THERMODYNAMIC RATING OF AN ENERGY EFFICIENT CHILLER CUM HEATER FOR METAL HYDRIDE STORAGE IN HYBRID PHOTOVOLTAIC -FUEL CELL (PV/FC) SYSTEM

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ABSTRACT

With dwindling energy resources which earth is having in the form of fossil fuels, today there is a scrupulous requirement of venturing alternative avenues, which can eventually share the ever-increasing energy demand. Solar photovoltaic is a reliable and clean source of energy. However due to its intermittent nature, it is vital to integrate solar photovoltaic with other sources of energy. Fuel cell technology because of its inherent environment friendly behavior has been an option that can fulfill this requirement. Present study deals with exploring the design challenges of integrating hydrogen fuel cell with solar photovoltaic. The continuous supply of hydrogen as fuel can be met in a safer and reliable manner through solid state storage of metal hydride system, with the hydrogen generated through an electrolyzer utilizing the PV (Photovoltaic) electricity. The challenges lie in dealing with the high-end exothermic reaction that occurs in the process of storing hydrogen in the metal hydride and the endothermic reaction that occurs in the process of extracting hydrogen. Therefore designing of an adequate cooling and heating arrangement for metal hydride storage system is also very important from efficient energy utilization point of view. Thermodynamic analysis of this cooling and heating circuit is reported for making an energy efficient PV/FC (Photovoltaic-fuel cell) system. The metal hydride unit is thermodynamically analyzed to critically ascertain the performance of the chiller that extracts the exothermic heat generation of the hydrides for the hydrogen storage to occur and the heater to achieve the reverse action. Several candidate approaches ranging from a simple back of the envelope calculations to sophisticated conjugate heat transfer analysis using CFD (Computational Fluid Dynamics) techniques are utilized to analyze the system. For the range of parameters considered, the study estimated the chiller and heater requirements of 250 W and 500 W respectively.

NOMENCLATURE

Abbreviation	Parameters
ΔH_r (kJ/mol)	Enthalpy of formation
C (kJ/kg K)	Specific heat
$\dot{q}'''_{H_2-MH}$	Heat generation
Ra_D	Rayleigh number
Pr	Prandtl Number
V	Kinematics viscosity
T_s	Outer cylinder surface temperature
Nu	Nusselt number
g (m/s^2)	Acceleration due to gravity
D_o(m)	Outer cylinder diameter
h_o (W/m^{2}K)	Heat transfer coefficient
k (W/m K)	Thermal conductivity
S (J/molK)	Entropy
R (J/mol K)	Universal gas constant
D_0 (m)	Characteristic diameter
F	Progress variable[13]
T (K)	Temperature
P (bar)	Pressure
MH	Metal hydride
PV	Photovoltaic
FC	Fuel cell
A (m^2)	Metal hydride cylinder area
U (W/m^{2}K)	Overall heat transfer coefficient between air and cylinder
H_g	Overall heat gain
H_s	Heat gain/loss by surrounding
H_{MH}	Heat generation inside metal hydride
C_{pw}(kJ/kg K)	Specific heat capacity of water
NL	Nominal litre
x	Cartesian axis direction
y	Cartesian axis direction
z	Cartesian axis direction
Special characters	
ε	Porosity factor
ρ	Density
Subscripts	
eff	Effective
g	Gain
sur	Metal hydride cylinder surface
amb	Ambient

INTRODUCTION

Energy demand is increasing rapidly in the world with increasing economic development. However, limited conventional sources and harmful emissions emphasize the need to develop new renewable and carbon free sources of energy. Thriving research activity in solar photovoltaic and hydrogen system encourages focusing and exploring both sources of renewable energy. Hydrogen production using PV power and storage in metal hydride leads to intensive research activities.

