International Journal of Engineering Research & Technology (IJERT)
ISSN: 2278-0181
Vol. 4 Issue 03, March-2015

Numerical Simulation of Metal Hydride ($MmNi_{4.6}Al_{0.4}$) Hydrogen Storage Reactor

P. M. Gavali[1]
PG scholar,
RIT, Sakharale

Dr. S. D. Yadav[2]
Associate Professor,
RIT, Sakharale

***Abstract* - This paper presents a numerical simulation of two-dimensional hydrogen storage reactor for storing capacity of $MmNi_{4.6}Al_{0.4}$ based metal hydride reactor. This reactor is of cylindrical configuration. Absorption of hydrogen in metal hydride reactor process is simulated in the FLUENT software. Simulation has been done for supply pressure of 20 bar and overall heat transfer coefficient 1000 W/m^2K. Reactor bed thickness is 7.5 mm made up of $MmNi_{4.6}Al_{0.4}$. Gravimetric density variation is presented in terms of wt % with respect to time. The numerical results shows, $MmNi_{4.6}Al_{0.4}$ absorb maximum hydrogen of 1.2 wt % at supply pressure of 20 bar and 1000 W/m^2K. These results are compared with the experimental data published in literature. Both results are very much similar.**

INTRODUCTION

Hydrogen is an ideal energy carrier which is considered for future transport, such as automotive applications. It is widely believed that hydrogen will within a few tens of years become the fuel that powers most vehicles and portable devices, i.e. hydrogen will become the means of storing and transporting energy. The reason is the depletion of oil and the relatively facile production of hydrogen from the various renewable sources of energy - hydroelectric, wind, solar, geothermal with water being the only raw material needed. To release the energy, hydrogen can be burned in an efficient and clean way in a fuel cell to form water again, or made to drive an electrochemical cell as in the commonly used nickel hydride battery. As concerns over air pollution and global warming increase, the incentive to switch to clean and efficient hydrogen economy becomes greater and the transition may occur well before oil reserves are depleted.

While hydrogen has many obvious advantages, there remains a problem with storage and transportation. Pressurized hydrogen gas takes a great deal of volume compared with, for example, gasoline with equal energy content - about 30 times bigger volume at 100 atmospheric gas pressure. Condensed hydrogen is about ten times denser, but is too much expensive to produce and maintain. There are also obvious safety concerns with the use of pressurized or liquefied hydrogen in vehicles. Solid fuel as chemical or physical combination with materials, such as metal hydrides, complex hydrides and carbon materials is another advance method for hydrogen storage. Each of these options possesses attractive attributes for hydrogen storage.

MATHEMATICAL MODELING

Darcy's equation

Darcy's law is a simple proportional relationship between the instantaneous discharge rate through the porous medium, the viscosity of fluid and the pressure drop over given distance.

$$Q = \frac{-k\,A\,(P_f - P_i)}{\mu\, L}$$

Kazeny – Carman equation

The Kazeny – Carman equation is often presented as permeability versus porosity, grain size and tortuosity. The definition of absolute permeability $k_{\ absolute}$ of porous material from Darcy's equation

$$Q = -k_{\ absolute}\ \frac{A}{\mu}\frac{dP}{dx}$$

Energy Balance Equation

As Newton's law of conservation states that energy can neither be created nor be destroyed, but it can be transformed from one form to another form. This law is to be implemented in the fluent for energy balance.

$$\frac{1}{r}\frac{\partial}{\partial r}\left[kr\ \frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[k\frac{\partial T}{\partial z}\right] + \frac{1}{r^2}\frac{\partial}{\partial \varphi}\left[k\ \frac{\partial T}{\partial \varphi}\right] + \dot{q} = \rho C_p\frac{\partial T}{\partial t}$$

Reaction Kinetics

$$\frac{dx}{dt} = C_a[exp^{\frac{E_g}{R_g T}}]\ [\frac{P_s - P_{eq}}{P_{eq}}][\frac{(x - x_f)}{(x_i - x_f)}]$$

This equation gives; rate at which fraction of concentration of the hydrogen is changing with respect to time. This equation states that, rate of change of concentration of the hydrogen with respect to time is depending upon- supply pressure, equilibrium pressure, fraction of hydrogen at initial state, fraction of hydrogen at final stage, activation energy etc.

