**International Conference on Applied Energy 2020**
**Dec. 1 - Dec. 10, 2020, Bangkok / Virtual**
**Paper ID: 0424**

# Numerical study of magnesium-based metal hydride reactor incorporating multi-phase heat exchanger for thermal energy storage system

Jing Yao[1], Pengfei Zhu[1], Jianwei Ren[2], Mehmet Fazıl Kapçı[3], Burak Bal[3], Sandra Kurko[4], Zhen Wu[1,] *, Zaoxiao Zhang[1,5,] *

1 School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an, 710049, PR China

2 Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa

3 Mechanical Engineering Department, Abdullah Gul University, Kayseri, Turkey

4 Center of Excellence for Hydrogen and Renewable Energy, University of Belgrade, Belgrade, Serbia

5 State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, 710049, PR China

* Corresponding author, Email: wuz2015@mail.xjtu.edu.cn (Zhen Wu) & zhangzx@mail.xjtu.edu.cn (Zaoxiao Zhang)

## ABSTRACT

Metal hydride based thermal energy storage system is regarded as a promising method due to its good reversibility, low cost, and no by-product. Multi-phase heat exchange has much higher heat transfer coefficient than single-phase fluid heat exchange, thus facilitating the steam generation. In this study, a two-dimensional model of the metal hydride reactor using multi-phase heat exchange is proposed to estimate the performance and its feasibility of application in the concentrated solar power system. The results show that the velocity of the heat transfer fluid should match well with the thermal conductivity of the metal hydride bed to maintain the heat flux at a relatively constant value. The match of thermal conductivity of 3 or 5 W/(m·K) and fluid velocity of 0.0050 m/s results in the heat flux up to about 19 kW/m$^2$, which is increased by 3 orders of magnitude than single-phase heat exchange. This study helps to facilitate the widespread application of metal hydride based thermal energy storage system in the concentrated solar power system.

**Keywords:** metal hydride; thermal energy storage; heat exchange; phase change material; power system.

## NONMENCLATURE

| | |
|---|---|
| *Abbreviations* | |
| CSP | Concentrated solar power |
| MH | Metal hydride |
| MH-TES | Metal hydride based thermal energy storage |
| MHR | Metal hydride reactor |
| PCM | Phase change material |
| TCS | Thermochemical storage |
| TES | Thermal energy storage |
| *Symbols* | |
| $C_p$ | Specific heat, J/(kg·K) |
| $H$ | Enthalpy, kJ/mol |
| $m$ | Transferred mass, kg |
| $T$ | Temperature, K |
| $\lambda$ | Thermal conductivity, W/(m·K) |
| $\rho$ | Density, kg/m$^3$ |
| $\phi$ | Volume fraction |
| $\mu$ | Viscosity, Pa·s |
| $\Delta H$ | Enthalpy change, kJ/mol |

## 1. INTRODUCTION

The development of human society depends on the energy consumption. During the recent years, more and more concentrated solar power (CSP) system has been built around the world, indicating the huge potential of solar energy market [1]. In the CSP system, due to the

Selection and peer-review under responsibility of the scientific committee of the 12th Int. Conf. on Applied Energy (ICAE2020).

various light condition and power demand of users over a day, thermal energy storage (TES) is always equipped to keep the balance between power generation and demand [2]. During the daytime, solar energy is collected and converted into thermal energy. Part of the thermal energy is used to generate power directly, while the rest is stored in the TES system. During the nighttime, the thermal energy stored in the TES system is released and used to generate power. The TES plays an important role in the control of power generation and the efficient utilization of solar energy. At present, sensible thermal storage, latent thermal storage and thermochemical storage (TCS) are three main approaches applied for the TES. The energy density of the sensible and latent thermal storage is about 108 and 360 kJ/kg, respectively [3]. Compared with these two approaches, the TCS is able to achieve significantly higher energy density, about 2800 kJ/kg for metal hydride $MgH_2$. Besides, the storage duration of the TCS can be indefinitely long in theory. Given these advantages, the TCS attracts extensive attentions [4].

Among all kinds of materials for TCS, metal hydrides (MH) have the advantages of good reversibility, low cost, no by-product and large experimental feedback, which are considered as a promising contender for the TES in the CSP system. The thermal storage process of the MH is achieved by a reversible chemical reaction. During the daytime, the heat from solar energy results in the hydrogen desorption of the MH. The hydrogen desorption reaction is endothermic, thus the thermal energy storage is realized. During the nighttime, hydrogen is supplied to the MH. The reaction between hydrogen and the MH occurs with the release of a large quantity of heat, indicating that the stored thermal energy is released.