Hybridization of solar photovoltaic with fuel cell is wiser choice for efficient utilization of solar PV power [1]. Hydrogen storage in metal alloy is much space efficient and safer [2]. But considerable amount of heat is liberated by absorption/desorption process of H_2 because of charging and discharging of hydrogen in metallic alloy during their endothermic and exothermic reactions [3]. Study of metal hydride cylinder temperature effect on hydrogen desorption process has been studied in details. This study explains the effect of inlet pressure and temperature on discharging rate. Similarly effect of water circulation temperature on metal hydride system explaining the H_2 discharging rate has also been studied. This study concluded an increase in the discharging of H_2 with increase water circulation temperature [4]. At a given temperature of absorption process, the H_2 absorbing rate and storage capacity of MH are increased with increasing inlet pressure of H_2. By lowering water circulation temperature the absorption rate and storage capacity increase and vice versa. Study of overall heat transfer coefficient on the absorption and desorption process reveals that absorption and desorption enhances with high heat transfer coefficients [5]. Studies have also been done for analyzing heat transfer process through different geometrical structures. Heat transfer for circular and elliptical geometries has been analyzed experimentally and theoretically in Ansys Design modeller [6]. The study of local heat transfer coefficient and temperature distribution within two concentric cylinders has been analyzed theoretically and experimentally [7].

From the reviewed literature of metal hydride charging and discharging, it can be seen that efficient system could be designed only by considering adequate coolant flow. This creates a need of efficient cooling or heating circuitry study that can be provided by a chiller/heater. Present study will make an attempt to explore design possibilities of such arrangements. The study presented here describes an analysis based on preliminary experiments backed up by CFD.

The experiments are carried out at CES, IIT Delhi Lab. Delhi is situated in north India and having geographical latitude of $28^{\circ}36^{'}$ and longitude of $77^{\circ}13^{'}$. Its elevation is 125m. The summer continues from March to June while winter prevails from November to February. The temperature variation is around 45 ℃ to 19 ℃ during summer and 31 ℃ to 4 ℃ during winter. To initiate the study for H_2 storage, a chiller of 165 W was selected for metal hydride charging operation. However the functioning of this chiller was successful during low ambient temperature conditions of 35 ℃ and below, it is not rendering the desired output during summer when the ambient temperature goes up to 45 ℃. This affects the chiller performance that relies on the ambient temperature which is function of seasonal variations. Therefore it is deduced to model /design cooling and heating circuit of metal hydride system with changing weather conditions.

SYSTEM DESCRIPTION

$LaNi_5$ metal alloy is used for the hydrogen storage in PVFC hybrid system. Metal hydride tank of 5000 NL (nominal litre) is used in the experiment as shown in Figure 1. The details of MH system are given in table 1. Metal hydride reaction is given as:

Charging/Discharging
$$\text{Metal} + x.H_2\ (\text{Metal}) \longleftrightarrow H_2 + \text{heat} \quad (1)$$
(Exothermic/endothermic reaction)

The temperature of the cooling fluid required for cooling the system during the charging, ranges from10 ℃ to 25 ℃ While heating the requirements ranges from 20 ℃ to 40 ℃ [8]. For this purpose two constant temperature baths are used, one bath for cooling and other bath is for heating. Water is used as cooling and heating media. A pump of 25 W is used to pump the water into MH cylinder described in Table 1.With the help of the opening/closing valves the flow of cold and hot water is controlled as shown in Figure 2.

Fig 1 Metal hydride storage system
1, 6 –Metal hydride cylinder 2- Fuel cell 3- Pressure transmitter 4-Pressure regulator 5-Hydrogen supply line 7-Electrolyzer 8-Water supply line 9- chiller/heater 10- hydrogen cylinder

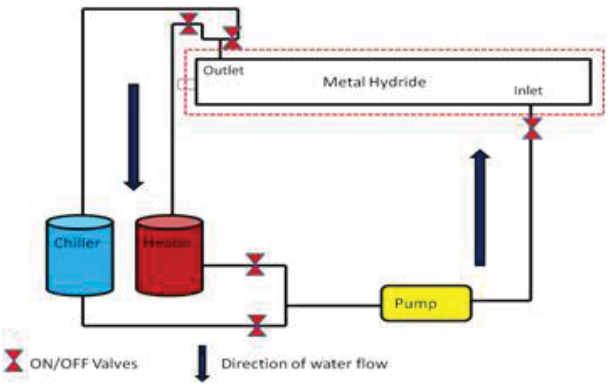

Fig 2 Water controlling unit of MH

Table 1 Description of MH cylinder

S. NO.	Parameters	Value
1	Metal alloy cylinder	7
2.	Outer cylinder	1
3.	Metal alloy	$LaNi_5$
4.	Material of cylinder	Stainless steel
5.	Length of cylinder (m)	0.93
6.	Diameter of outer cylinder (m)	0.168
7.	Diameter of inner cylinder (m)	0.50
8.	Heat transferring fluid	Water

