat transfer coefficient for free convection to air at atmospheric pressure and moderate temperature for vertical cylinder (the heat transfer coefficient is 5 $W/m^2 \cdot ºC$).

The above boundary conditions are applied and the transient problem solved using ANSYS solver. Results are obtained in the form of temperature distribution in metal hydride reactor (See Fig. 5). The maximum temperature rise during hydriding process is 422 ºC in first 20 minutes. Fig. 6 shows temperature profile with respect to time, which clearly indicate that the temperature rises up to 290°C in the first 5 minutes only.

Based on the study, an optimal strategy for operating the reactor is devised. Essentially, after first 5 minutes of hydriding (by which time the temperature increases to 290 ºC as per FEM study), the flow of hydrogen is switched off and the reactor allowed to cool by natural convection and radiation to its optimal operating temperature of 220°C.

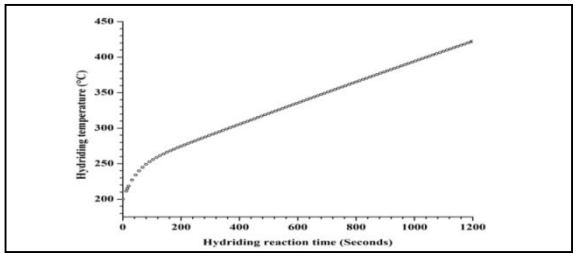

Fig. 5 : Temperature profile during hydriding process

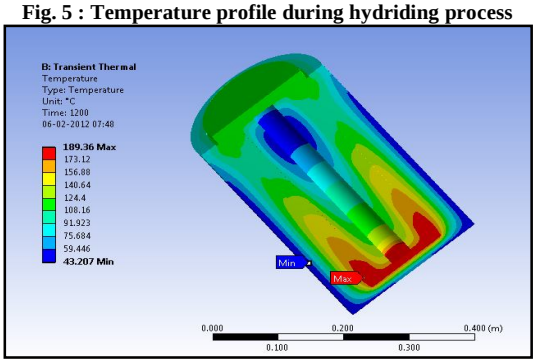

Fig. 6 : Temperature distribution during dehydriding process at time, t=1200 sec, after initialation of dehydriding

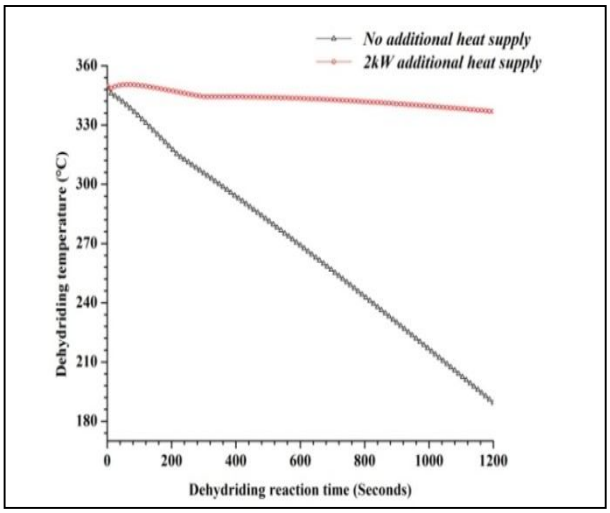

Fig. 7 : Temperature profile during dehydriding process

2) Dehydriding process:

For the dehydriding reaction, hydrogen is released from Mg hydride alloy bed through the porous filter. This reaction is an endothermic chemical reaction. Hence, it desorbs hydrogen by absorbing heat (75 kJ per mole of hydrogen). Therefore, temperature decreases during dehydriding process. This reaction occurs at a temperature of 350 ºC and a pressure of few atmospheres. Maximum 80 to 90 % moles of hydrogen desorbs within the first 20 minutes. Hence, for transient thermal analysis, we consider 1200 sec for the dehydriding reaction. Desorbed total number of moles of hydrogen is 37.5 moles. Therefore, total heat absorbed is 2.34 kW during dehydriding reaction. Hence, for transient thermal analysis, initial and boundary conditions are fixed as below:

- Initial temperature of reactor is 350 ºC.
- Heat sink on metal hydride bed is 2.34 kW.
- Dehydriding reaction time is 1200 sec.
- Free convection and radiation heat transfer boundary condition on outer cylinder are assumed. For simplicity, we use heat transfer coefficient for free convection to air at atmospheric pressure and and moderate temperature for vertical cylinder (the heat transfer coefficient is 5 $W/m^2 \cdot ºC$).

Applying above initial/boundary conditions and solving the transient thermal problem using ANSYS solver, the temperature profile is obtained as a function of time, see Fig. 7. The maximum temperature drop during dehydriding process is computed as 189ºC in first 20 minutes. Since for continuous dehydriding process, we have to maintain constant temperature 350ºC, an external heat needs to be provided to the reactor. The optimal extra external heat source is computed as 2 kW using FEM analysis. Fig. 7 shows temperature profile with respect to time for the dehydriding process.

IV. CONCLUSIONS

Based on this work, following conclusions are derived:

- Geometrical model of reactor is developed using Pro/Engineer Wildfire and transient thermal analysis is carried out using ANSYS software.
- Temperature profile of reactor is computed for hydriding process and maximum temperature rise from 200 º C to 422 º C is seen in first 20 minutes.
- Similarly, temperature profile of reactor is computed for dehydriding process and temperature is seen to drop to 189 ºC from 350 ºC in first 20 minutes.
- For dehydriding reaction, the optimal external heating requirement is worked out as 2 kW.

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