Modeling and Simulation of Hydrogen Storage Device for Fuel Cell Using COMSOL Multiphysics

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Abstract: In this paper, a 2D dynamic Simulation for a portion of metal hydride based hydrogen storage tank was performed using Computational Software COMSOL 4.0a Multiphysics. The software is used to simulate the diffusion and heating of hydrogen and metal hydride powder in both radial and axial directions. The model consists of a system of partial differential; equations (PDE) describing two dimensional heat and mass transfer of hydrogen in a porous matrix. The phenomenon of hydrogen absorption/ desorption is accompanied by thermal effects, such as heat release during absorption or heat Consumption during desorption. The thermal effects influence the temperature distribution in the metal hydride, and conversely the temperature distribution affects the rate of hydrogen release or consumption. The effects of different parameters such as temperature, pressure, thermal conductivity, permeability and internal geometries inside the hydride tank on the outflow/inflow of hydrogen gas were investigated.

Keywords: Hydrogen storage, Metal hydride, Absorption, Desorption, Heat transfer.

1. Introduction

Hydrogen is the most abundant element in the universe. It has great potential as an energy source and can be easily generated from renewable energy sources [1].yet storage has been the major problem to hydrogen economy which limit its wide usage and commercialization. Many technologies are developed. Hydrogen can be stored in high pressure metal and composite storage tanks. It is also by cooling it to its liquid form and containing it in super insulated tanks[2,3]. These method have a drawbacks and not practical for everyday use. Storing hydrogen in metal hydride bed proved to be effective and promising, and it continues to receive major boost among the researchers throughout the world.

This paper presents a model of hydrogen storage in a packed bed reactor , where hydrogen is stored in a packed bed of metal hydride and is absorbed/ released by application of cooling/ heating, metal hydride technology uses metal alloys to absorb hydrogen under moderate pressure and temperature and creating hydrides. A metal hydride tanks contain a granular metal which absorbs hydrogen and releases it with the application of heat from heat transfer fluid. Several mathematical models for the description of hydrogen absorption/desorption in a metal hydride bed reactor in 2D and 3D are available in the literature using different approaches[1-6]. This paper aim to investigate the metal hydride hydrogen storage tank(MHST) on the outflow/nflow of hydrogen gas. And also the flowrate of hydrogen inside the metal hydride reactor was determined.

Mathematical simulation have been achieved through the description of transport phenomenon by partial differential equations(PDEs) using COMSOL Multiphysics. This paper provides an important insight to the fundamental understanding of multiphysics coupling phenomenon during hydrogen absorption/desorption process. Mathematical model, results of simulation with COMSOL Multiphysics software and effect of thermal conductivity and heat contact resistance were presented and discussed.

2.0 . Use of COMSOL Multiphysics

The absorption and desorption of metal hydride and hydrogen gas flow in and out of the tank are affected by heat , mass and momentum transfer. The transfer processes are unsteady and depend on spatial coordinates. Therefore , the model is represented by non- stationary partial differential equations. Analytical solution of such equation is not feasible. Therefore, the computational fluid dynamic(CFD) Software, COMSOL Multiphysics 4.0a was used to numerically solve the model equations and investigate the time evolution of the parameter

characterizing the process(temperature, pressure, velocity, density and hydrogen flowrate). The geometry used in the modeling is presented in figure1 below. The geometry was built in a rectangular shape and split into two computational domains. One domain represent packed bed and the second domain represent walls of the storage tank. the mesh used has 285 points and 496 triangular element,leding to 2345 degrees of freedom, the element size is normal , the solver used is (UMFPACK) solving PDEs in an interval 0:600s with time step of 10s.the geometry of metal hydride hydrogen bed reactor is illustrated in figure 1, figurea2,3 shows profile distribution of pressure and temperature inside the MHST during absorption, figure 4,5 shows profile distribution of temperature, pressure during desorption of hydrogen.