NUMERICAL ANALYSIS

In the present study the test module is a water jacketed assembly of hermitically sealed MH cylinders as shown in Fig. 1. The MH cylinders are of diameter 50 mm and length 930 mm with the coolant jacket of diameter of 168 mm and length 930 mm. The conjugate heat transfer taking place through the metal hydride and the coolant circulating through the outer envelope of the metal hydride cylinders is estimated through CFD (Computational Fluid Dynamics). For the CFD analysis the coolant flow is treated as a convective boundary condition with a heat transfer coefficient and temperature of coolant at the inlet corresponding to actual known test conditions as shown in Table 2.

Table 2 Inlet water temperature

Process	Water inlet temperature (°C)
Charging	20
Discharging	30

The coolant flow conditions used in the experiments with their corresponding maximum and minimum observed temperature variations during summer and winter conditions of Delhi (where the experiments are carried out) are given in Table 3 and Table 4.

Table 3 Heat transfer coefficient during charging

Parameter	Tavg (°C)	Ra	Nu	$h_o\,(\frac{W}{m^2K})$
Summer max	32.5	1.04×10^7	28.29	4.5
Summer mini	19.77	4.43×10^5	11.47	1.77
Winter max	25.55	4.7×10^6	22.43	3.57
Winter min	12.15	9.0×10^6	27.16	4.05

Table 4 Heat transfer coefficient during discharging

Parameter	T_{avg} (°C)	Ra	Nu	$h_o\,(\frac{W}{m^2K})$
Summer max	37.5	5.13 x 10^6	22.95	3.76
Summer min	24.55	4.66 x 10^6	22.33	3.55
Winter max	30.5	4.61 x 10^5	11.60	1.84
Winter min	17.15	1.28 x 10^7	30.11	4.64

Calculation of heat transfer coefficient through outer cylinder

Calculation of heat transfer coefficient is done for different ambient conditions. Two extreme temperatures of summer and winter are chosen from the Meteonorm 7 software [9]. The value of maximum and minimum temperature in summer and winter is given in table 5 as:

Table 5 Inlet water temperature of MH

Season	T_{max} :(	T_{min} :(
Summer	44.1	19.1
Winter	31.1	4.3

For the CFD analysis it assumed that that outer cylinder temperature is equal to metal hydride when it is charged (20 °C) [8]

_t e over metal hydride cylinder is taken as:

_t e L Xik E XW c X / 6 (2)

Rayleigh number for metal hydride cylinder is estimated as:

H L e kXi Xfi cH/ / t· (3)

Nusselt number is governed by following correlations [10] as:

Nu= r x E 4 7< ;, 6 2 / e5>@ 11 5 2 4 .3 Á i (4)

Heat transfer coefficient between metal hydride cylinder and ambient air is calculated as:

D4 L ‰, Nu (5)

Where k and h_o are thermal conductivity and heat transfer coefficient respectively.

The coolant flowing through the outer envelope enters the metal hydride cylindrical bank with certain velocity and at a predefined temperature. The coolant after passing through the metal hydride cylinders comes out through the outlet at certain conditions which is estimated through this CFD simulation.

The metal hydride system is subjected to conjugate heat transfer phenomenon as it interacts with the ambient through natural convection. The metal hydrides react with pressurized hydrogen under different operating conditions. The turbulent forced convection of the coolant helps in mitigating the energy generated or absorbed during the exothermic and endothermic reactions respectively.