Van't Hoff Equation

The Van't Hoff equation in chemical thermodynamics relates the changes in equilibrium constant k of a chemical reaction to the standard enthalpy change $\Delta\, H$ for the process

$$\frac{d(\ln k)}{dT} = \frac{\Delta H}{RT^2}$$

$$\frac{P_{eq}}{P_{atm}} = \exp\{\frac{\Delta S}{R_u} - \frac{\Delta H}{R_s T} + (\varphi_s \pm \varphi_0)\ \tan[\pi\left(\frac{x}{x_f} - \frac{1}{2}\right)] \pm \frac{\varphi}{2}\}$$

Nomenclature

A – area [m^2]
C_a - Reaction rate constant [S^{-1}]
μ- dynamic viscocity [kg/ms]
L – length of reactor [m]
Cp -specific heat [J/kgK]
k- Permeability
E_g -activation energy of the reaction [J/molH$_2$]
H -enthalpy of reaction [J/molH$_2$]
K -coefficient of Darcy law [m^2]
m -mass of hydrogen absorbed [kg]
m_f- mass flow rate of the cooling fluid [kg/s]
MH_2 -molecular weight of hydrogen [kg/kmol]
P- pressure [bar]
Q- heat [J]
r -radius of the reaction bed [m]
R_u- ideal gas constant [J/molH$_2$ K]
S -entropy of absorption [J/molH$_2$ K]
t- time [s]
T- temperature [K]
U -overall heat transfer coefficient [W/m$_2$ K]
V -velocity [m/s]
ρ- density [kg/m^3]
X- hydrogen concentration (H/M)
Greek symbols
ε- porosity
ϕ -hysteresis factor
ϕ_s- slope factor
Subscripts
a- absorption
e- effective
eq -equilibrium
f- final, fluid
g- gas
i- inlet, inner
m- metal
o- outer
r -radial
z- axial
0- initial

Pressure Composition Isotherms

Figure 1 shows typical pressure- composition-isotherm (P-C-T diagram) for metal- hydrogen reaction. Equillibrium state is defined by hydrogen pressure (P_b), temperature(T), and hydrogen concentration in metal. Equillibrium diagram is to be represented three-dimensional curve. Figure 1 may be regarded as two cross sections vertical to the temperature axis of three dimentional curve. While horizontal axis represent hydrogen concentration. This hydrogen concentration is expressed by ratio of the number of hydrogen atoms to that of metal atoms within metals.

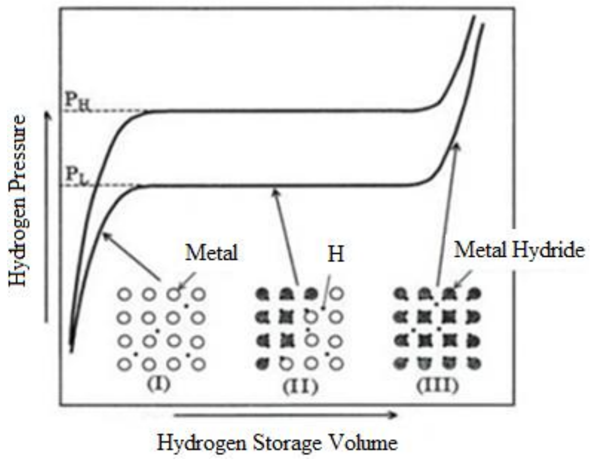

Fig. 1: Pressure Compsition Isotherm (P-C-T diagram) for the metal hydrogen reaction

I. A solid solution of hydrogen
II. A coexistent region of hydrogen solid solution and metal hydride
III. Metal hydrie

Hydrogen is readily absorbed in metal to form a solid solution, if the surface of metal is clean.It is known that the amount of hydrogen contained in solid solution increases in proportion to a square root of hydrogen pressure, and in the P-C-T diagram, area of solid solution corrosponds to steep rise of equillibrium pressure. When hydrogen in metal solid solution rises to certain level, part of solid solution turns into metal hydride. Further increase in concentration of hydrogen leads to increase in metal hydride in solid solution.