3. Figures

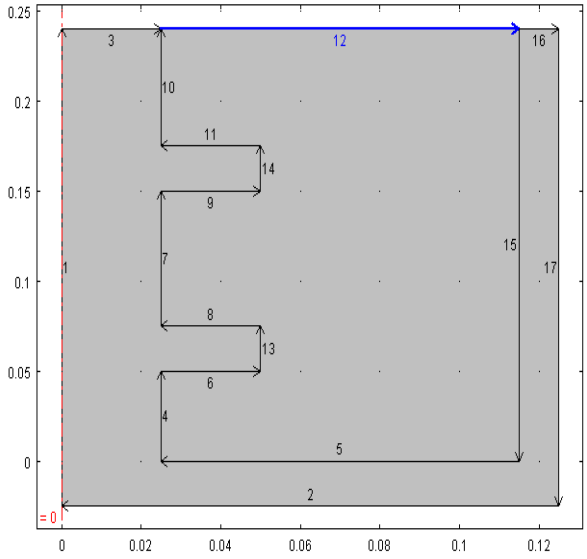

Figure1- Geometry used in modeling MHHST ,(subdomain1-porousmedia,subdomain2-internal wall)

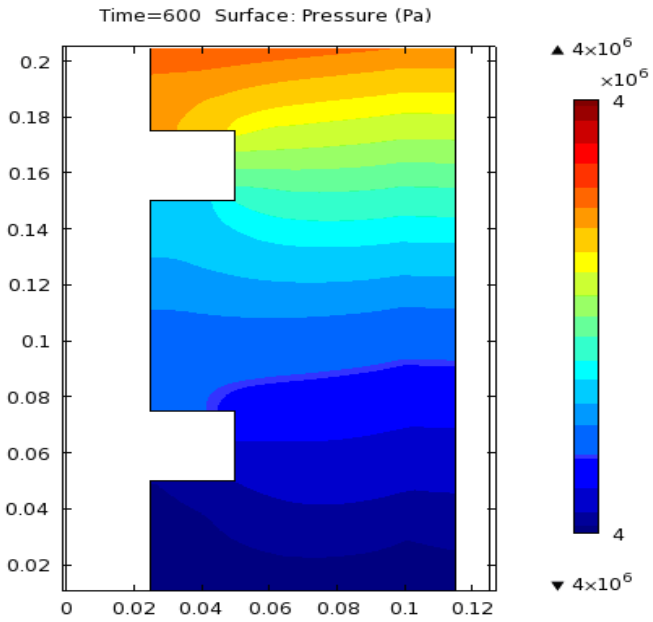

Figure 2-pressure distribution in MHHSTduring absorption

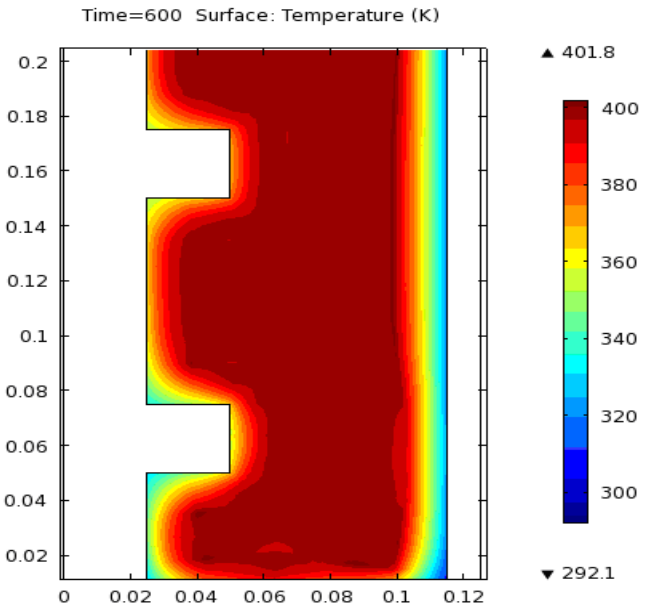

Figure3Temperaturedistribution in MHHST during absorptin in MHHST during absorption.

