

## **An Analysis of Coupled PEM Fuel Cell – Metal Hydride Hydrogen Storage Tank System**

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### **Abstract**

Thermal coupling of PEM fuel cells (PEMFC) and metal hydride hydrogen storage tanks is an interesting possibility. While, hydrogen desorption from metal hydrides is an endothermic process, the fuel cell generates considerable amount of waste heat to be rejected. Hence one can visualize a self-sustainable system by utilizing the fuel cell heat output at the metal hydride storage device for hydrogen desorption. Moreover, the metal hydride device can also act as a thermal compressor to deliver hydrogen at higher pressures which can improve the performance of the fuel cell. Due to the difference between the rates of desorption of hydrogen from the metal hydride bed and consumption of hydrogen in the fuel cell, an interface between the two components needs to be introduced. In the case studied in this paper, the interface is a gas buffer tank together with a control valve to deliver hydrogen at preset pressure and varying flow rate as demanded by the fuel cell. Such a system has been analyzed for different operating conditions and load requirements.

### **Keywords**

Hydrogen Storage, Metal Hydride, Heat and Mass Transfer, Simulation, PEM Fuel Cell, Thermal Coupling.

### **Introduction**

In the near future, issues related to climate change, scarcity of fossil fuels, energy security concerns, environmental problems etc are expected to create new opportunities for hydrogen based power sources. One of the major barriers that has prevented the widespread use of hydrogen as a fuel is the difficulty involved in its storage and portability. Hence developing efficient, reliable and safe hydrogen storage system is of topical interest.

Especially for fuel cell applications in automobiles, development of efficient onboard hydrogen storage systems is of prime importance. A simple mode of storing hydrogen is in the form of a compressed gas in high pressure cylinders. These cylinders are heavy, occupy large space, and both storage and re-fueling can be dangerous because of the high pressure. Hydrogen storage in liquid state at cryogenic temperatures demands super-insulated containers, with special attention to prevent hydrogen boil off. While solid state hydrogen storage using materials like in carbon nanotubes, complex hydrides and metal organic frameworks is in research phase, use of metal hydrides (MH) has reached a stage of field trials. In metal hydrides, hydrogen can be stored reversibly in the solid state at relatively low pressures and normal temperatures and hence it is an attractive option for the automotive and portable applications.

A comprehensive review of the thermal management and control aspects of fuel cells is made by Faghri and Guo [1]. A detailed discussion on the heat and mass transfer issues related to solid state hydrogen storage is made by Srinivasa Murthy [2].

There have been many reports on the thermal coupling of hydrogen storage devices and PEMFC. Thermally coupled high temperature PEMFC and an alanate hydrogen storage tank have been analyzed using the software package gPROMS by Pfeifer et al [3]. The pre-heating and temperature hold-times before starting the fuel cell were found to have a considerable influence on the operation due to the possible break-down of hydrogen pressure in the tank. The heat transfer characteristics were investigated by changing the geometries of the tanks. An optimum system temperature of 185 C and a fuel cell total power of 1 kW were found to fit to a 2 kg alanate tank from efficiency considerations. Jiang et al [4] simulated the MH hydrogen storage and PEMFC using the Virtual Test Bed (VTB) and compared both thermally coupled and uncoupled conditions. MacDonald and Rowe [5] studied the ability of thermally coupled metal hydride storage systems to supply hydrogen to a fuel cell with a time varying demand. A two-dimensional mathematical model was utilized to compare different heat transfer enhancements and storage tank configurations. A metal hydride storage unit was thermally integrated with a water-cooled PEMFC stack by Forde et al [6] who identified the metal hydride temperature as a useful system control parameter. Different control strategies for regulating the water flow from the fuel cell to the metal hydride were investigated. The results demonstrated how the amount of cooling water from the fuel cell used for heat exchange with the metal hydride affected the time for the fuel cell to reach the operating temperature. The main conclusion was that the ramp-up of the fuel cell power was not significantly influenced by the control strategy. However, in order to ensure full utilization of the hydrogen storage capacity in the metal hydride it was necessary to keep the average metal hydride temperature above a certain temperature.