PROBLEM DEFINITION

The governing equations are solved with a fully implicit finite volume numerical scheme embodied in a general purpose code FLUENT. Fig. 2 shows that, the schematic of cylindrical reactor which is going to be analyzed for hydrogen storage weight percent.

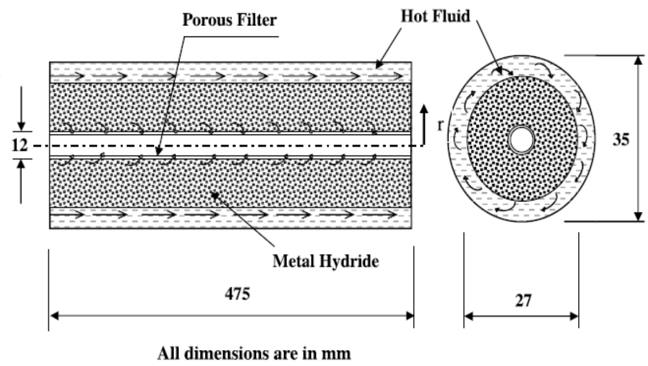

Fig. 2 Hydrogen storage reactor

The solution method involves the integration of the governing differential equations over finite control volume and transforming them into a general algebraic form.

RESULT AND DISCUSSION

From literature, it is clear that overall heat transfer rate affect the hydrogen absorption capacity. P Muthukumar and Manvendra Umekar published their work under title "Study of coupled heat and mass transfer during absorption of hydrogen in $MmNi_{4\cdot6}Al_{0\cdot4}$ based hydrogen storage device". With overall heat transfer coefficient 750 W/m^2K and 20 bar supply pressure, Obtained results have been plotted on the graph [Time (s) v/s Hydrogen Storage Capacity (wt %)].

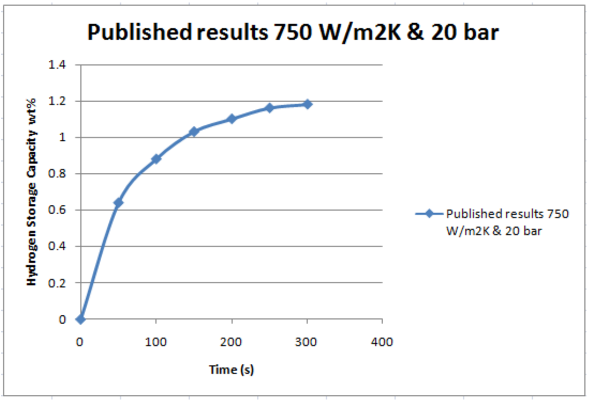

Fig 3: Time(s) v/s Hydrogen Storage Capacity (wt.%)
(Overall Heat Transfer Coefficient 750 W/m^2 K, 20bar)

This graph has time (in seconds) on X axis while hydrogen storage capacity (in wt %) on Y axis. As time increase hydrogen storage capacity goes on increasing and became stable on further increase in time.

From above graph it is clear that, it takes 300 seconds to absorb 1.18 wt % of hydrogen at charging pressure of 20 bar. This system is to be modified from overall heat transfer coefficient point of view.

Simulation is completed; by keeping all other parameters constant except, overall heat transfer coefficient. Overall heat transfer coefficient increased up to 1000 W/m^2K. Results are plotted as below-

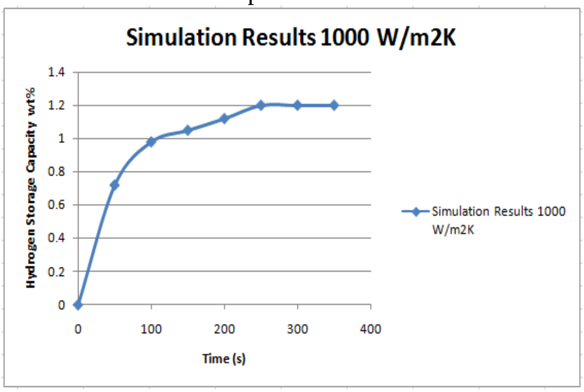

Fig. 4: Time(s) vs Hydrogen Storage Capacity (wt %)
(Overall Heat Transfer Coefficient 1000 W/m^2 K, 20 bar)