The pressure and temperature inside the metal hydride cylinder is governed by the Van't Hoff equation [11] as follows:

@ TL/Te A L F ¿W/V E ¿L/VX (6)

Values of ¿ and § is given in Table 6 [12]:

Table 6 Enthalpy and Entropy of formation of $LaNi_5$

Process	¿ (kJ/mol)	§(J/molK)
Absorption	-31.84	-111
Desorption	31.84	111

Since the metal hydride cylinders are secured in a hermitically sealed cylindrical jacket therefore experimental estimation of the actual flow conditions of the coolant flowing through the system is cumbersome. Also the heat generated in the cylinder through the solid metal alloy complicates the situation of temperature estimation. CFD is therefore chosen as a reliable tool to measure the flow condition under this situation. The computational solution of any fluid dynamics problem requires approach into the conservation of mass, momentum and energy (Navier-Stokes) equations. These equations are as follows:

ˇ L r (7)

Oˇ L F ˇ E Jˇ6 (8)

Oˇ L ˇ: ˇ ;F ˇ (9)

where, ρ is the density of the fluid, p is the pressure acting in the direction of flow, F is the net body force acting over the domain and, v is the free stream velocity acting in x-direction, y-direction and z direction.

Turbulent flows at realistic Reynolds numbers are characterised by a large range of turbulent length and time scales. The Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) of such turbulent flows would require very high computing power and hence such methods are restricted and a reduced simulation complexity is adopted by time averaging the turbulence effects considering mean quantities of the flow. With the introduction of time averaging procedure, the instantaneous velocity L E (where, V and v' are mean and fluctuating components of velocity) and instantaneous temperature L _t cp _E (where, $T_{average}$ and t' are mean and fluctuating components of temperature). By substitution of v and T in equation 3, 4 and 5 respectively results in average equations (RANS) for incompressible flow as follows:

$$\nabla.V = 0 \quad (10)$$
$$\rho\nabla V.V = F - \nabla p + \mu\nabla^2 V + V\tau \quad (11)$$
$$\rho\nabla v.E = \nabla(k\nabla T_{avergae}) - \nabla.p \quad (12)$$

Using energy balance of metal hydride it is found that-

$$(\rho C)_{MH}\frac{\partial T}{\partial t} = -\frac{[H]m}{2}\Delta H_r\frac{\partial F}{\partial t} + k_{eff}\nabla^2 T + \dot{q}'''_{MH-H_2} \quad (13)$$

Using energy balance of hydrogen system, it is found that

$$(\rho C)_{H_2}\frac{\partial T}{\partial t} = \frac{\partial p}{\partial t} + k_{eff}\nabla^2 T + \dot{q}'''_{H_2-MH} \quad (14)$$

The heat generated by the metal hydride cylinders are calculated on the basis of the molar heat generation as shown below

Enthalpy of formation of metal hydride is 31.84 kJ/mol.

H_2 flow rate in metal hydride 100 NL/hr

So heat liberation by hydrogen absorption/ desorption is 37 W.

The above sets of equations are solved using finite volume approach by imposing appropriate boundary conditions. The computational domain is discredited with tetrahedral meshing of 269783 cells. Figure 3 depicts the meshed geometry under investigation. The test section geometry is developed in ANSYS DesignModeler [13]. The discretized control volumes are solved using Fluent as the solver. Figure 4 shows the grid of the geometry in details.

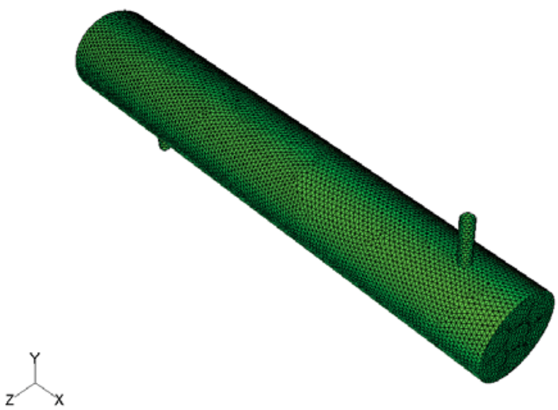

Figure 3 Metal hydride meshed circuit with coolant circuit

Figure 4 Metal hydride kit with coolant circuit

RESULTS AND DISCUSSION

The computational model was run to achieve initial grid independence to optimize the number of cells to 269783. The model converged with a mesh of 109697 tetrahedral mesh volumes for the cylinder jacket with inlet and outlet system and 160086 tetrahedral mesh volumes for the metal hydride and with an approximate grid length of 0.508 mm. After stabilizing the mesh, the computational model was run by varying the different input parameters including the seasonal temperature variations and the coolant flow rate. The velocity vectors for a typical condition of maximum summer temperature are shown in Figure 5