A simplified coupling strategy is the main emphasis of the present paper. Here, the MH storage device is coupled to the PEMFC through a hydrogen buffer tank and a flow control valve. The performance of such a device is studied with the example of a 2 kW capacity power pack.

## **Model Description and Solution**

Modeling of the PEMFC:

Here, a part of a fuel cell corresponding to one turn of flow field channel has been modeled. This contains one inlet channel, a current collector and an outlet channel in place of complete fuel cell stack to reduce computational efforts without compromising accuracy. Two-dimensional above-the-channel model has been used for analysis. The modeled section of the fuel cell consists of three sub-domains: an anode, a proton exchange membrane and a cathode. Each of the electrodes is in contact with an interdigitated gas distributor, which has an inlet channel, a current collector and an outlet channel. The fuel cell model adapted here is similar to that reported by Grujicic and Chittajallu [7] and hence is not described here. The solution is obtained by using COMSOL Multiphysics<sup>TM</sup> [8] with a stationary non-linear solver.

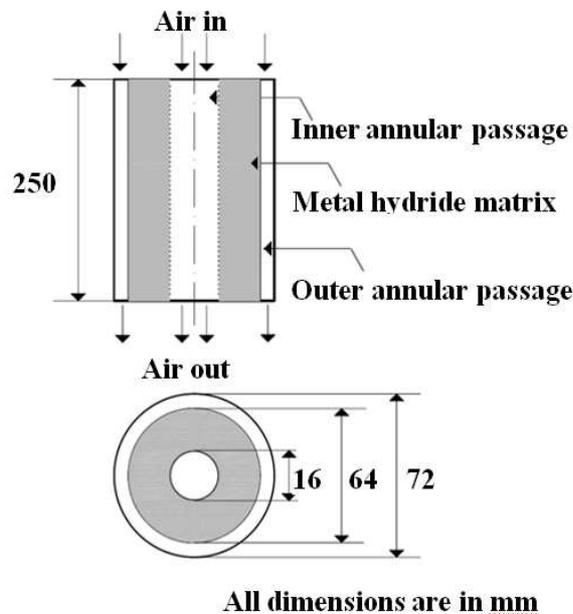
Modeling of the MH tank:

As already mentioned, heat transfer plays a crucial role in the performance of metal hydride hydrogen storage system. Mohan et al [9,10] have discussed in detail the MH storage device simulation procedure using COMSOL Multiphysics<sup>TM</sup>. MacDonald and Rowe [5] have studied various heat transfer enhancements and concluded that a finned cylinder yields higher pressures and occupies more space, while the annular case yields acceptable pressures and requires less

2<sup>nd</sup> European Conference on Polygeneration – 30<sup>th</sup> March -1<sup>st</sup> April 2011 – Tarragona, Spain space. Hence an annular configuration of a cylinder as shown in Figure 1 has been used for the hydrogen storage tank. LaNi<sub>5</sub> is chosen for its favourable storage properties at the heat rejection temperatures of the PEMFC. A dynamic simulation model is adapted and COMSOL Multiphysics<sup>TM</sup> [8] with a time-dependent solver is used for solution.