Comparison of all results gives that, metal hydride reactor gives best results for 20 bar supplied pressure and 1000 W/m^2K overall heat transfer coefficient. Results obtained from 20 bar pressure and 750 W/m^2K gives better results than results obtained from 10 bar supply pressure and 1000 W/m^2K heat transfer coefficient.

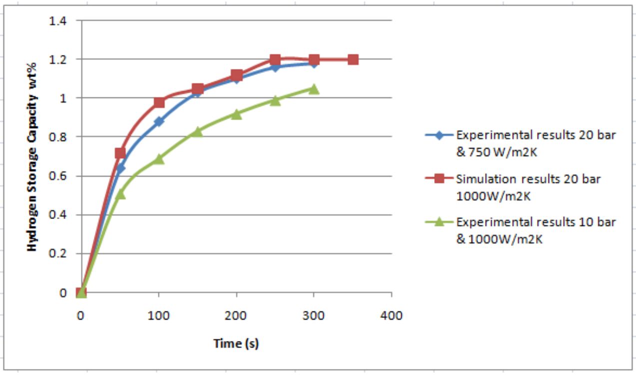

Fig. 5: Time(s) v/s Hydrogen Storage Capacity (wt %)

CONCLUSION

This paper concludes that, $M_m Ni_{4.6} Al_{0.4}$ metal reactor for hydrogen storage is best suitable material for hydrogen storage. Time required to store hydrogen is reduced to greater extend at supply pressure of 20 bar as compared to 10 bar pressure. With 1000 W/m^2K overall heat transfer coefficient better results are obtained as compared to 750 W/m^2K overall heat transfer coefficient. With $M_m Ni_{4.6} Al_{0.4}$ as metal, it takes half time to store same amount of hydrogen at 20 bar pressure as compared to 10 bar supply pressure. $M_m Ni_{4.6} Al_{0.4}$ material gives better performance for 20 bar supply pressure and 1000 W/m^2K overall heat transfer coefficient.

REFERENCES

1. Sarang A. Gadre, Armin D. Ebner, Karen D. Daniel, Shaheen A. Al- Muhtaseb, Charles E. Holland and James A. Ritter (2002) "Modeling The Discharge Behavior of A Metal Hydride Hydrogen Storage System" Fuel Chemistry Division Preprints 2002, 47(2), 792.
2. P. Muthukumar, A. Satheesh, U. Madhavakrishn and Anupam Dewan (2009), "Numerical investigation of coupled heat and mass transfer during desorption of hydrogen in metal hydride beds", Energy Conversion and Management 50 (2009) 69–75
3. Michael C. Georgiadisa,b, Eustathios S. Kikkinidesc,d, and Athanasios K. Stubose(2005) "On The Optimization Of Hydrogen Storage In Metal Hydride Beds" European Symposium on Computer Arded Process Engineering – 15 L. Puigjaner and A. Espuña (Editors) © 2005 Elsevier Science B.V.
4. E. Tzimas, C. Filiou, S.D. Peteves And J.-B. Veyret Petten(2003), "Hydrogen Storage: State-Of-The-Art And Future Perspective" The Netherlands European Communities
5. R.J. Westerwaal and W. G. Haije (2008)"Evaluation solid-state hydrogen storage systems Current status" April 2008
6. Apurba Sakti (2007) "Modeling A Metal Hydride Hydrogen Storage System" EGEE 520, Mathematical Modeling of EGEE systems Spring 2007
7. P. Muthukumar,M. Prakash Maiya and S. Srinivasa Murthy (2005)," Experiments on a metal hydride-based hydrogen storage device", International Journal of Hydrogen Energy 30 (2005) 1569 – 1581