Many heat transfer cell designs have been employed in the metal hydride reactor (MHR), such as multi-tubular, helical coil heat exchanger, adding expanded graphite or metal foam, compacted disc of the MH [5]. However, the researches mentioned above focused on the structure design of heat exchanger and the thermal conductivity improvement of the MH bed. Little attention is paid to how to enhance the heat transfer fluid. The boiling heat transfer of fluid has higher heat transfer coefficient than single-phase fluid heat exchange [6]. Meanwhile, the steam generated by boiling process is compatible with the subsequent Rankine cycle in the CSP system. In addition, considering the interval of hydrogen absorption and desorption process in the MHR, storing a small part of heat in the phase change material (PCM) during hydrogen absorption process is beneficial to the temperature control and the rapid startup of the high temperature MH during the hydrogen desorption process.

Therefore, a two-dimensional model of the MHR using multi-phase heat exchange (including boiling heat transfer and PCM heat storage) is proposed to estimate the performance of the MH-TES and its feasibility in the CSP application in this study. Based on the developed model, the effects of some key parameters are predicted to optimize the performance. This study contributes to the performance improvement and the efficient design of the TES in the practical application of the CSP system.

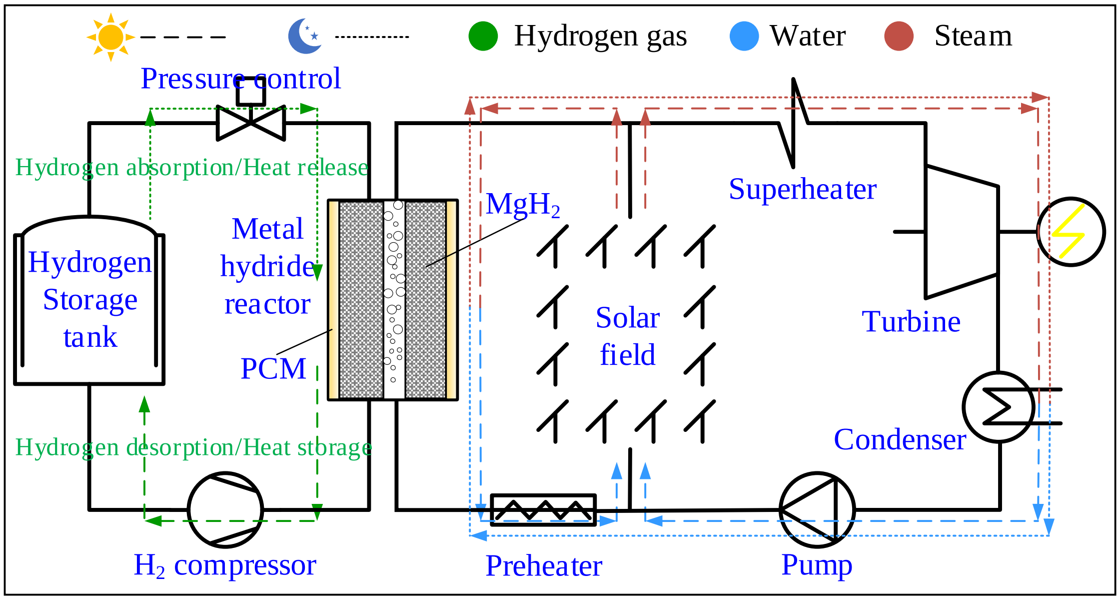

Fig. 1 The schematic diagram of the CSP system coupled with the MH-TES using multi-phase heat exchange.

## 2. MODEL DEVELOPMENT

Fig. 1 illustrates the schematic diagram of the CSP system coupled with the MH-TES using multi-phase heat exchange. During the daytime, the solar field is equivalent to a boiler for generating steam. Part of the steam is used for power generation, while the others drive the hydrogen desorption reaction of the MH to achieve the thermal energy storage. When considering the heat dissipation to external environment, the approach of storing part of heat into the PCM could maintain the temperature of the MHR at high level. In this way, relatively high temperature is prepared for hydrogen absorption process without extra heat device.

During the nighttime, heat released by hydrogen absorption reaction is used for steam generation. The subcooled water at 3.5 MPa (with saturation temperature of 242.5 °C) is first heated to 220 °C by preheater, and then turned into steam in the MHR. The boiling process of the liquid significantly increases the heat transfer coefficient. It should be noted that the outlet fluid of the MHR may not be converted into steam completely. The superheater can complete the evaporation of the liquid and prevent the droplets from entering the turbine. Besides, many parallel reactors can be combined to store the heat from solar energy for a large system.