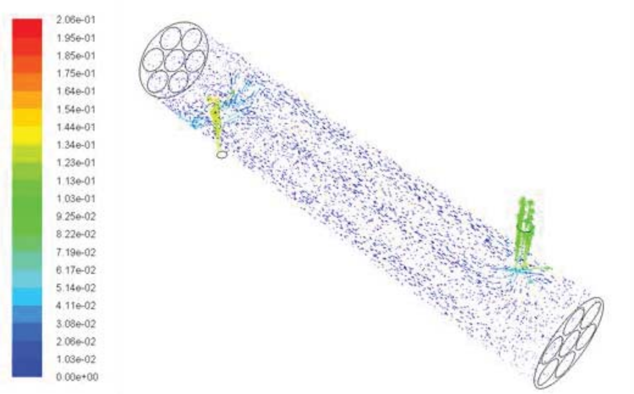

Figure 5 Velocity contours in m/s of the coolant flow along the metal hydride cylinders from inlet to outlet – For summer during exothermic heat generation

Figure 6 and Figure 7 show the temperature map of the water jacket during charging at maximum temperature of the summer day and discharging at minimum temperature of the winter day respectively as mentioned in the range of parameters. It can be observed that for both charging and discharging the cooling and heating capacity of the coolant is strongly governed by the external free convection. The pattern depicts the impression of an induced Rayleigh Bernard flow which would have been visible with an extended boundary simulation of the ambient [14]. Figure 8 and Figure 9 shows the variation of temperature over the metal hydride cylinders during the exothermic and endothermic reactions that generate or absorbs heat in the process. The internal coolant flow over the metal hydride cylinders explains the cooling/ heating mechanism in an elaborate manner. Figure 10 to 13 shows the effectiveness of the fluid to absorb or generate heat during summer and winter respectively. As the fluid travels from the inlet to outlet it swaps the energy distribution showing efficient mode of cooling or heating. This energy swap is governed by solid metal hydrides heat generation or absorption during the charging and discharging through pressurized hydrogen.

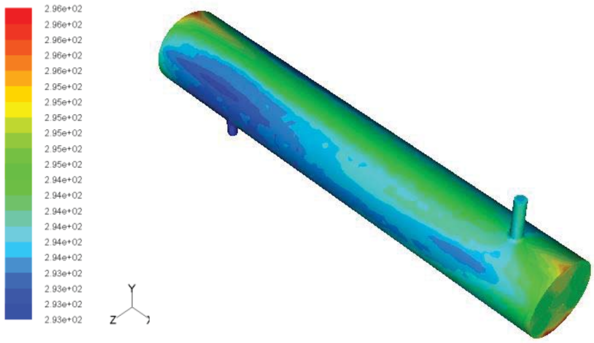

Figure 6 Temperature distribution in K of the cylinder jacket with water circulated from inlet to outlet – For summer during metal hydride charging

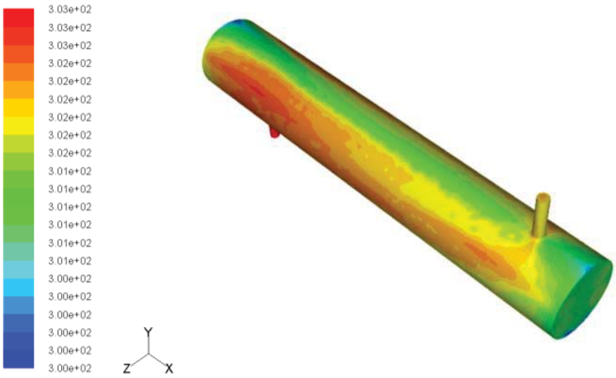

Figure 7 Temperature distribution in K of the cylinder jacket with water circulated from inlet to outlet – For winter during metal hydride discharging