**Table 1 Properties of LaNi<sub>5</sub> [5]**

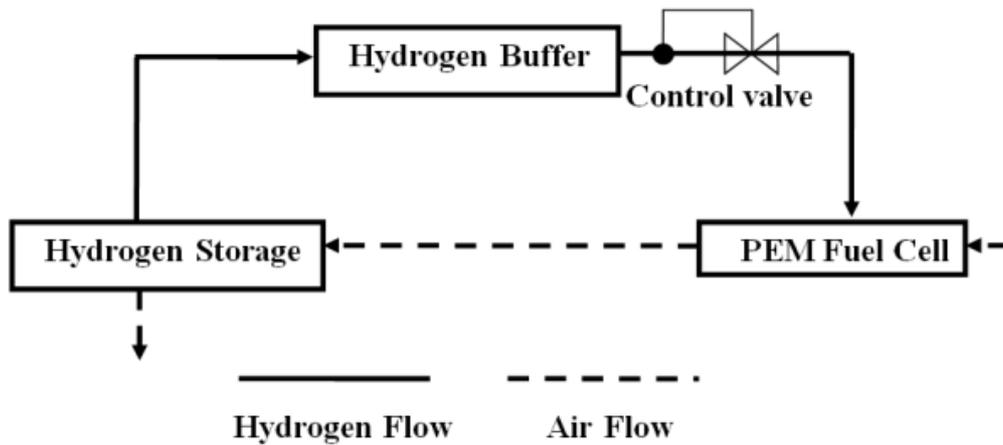
Property	Value
Saturated Density	8527 kg.m <sup>-3</sup>
Empty Density	8400 kg.m <sup>-3</sup>
Specific Heat	419 J.kg <sup>-1</sup> .K <sup>-1</sup>
Eff. Thermal Conductivity	1.32W.m <sup>-1</sup> .K <sup>-1</sup>
Permeability	10 <sup>-8</sup> m <sup>2</sup>
Heat of formation of MH	-1.539x10 <sup>7</sup> J.kg <sup>-1</sup>
Porosity	0.5
Molecular weight	432 kg.kmol <sup>-1</sup>



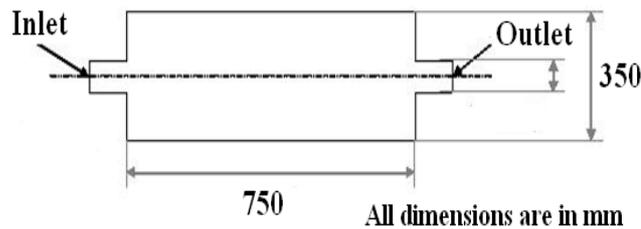
**Fig. 1 Schematic of the hydrogen storage device**

Coupling of the Two Components:

Figure 2 illustrates the schematic of the coupled system. The fuel cell consumes hydrogen and humidified air to produce electrical power and also heat due to certain irreversible losses. In the present case this heat in the form of hot air which is passed through the outer and inner annular passages of hydrogen storage system to provide heat required to desorb hydrogen from the MH bed. The hydrogen thus produced is supplied to the PEMFC via the buffer tank. The buffer is introduced between the two systems since the rate of desorption of hydrogen from the metal hydride storage tank and the rate of hydrogen required by the fuel cell are different and also transient. The supply of hydrogen to the fuel cell is at constant pressure and the flow rate is adjusted by a control valve which is actuated by the feedback sensors monitoring the fuel cell load. Figure 3 shows the buffer tank in which both the quantity and pressure of hydrogen vary with time.



**Fig. 2 Schematic of the coupled system**



**Fig. 3 Schematic of the hydrogen buffer**

## Results and Discussion

For example, it is assumed that the 2 kW power pack operates for two hours at 0.7 V. The various parameters computed as mentioned above are as follows:

- Mass of hydrogen consumed in 2 hours in the PEMFC stack = 0.214 kg
- Amount of heat released by PEMFC stack in 2 hours = 14400 kJ
- Initial weight of the metal hydride bed = 4.21755 kg
- Final weight of the metal hydride bed = 4.154744 kg
- Amount of hydrogen desorbed by a single MH storage tank = 0.0628 kg
- Number of storage tanks required =  $0.214/0.0628 = 4$
- Amount of heat required for desorption = 3293.46 kJ

It may be noted that the heat rejected by the PEMFC is over 4 times higher than that needed to drive the MH storage device.

PEMFC Performance:

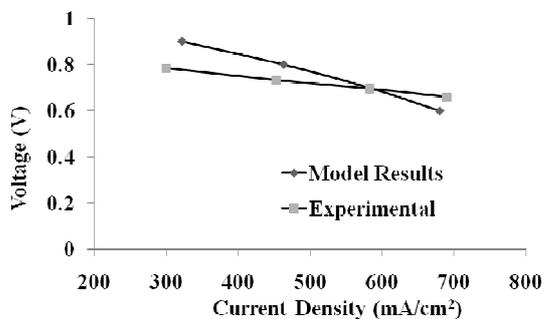
In order to validate the model, the simulation results for constant stack temperature of 72° C are compared with the published experimental data (Laurencelle et al [11]) in Figure 4. When the current density is less than 0.58 Acm<sup>-2</sup>, the output voltage in the model is greater than the

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 experimental results. After the current density exceeds  $0.58 \text{ Acm}^{-2}$ , the output voltage in the model is less than the experiment results. Over the parameter range of interest, the variation was within about  $\pm 8\%$ . Even though the theoretical model is quite rigorous, the actual fuel cell is a complicated device and hence it is difficult to precisely predict its performance by a steady state model.