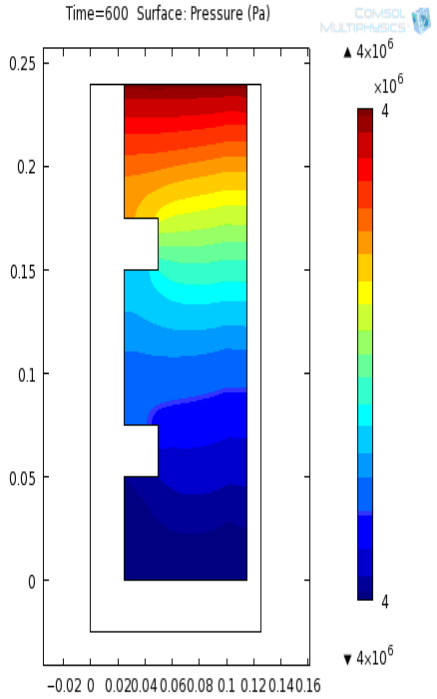

Figure4- pressure distribution during desorption

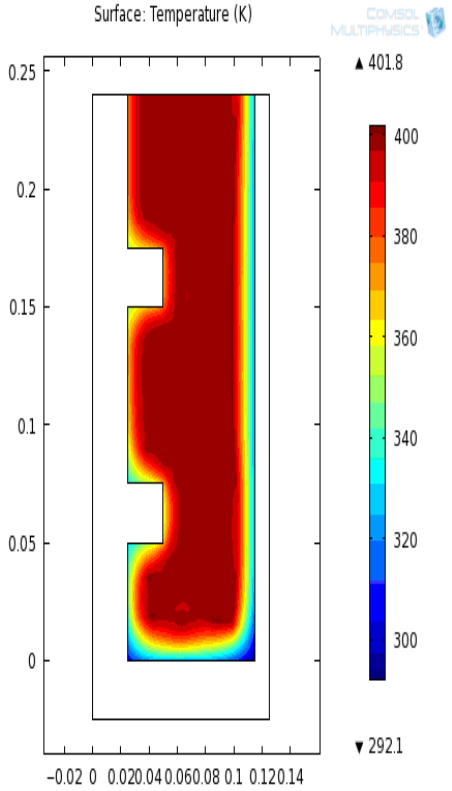

Figure5- Temperature distribution during desorption.

4.1Mathematical model

Two-dimensional non-stationary mathematical model of the metal hydride reactor for hydrogen storage consists of mass, momentum and energy balance equations together with constitutional equation for pressure and temperature.

4.2Mass balance

The mass conservation equation of the solid metal hydride:

$$(1-\varepsilon)\frac{\partial \rho_s}{\partial t} = m$$

Mass balance equation for hydrogen gas:

$$\varepsilon \frac{\partial \rho_g}{\partial t} + \nabla(\rho_g u_g) = m$$

where ρ_g denotes the density of the hydrogen gas in the reactor during the desorption process. Hydrogen density is determined using the perfect gas law. Velocity of hydrogen gas (u_g) is calculated using the Darcy's law (Jemni *et al*., 1995):

$$u_g = \frac{K}{\mu_g}\nabla P_g$$

Where K is permeability, μg is gas viscosity, Pg is gas pressure.

Distribution of hydride powder particles by size and shape makes widening and smoothing of adsorption/desorption curves. Complex mechanism of hydrogen reaction with metal hydride is not well known, and macrokinetics expressions are obtained from experimental data for each particular metal hydride powder.

Equation for hydrogen kinetics (hydrogen mass desorbed, *m*, per unit time and per unit volume) is given by (Dhaoua *et. al.* 2007):

$$m = C_d \exp\left(-\frac{E_d}{R_g T}\right)\frac{P_g - P_{eq}}{P_{eq}}\rho_s$$

For the $LaNi_5$–Hydrogen system C_d = 9.57 1/s; E_d = 16.420 KJ/ mol of H2.