Fig. 2 presents the configuration of the designed MHR and the structured grid for simulation. In the center of MHR, a tube of 3 mm in radius is installed for heat transfer flow. Outside this tube, an annular tube with outer radius of 35 mm and inner radius of 3 mm is placed for MH bed. Then, a PCM layer of 3 mm surrounds the MH bed. The height of MHR is 70 mm. The thermal properties of the $MgH_2$ bed (MH) and $NaNO_3$ (PCM) are listed in the Table 1 [7].

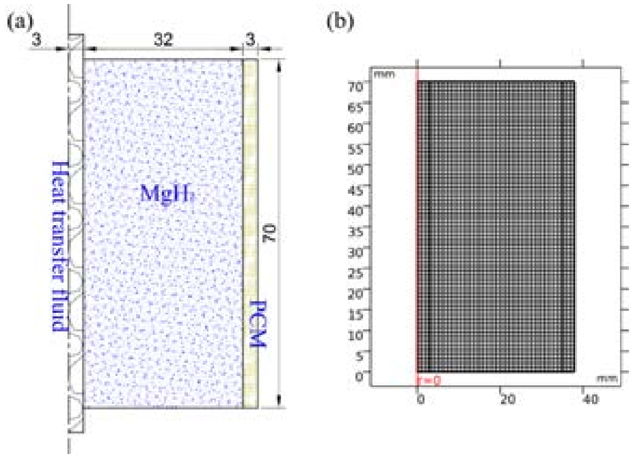

Fig. 2 The configuration of MHR (a) and the structured grid for simulation (b).

Table 1 The thermal properties of $MgH_2$ bed (MH) and $NaNO_3$ (PCM) [7].

| Property | Value |
|---|---|
| $MgH_2$ (MH) | |
| Thermal conductivity | 0.48 W/(m·K) |
| Specific heat | 1545 J/(kg·K) |
| Density | 1800 kg/m$^3$ |
| Porosity | 0.74 |
| Rate constant | $2.9\times10^8$ 1/s |
| Activation energy | 130 kJ/mol |
| Reaction enthalpy | -75 kJ/mol |
| Reaction entropy change | -135.6 J/(mol·K) |
| Saturated mass content of hydrogen | 0.06 |
| $NaNO_3$ (PCM) | |
| Melting temperature | 307 °C |
| Thermal conductivity | 0.5 W/(m·K) |
| Specific heat | 1820 J/(kg·K) |
| Density | 2260 kg/m$^3$ |

## 3. RESULTS AND DISCUSSION

In this model, the PCM is employed to store part of heat during the hydrogen desorption process to maintain the MHR at high temperature until hydrogen absorption process. When the hydrogen absorption process starts, the initial condition of the PCM can be completely melted ($\vartheta$=1, good heat preservation) or solidified ($\vartheta$ =0, poor heat preservation) or in-between position.

Fig 3 displays the distributions of void fraction (in the heat transfer fluid, 0<$x$<3 mm), reaction fraction (in the MH bed domain, $3 \leqslant x \leqslant 35$ mm), and melting fraction (in the PCM domain, 35<$x$<38 mm) at initial melting fraction $\vartheta$=0 and 1. It is found that part of heat

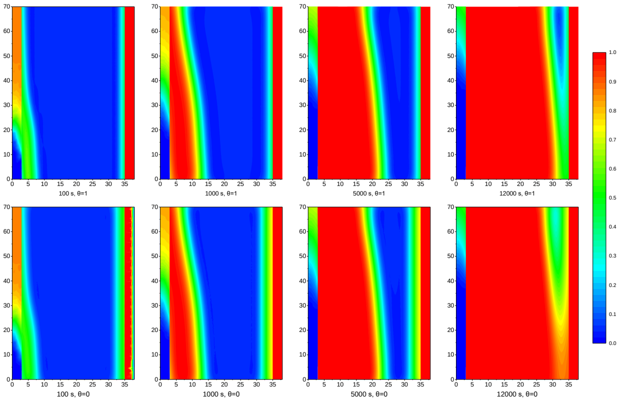

Fig. 3 The distributions of void fraction, reaction fraction, and melting fraction at initial melting fraction $\vartheta$ =0 and 1.

released by hydrogen absorption reaction is stored in the completely solidified PCM, thus increasing the reaction fraction of the MH. Nevertheless, the PCM has an impact on the MH bed which is close to the PCM only. In addition, the void fraction of heat transfer fluid achieves high level at the beginning, and then reduces over time. This can be explained by the low thermal conductivity of the MH bed and the increasing thermal resistant between the heat transfer fluid and heat source of reaction. Therefore, increasing the thermal conductivity of the MH bed is effective to optimize the heat transfer performance.