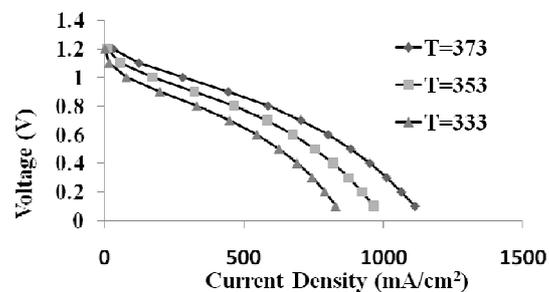
Hydrogen supply pressure and operating temperature are two important parameters which influence the performance of the PEMFC. In fact, the hydrogen delivery pressure of the MH storage device depends on the desorption temperature, i.e. that of heat supply.

The PEMFC performance is known to improve at elevated temperatures, although this cannot be predicted simply by the equations describing the polarization curves. Increased temperature results in higher potential loss and lower performance. However, increased temperature also yields higher exchange current density and significantly improves mass transfer properties. Figure 5 shows the polarization curves which indicate voltage gain with increased temperature. From Figure 6, it can be seen that the maximum power delivered also increases with temperature.

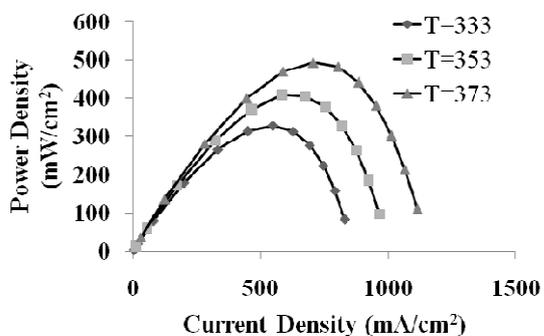
An increase in the operating pressure results in higher cell potential due to an increase in exchange current density caused by increased concentration of reactant gases in the electrodes. Exchange current density is proportional to surface concentration, which in turn is proportional to pressure. In addition increased pressure may also have an effect on limiting current density by improving mass transfer of gaseous species. Figure 7 shows the polarization curve at different pressures. From Figure 8, it can be inferred that the maximum current density which can be drawn by the fuel cell increases with pressure.



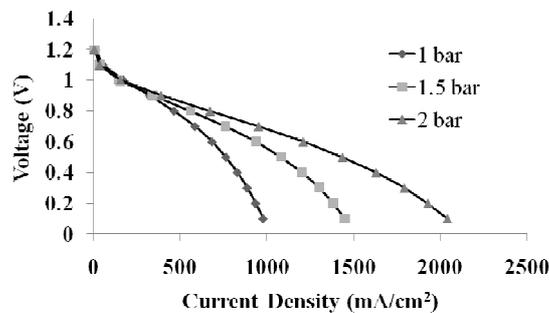
**Fig. 4 Validation of PEMFC simulation**