Equilibrium pressure P_{eq} can be calculated from modified van't Hoff equation (Nishizaki T., *et.al,* 1983)):

$$\ln(P_{eq}) = \frac{\Delta H}{RT} - \frac{\Delta S}{R} + (\phi - \varphi_0)\tan\left[\pi\left(\frac{C}{C_m} - \frac{1}{2}\right)\right] + \frac{\beta}{2}$$

where, φ (0.35) and β (0.25) are the plateau flatness factor and the plateau hysteresis factor .

4.3Momentum balance

Momentum balance equation includes Darcy's term to account for momentum transfer due to pressure gradient in the metal hydride porous media:

$$\frac{\partial(\rho_g \varepsilon)}{\partial t} + \nabla\left(-\rho_g \frac{K}{\mu_g} \nabla P_g\right) = 0$$

where:

Permeability K and porosity ε are related by equation:

$$K = C_k \cdot d_p^2 \left(\frac{\varepsilon}{1-\varepsilon}\right)^2$$

Where d_p is metal hydride particle diameter and constant C_k=2.37x10^{-3}.

4.4Energy balance

Energy balance equation, describing temperature evolution of the hydrogen – porous bed system:

$$\frac{d}{dt}\left(\varphi \rho_g C_{pg} T + (1-\varepsilon)\rho_s C_{ps} T - \varepsilon \frac{\rho_g RT}{M_{H_2}}\right) +$$
$$\nabla\left(\rho_g C_{pg} uT - \lambda_e \nabla T\right) + (1-\varepsilon)(-\Delta H)\rho_s m = 0$$

Effective thermal conductivity of metal hydride bed traditionally expressed as:

$$\lambda_e = \varepsilon \lambda_g + (1-\varepsilon)\lambda_s$$

4.4 Boundary condition

The following boundary conditions are properly implemented in the software during simulation:
Inlet/outlet, wall, flux, and isolation, and they are considered for heat, mass and momentum transfer for both absorption/desorption in the geometry used.
Initial Conditions:
Absorption
P-ini = P = 40bar,T-ini = 293K
Desorption
P-ini =P =10bar,T-ini = 333K

5. **Results**

The input data used in this simulation are presented in the table 1 below, the value of thermal conductivity,permability and heat transfer coefficient were also presented;
Table 1-variables used for the simulation

Rho_s	6360kg/m^3	Bulk density of metal hydride at saturation
Rho_emp	6000kg/m^3	Bulk density of metal hydride
Cps	419J/Kg/K	Solid specific heat capacity
Pg	P	Gas pressure
Cpg	14890J/Kg/K	Gas Specific heat capacity
K_e	1.32W/m/K	Permeability
epsilon	0.5	porosity
T-ini	293K	Initial temperature
Rg	8.314J/mol/K	Universal gas constant
Ca	59.187[1/s]	Absorption constant
Cd	9.57[1/s]	Desorption constant
Ea	21139.6[J/mol]	Absorption activation energy
H1	150w/m^2/k	Heat source
P-ini(abs)	40bar	Initial pres
Peqa	1000[Pa]*exp(17.6083 704.6[K]/T)	Equilibrium gas pressure of absorption
Peqd	1000[Pa]*exp(17.4783 704.6[K]/T)	Equilibrium pressure

The simulation was done for 600s , after input all the parameter in the software, allocating properly all the initial boundary conditions, initialize the mesh. The distribution of hydrogen gas pressure,, hydrogen concentration in the metal hydride, and temperature for both absorption/ desorption are varied along time. the following results were obtained.
Figure6 shows the pressure distribution in the MHHST during absorption, pressure in the bed increases as a result of increase in temperature

of the bed and heating fluid, the equilibrium pressure strongly depend on temperature.