In this study, the thermal conductivity of the MH is increased from 0.5 to 1, 3 and 5 W/(m·K) by adding expanded graphite to investigate the effect of the MH thermal conductivity. As seen in Fig. 4, in the tube, the subcooled heat transfer fluid is first heated from 220 °C to saturation temperature. Then the heat transferred to fluid is used for its evaporation which takes a lot of heat. In Fig. 4(a), the low thermal conductivity leads to insufficient heat transfer to the fluid. The fluid reaches the saturation temperature at vertical distance of 30 mm under 0.5 W/(m·K), and at vertical distance of 15 mm under 1 W/(m·K). By comparison, the vertical distance for reaching saturation temperature is only 3 mm at the thermal conductivity of 3 and 5 W/(m·K).

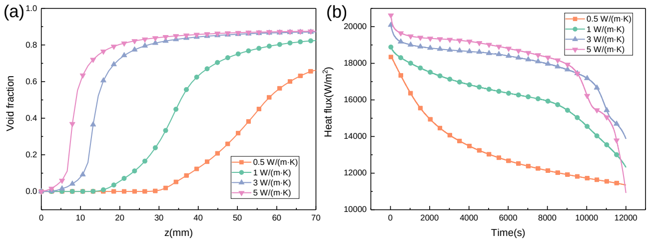

Fig. 4 The variation of void fraction at 5000 s (a) and the heat flux from the MH to heat transfer fluid (b) at different thermal conductivities

The heat flux from the MH to heat transfer fluid, which is also equivalent to the average heat transfer coefficient, is calculated, as shown in Fig. 4(b). At low thermal conductivity of 0.5 W/(m·K), the heat flux reduces from 18.3 to 11.3 kW/m$^2$ fast because large thermal resistant limits the heat flux from the MH to heat transfer fluid. At higher thermal conductivity of 3 and 5 W/(m·K), the heat flux reduces at low speed before the hydrogen absorption reaction is complete. The heat flux decreases from about 20 to 18 kW/m$^2$ before 10000 s under the thermal conductivity of 5 W/(m·K). The low reduce speed not only enhances the heat transfer between the MH bed and heat transfer fluid and accelerates the reaction during the whole hydrogen absorption process, but contributes to the stability of the steam quality, thus simplifying the operation of superheater. Therefore, increasing the thermal conductivity of the MH bed is an important auxiliary method to obtain better performance of heat transfer when multiphase heat exchange is adopted in the MH-TES.

## 4. CONCLUSIONS

In this paper, a two-dimensional model of the MHR using multi-phase heat exchange is established to describe the heat and mass transfer behavior and estimate the heat transfer performance. Based on the developed model, the effects of the key parameters on the heat transfer performance of the MHR are investigated for performance optimization. It is found that the fluid velocity should match well with the thermal conductivity of the MH bed to keep the uniform heat exchange during the hydrogen absorption process. For the thermal conductivity of 3 or 5 W/(m·K), the fluid velocity of 0.0050 m/s can maintain the heat flux at 19 kW/m$^2$, and 0.0025 m/s with 0.5 W/(m·K) corresponds to 10 kW/m$^2$.

## ACKNOWLEDGEMENT

This work was supported by the Natural Science Foundation of Shaanxi Province (No. 2020JM-014) and China-Central Eastern European Countries Higher Education Institutions Consortium (No. 202006).

## REFERENCE

[1] Palacios A, Barreneche C, Navarro ME, Ding Y. Thermal energy storage technologies for concentrated solar power – A review from a materials perspective. Renew Energy 2020;156:1244–65.

[2] González-Roubaud E, Pérez-Osorio D, Prieto C. Review of commercial thermal energy storage in concentrated solar power plants: Steam vs. molten salts. Renew Sustain Energy Rev 2017;80:133–48.

[3] Ayub I, Nasir MS, Liu Y, Munir A, Wu Z, Yang F, et al. Numerical modeling and performance comparison of high-temperature metal hydride reactor equipped with bakery system for solar thermal energy storage. Int J Hydrogen Energy 2020.

[4] Sunku Prasad J, Muthukumar P, Desai F, Basu DN, Rahman MM. A critical review of high-temperature reversible thermochemical energy storage systems. Appl Energy 2019;254:113733.

[5] Wu Z, Yang F, Zhang Z, Bao Z. Magnesium based metal hydride reactor incorporating helical coil heat exchanger: Simulation study and optimal design. Appl Energy 2014;130:712–22.

[6] Tong LS. Boiling Heat Transfer And Two-Phase Flow. CRC Press; 2018.

[7] Mellouli S, Abhilash E, Askri F, Ben Nasrallah S. Integration of thermal energy storage unit in a metal hydride hydrogen storage tank. Appl Therm Eng 2016;102:1185–96.