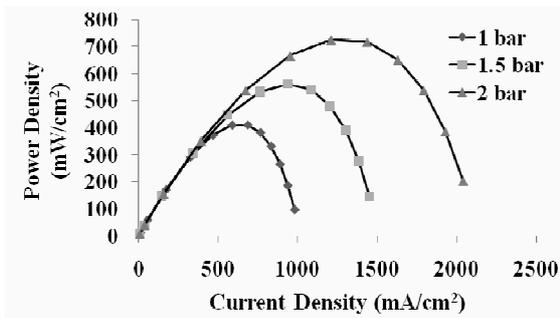
**Fig. 5 PEMFC Performance**



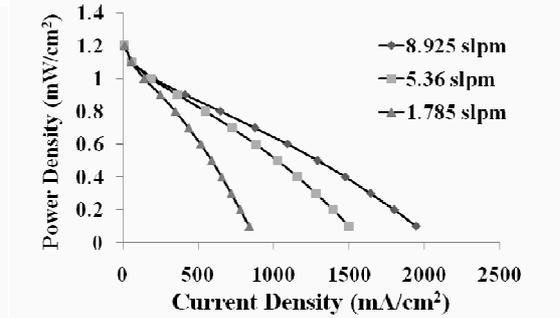
**Fig. 6 PEMFC Performance**



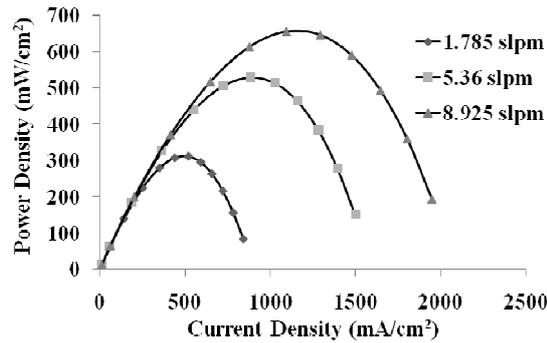
**Fig. 7 PEMFC Performance**



**Fig. 8 PEMFC Performance**



**Fig. 9 PEMFC Performance**



**Fig. 10 PEMFC Performance**

Figures 9 and 10 show the performance of the PEMFC for different flow rates of hydrogen. As can be expected the power delivered is proportional to the fuel flow rate.

The power produced by the PEMFC is expressed as a function of the pressure and temperature as follows:

$$W = -1.05594 + 1.385369 * P + 0.004735 * T$$

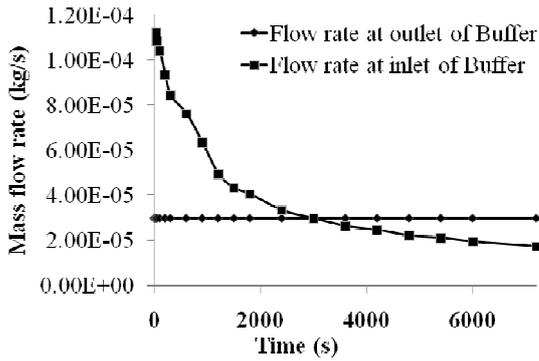
This correlation, valid for pressures between 1 bar to 3 bar and temperatures between 273K and 383K, gives the power output of system in kW as a function of the pressure (bar) of the inlet gases and operating temperature (K) of the fuel cell. In order to operate the power system at different load conditions one can fix the temperature at which the fuel cell is operating and vary the pressure through the valve as per the load requirement.

Performance of the Coupled System:

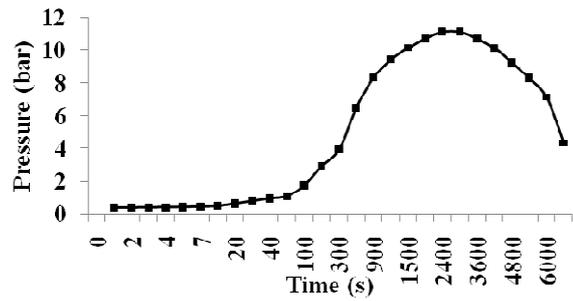
Three different cases of loading of the fuel cell have been considered to demonstrate the operation of the coupled system:

*a) Constant Load*

Figure 11 shows the mass flow rate of hydrogen to the fuel cell and the rate at which the hydrogen is desorbed from the metal hydride bed. Initially the rate of desorption in the metal hydride bed is greater than the rate of hydrogen required by the fuel cell. Hence more hydrogen is available than is required by the fuel cell. It can be seen that the rate of desorption decreases with time and after a certain point in time the rate of desorption is less than the rate of consumption of hydrogen by the fuel cell.