Figure7 shows the temperature distribution in the bed varied along time , there is a gradual increase in temperature due to the exothermic nature of the reaction between hydrogen and metal hydride

Figure8 shows the concentration of hydrogen in metal hydride , there is rapid increase in the concentration of hydrogen in metal hydride at different time interval.

Figure9,10,and 11 shows pressure, temperature and concentration distribution of hydrogen in metal hydride bed. There is decrease in temperature, pressure and concentration of hydrogen in metal hydride bed during desorption at different time intervals.

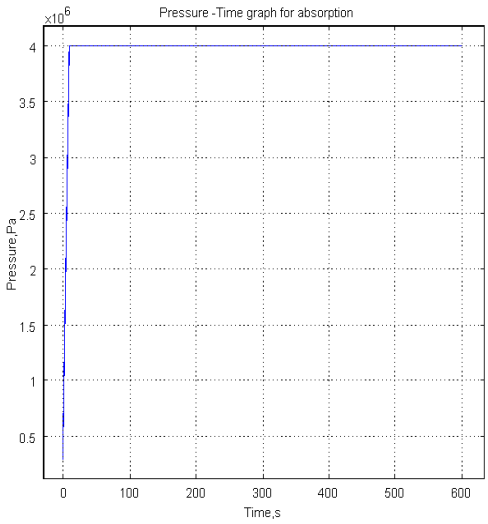

Figure6-Pressure distribution with time in 600s during absorption

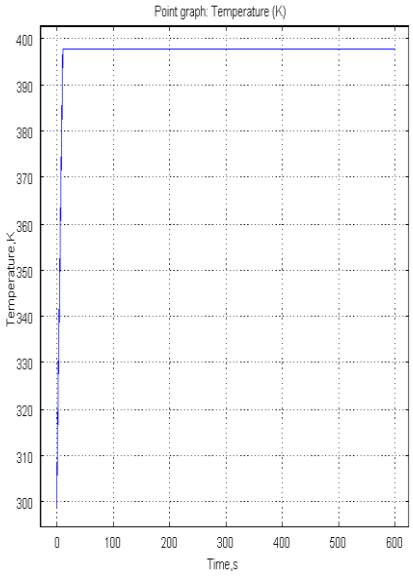

Figure7-Temperature distribution with time in 600s during absorption

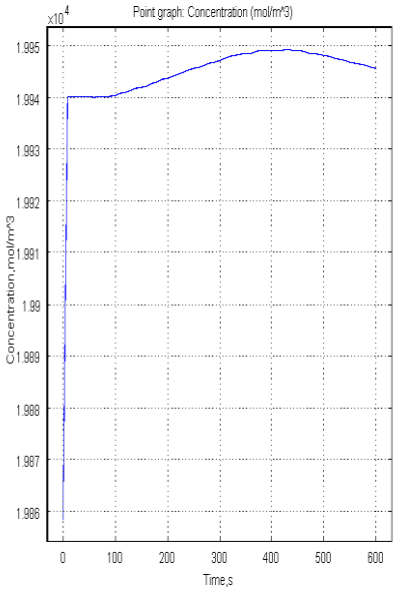

Figure8- Concentration of hydrogen in metal hydride with time during absorption

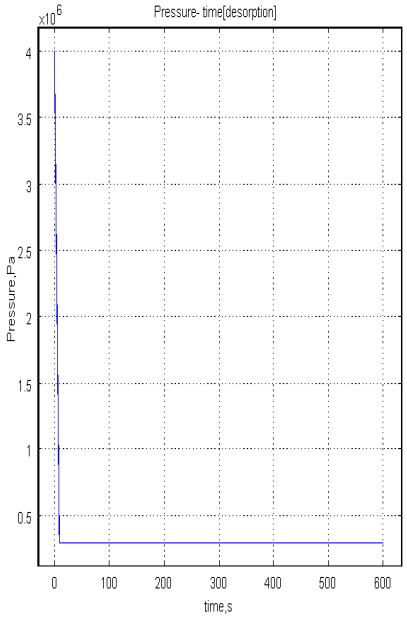

Figure9- Pressure distribution in MHHST with time during desorption

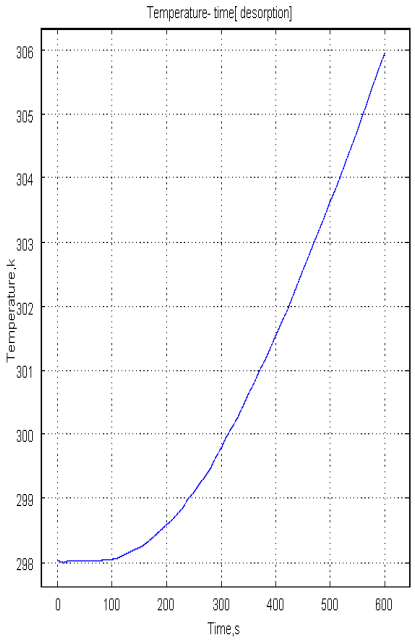

figure10-Temperature distribution in MHHST during with time desorption

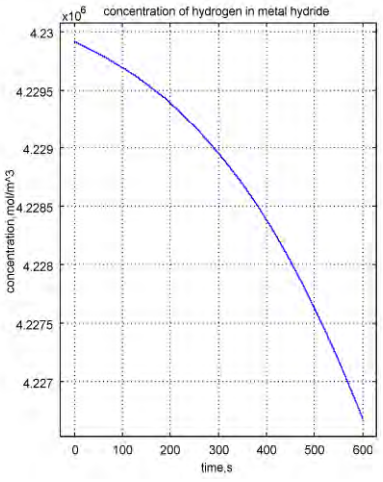

Figure11-concentration distribution of hydrogen in metal hydride with time during desorption

6.Effect of thermal Conductivity and Heat contact resistance on MHHST.

Thermal Conductivity of a metal hydride bed has a direct impact on the performance of hydrogen reactors. Varied thermal conductivities of absorption/ desorption process increases the accuracy of result obtained better than fixed thermal conductivities. Contact resistance depends on powder properties mainly size and packing density and wall properties. Lower heat contact resistance yields short absorption time and vice versa for desorption process.