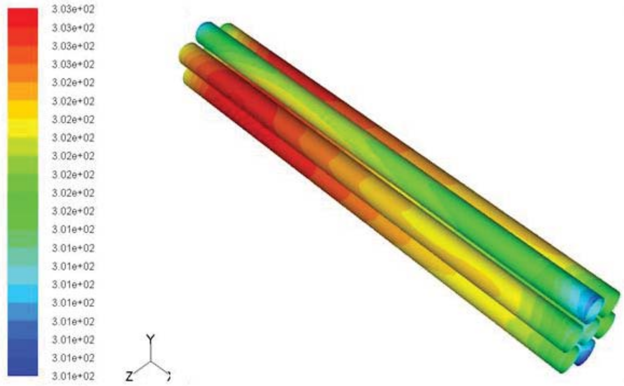

Figure 8 Temperature distribution in K of the metal hydride cylinders with water circulated from inlet to outlet – For summer during metal hydride charging

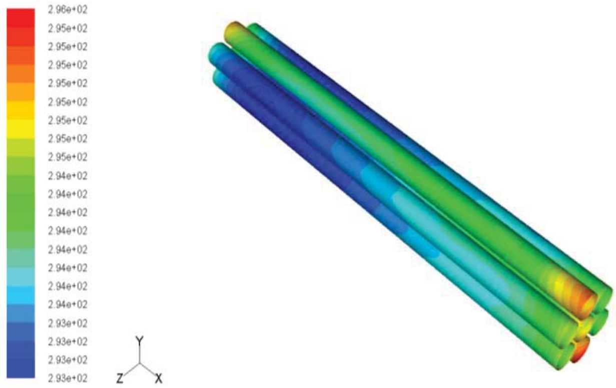

Figure 9 Temperature distribution in K of the metal hydride cylinders with water circulated from inlet to outlet – For winter during metal hydride discharging

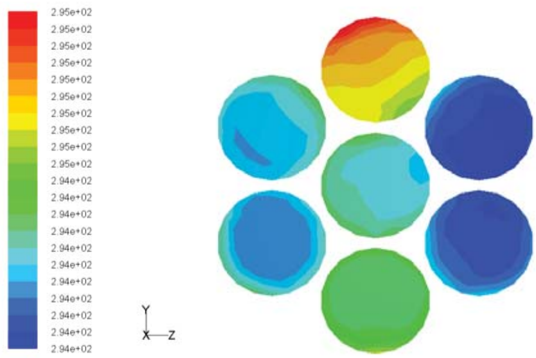

Figure 10 Temperature distribution in K of the inlet side of the metal hydride cylinders with water circulated from inlet to outlet – For summer during exothermic heat generation

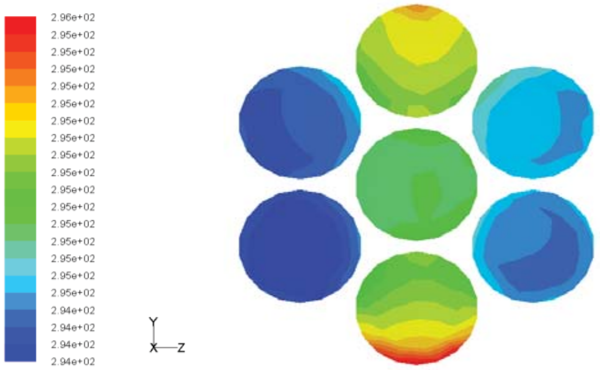

Figure 11 Temperature distribution in K of the outlet side of the metal hydride cylinders with water circulated from inlet to outlet – For summer during exothermic heat generation