**Fig. 11 H2 flow rates in and out of the buffer tank**

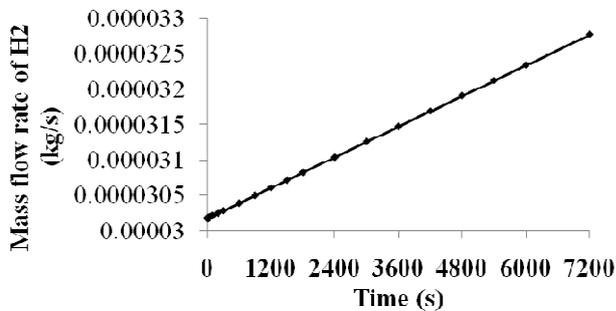


**Fig. 12 Variation of H2 pressure in the buffer with time**

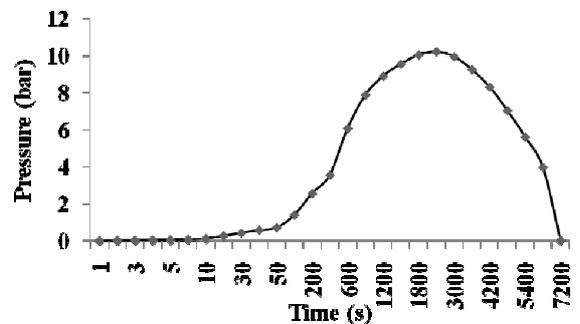
Figure 12 shows the pressure of hydrogen in the buffer as a function of time. Since the rate of hydrogen production decreases continually the amount of hydrogen in the buffer first increases and then it decreases. There is some amount of hydrogen still left in the buffer after the operation of the fuel cell for two hours.

*b) Linearly Increasing Load*

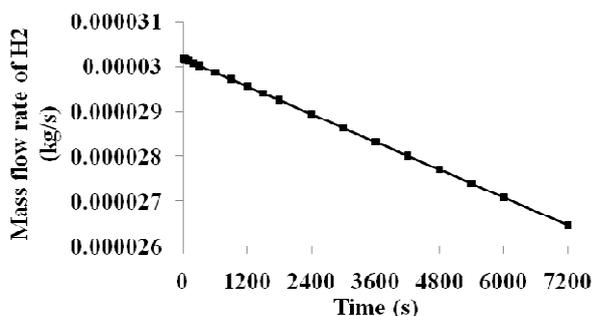
Figure 13 shows the flow rate of hydrogen consumed by the fuel cell in case of a linearly increasing load. As seen in the figure, the mass flow rate of hydrogen increases with time. Figure 14 shows the pressure of hydrogen in the buffer as a function of time. The pressure peaks earlier in this case than the constant load case as hydrogen is consumed at a faster rate. Also one can see that the hydrogen in the buffer is almost consumed.



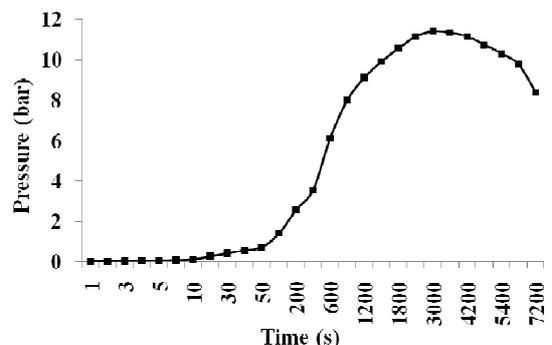
**Fig. 13 Mass flow rate requirement of PEMFC**



**Fig. 14 Variation of H2 pressure in the buffer with time**



**Fig. 15 Mass flow rate requirement of PEMFC**



**Fig. 16 Variation of H2 pressure in the buffer with time**

c) *Linearly decreasing load*

Figure 15 shows the flow rate of hydrogen demanded by the fuel cell in case of a linearly decreasing load. Figure 16 shows the pressure of hydrogen in the buffer as a function of time.

### Concluding Remarks

A simple strategy for coupling a PEMFC with a solid state MH hydrogen storage device using a hydrogen gas buffer between the two components is proposed. The performance of such a system is demonstrated for the case of two hour operation of a 2 kW peak capacity PEMFC.

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### Acknowledgements

The support of United States Department of Energy, Office of Energy Efficiency & Renewable Energy – Fuel Cell Technologies Program Office through Argonne National Laboratory is gratefully acknowledged.