7.Conclusion

ln this paper, the objectives of the work has been verified with the simulation results obtained. The simulation of heat and mass transfer for MHHST with internal geometry was done. Heat transfer,mass transfer, and momentum transfer modules were effectively incorporated in COMSOL Multiphysics 4.0a software.

Absorption of hydrogen in metal hydride occur faster at a lower temperature and higher pressure due to the exothermic nature of the reaction, and desorption occurs at higher temperature and lower pressure due to the endothermic nature of the desorption process. Concentration increases with absorption of hydrogen and decreases with desorption of hydrogen .

8.References

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9.**Acknowledgement**
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10. **Nomenclature**

C	Kinetic constant [1/S]
C_p	Specific heat [J/kg/K]
E	Activation energy [J/mol]
h	Overall heat transfer coefficient [W/m^2/K]
K	Permeability [m^2]
m	Source term [Kg/ m^3/S]
M	Molecular weight [kg/mol]
P	Pressure [Pa]
Rg	Universal gas constant [J/mol/K]
T	Temperature [K]
t	Time [S]
v	Gas velocity [m/s]

Greek symbols:

Λ	Thermal Conductivity [W/m/K]
ΔH	Enthalpy [J/mol]
ΔS	Entropy [J/mol/K]
E	Porosity [-]
μ	Dynamic viscosity [kg/m/s]
ρ	Density [Kg/m^3]
ΔG	Gibb's energy [J]

Subscripts:

a	Absorption
d	Desorption
e	Effective
eq	Equilibrium
f	External fluid
g	Gas
s	Hydride
ss	Saturation
0	Initial