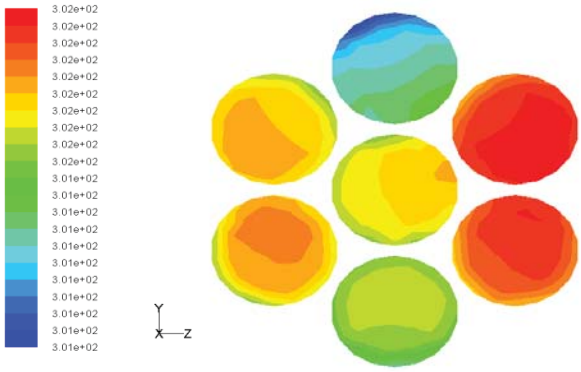

Figure 12 Temperature distribution in K of the inlet side of the metal hydride cylinders with water circulated from inlet to outlet – For winter during endothermic heat absorption

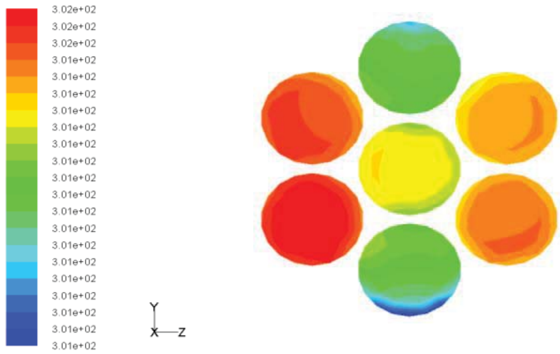

Figure 13 Temperature distribution in K of the outlet side of the metal hydride cylinders with water circulated from inlet to outlet – For winter during endothermic heat absorption

Estimation of Chillier rating

Energy balance for the metal hydride and chiller /heater system is described as follows:

Cooling /heating to be provided by chiller /heater = cooling or heating load of the system (15)

To maintain constant water temperature inside metal hydride the heating load should be equal to cooling provided by the chiller.

Source of heat gain or loss in system for charging during summer/winter is equal to heat generation by the MH and heat gain by surrounding.

$$H_g = H_s + H_{MH} \quad (16)$$

Where, H_g is overall heat gain by the MH system.

H_{MH} is heat generation by metal hydride and H_s is heat gain/loss by surrounding, which is given as:

$$H_s = UA\Delta T \quad (17)$$

Where U is overall heat transfer coefficient and A is area of metal hydride cylinder and ΔT is temperature difference.

COP (Coefficient of performance) of chiller is given as:

$$COP_{Chiller} = \frac{\text{Cooling capacity}}{\text{Work input}} \quad (18)$$

Ideal COP of the chiller in summer condition is governed by:

$$COP = \frac{T_L}{T_H - T_L} \quad (19)$$

T_L is cooling temperature which is 20 ℃ for absorption process, which is chiller water temperature and T_H is sink temperature, which ambient temperature.

The COP of commercially available chiller is given =1.33 [15]

CFD results shows that heating load on the system in summer for charging process of H_2 is 167 W.

According to calculations compressor should be at least 126 W. But in summer the compressor COP will decrease due to high sink (ambient) temperature [16]. Therefore by considering the above thermodynamic criteria of cooling requirement a factor of 2 is envisaged and 250 W chiller is proposed. This will ascertain a smooth functioning of the system without any discontinuities.

Estimation of heater rating

Running on the same line CFD analysis predicted the cooling load requirement to be 203W.

COP of electric heater is given as:

$$COP_{Heater} = \frac{\text{Heating capacity}}{\text{Work input}} \quad (20)$$

Thermodynamically COP of electric heater is unity, which predicts the heater rating to be at least 203 W. Commercially available electric heater has minimum rating of 500 W, hence a 500 W electric heater is selected for heating.

CONCLUSION

This study attempts to look at a catalogue approach for selecting an energy efficient chiller cum heater system capable of operating under varying ambient conditions due to the seasonal changes throughout the year. The CFD study of the metal hydride system has been done successfully. According to the present study rating of chiller and heater are estimated as 250 W and 500 W respectively. The results predicted by the above study of metal hydride system are used to install a water chiller/heater in the Centre for Energy Studies, IIT Delhi. The metal hydride system is working satisfactory with this chiller/heater.

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