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# Numerical Aimulation of Hydride Reactor Magnesium with Storage of Heat of Reaction in Phase Change Material

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## Abstract

The objective of this manuscript is to study the possibility of improving the thermal performance of an Evacuated Tube Solar Collector with the integration of a Phase Change Material (PCM). A 2D mathematical model has been proposed. In addition, the feasibility of thermal coupling was studied. The objective of this study is to store all of the heat released during the absorption of hydrogen in a phase change material "$Mg_{69}Zn_{28}Al_3$"

For this, in this present study, we wanted to study the possibility of store the heat, released during hydrogen charging, in a phase change material (PCM), to restore it during the desorption step of the reactor The various results obtained will be presented and discussed**.**

Keywords: $Mg_{69}Zn_{28}Al_3$; phase change material; magnesium hydride; absorption; melting.

## 1. Introduction

Several studies have been carried out [1, 2] in order to predict heat transfer and mass for several configurations of the metal hydride reactors. Among these studies, we cite that of Choi, Mills [1], Gopal and Murthy [3], Mat and Kaplan [4-6]. These authors have developed two-dimensional models governing transfers of heat and mass, during sorption phenomena, in a metal reactor hydrogen. These models take into account the variation of the pressure in the reactor and of the temperature difference between the solid and the gas. Ben Nasrallah [7] et al. [8] have shown that these variations can be negligible. Askri and Mellouli [9, 10] developed a two-dimensional mathematical model describing the influence of different configurations of heat exchangers on heat transfers in a reactor containing $LaNi_5$. Three-dimensional models are also available. Chung et al. [13, 14] show that the presence of a volume of hydrogen gas in the part upper tank can decrease reaction times of the reactor.

Magnesium hydride has been studied numerically by Ph. Marty et al. [12] then by Chaise et al. [11]. Regarding radiation, little work has been published from causes the hydrides studied to react at low temperature levels (<100 ° C). However, for magnesium hydride, Askri et al. [2] found that this mode of heat transfer could influence the charging time. The analysis of this work makes it possible to consider the following hypotheses:

- Hydrogen behaves like an ideal gas between the pores of the hydride,
- The temperature of the gas is locally the same as that of the powder,
- The flow is considered to be laminar between the powder grains,
- The sensitive energy of the hydrogen entering the tank is negligible compared to reaction energy.

## 2. Description of the model used

The digital model developed is a two-dimensional model axisymmetric on two adjacent domains, one corresponding to the hydride of magnesium, the other to the phase change material (Figure.1). Indeed, this model allows taking into account the kinetic and thermodynamic behavior of hydride with an PCM.

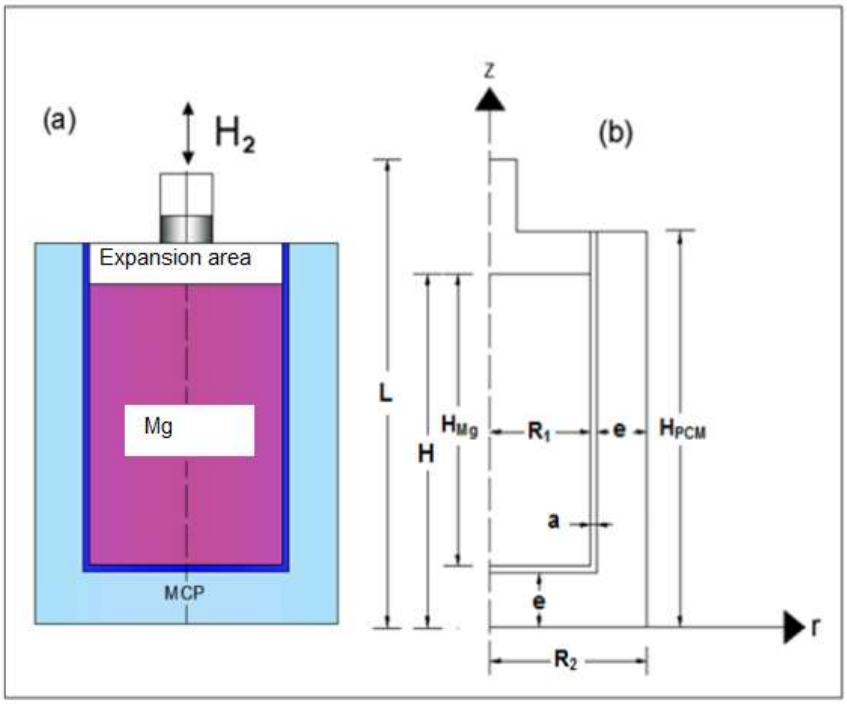


**Figure .1. Configuration of the reactor in 2D (a), Axisymmetric section of the reactor (b).**

## 3. Numerical calculation method

The numerical resolution method was performed using Fluent® 6.3 software, which uses the finite volume method. This method is based on solving the equations of conservation as an equation of energy in a discretized Eulerian space. In an element of volume (EV), the temporal variation of the temperature is calculated as sum of flows through an elementary volume. The flow is divided into two terms, one conductor and another as a source term. The quantities are stored at mesh center. The values are calculated at the faces by interpolation. The method used in the calculations is an implicit scheme**.**

## 4. Initial and boundary conditions

### 4.1 Initial conditions

Initially, the temperatures: of magnesium, gas and the PCM domain ($Mg_{69}Zn_{28}Al03$) are assumed to be uniform across the reactor:

$$T_{magnésium} = T_{H2} = T_{MCP} = T_{solidus} = 607\,k$$

- The hydrogen pressure applied is 8 bars.
- The initial pressure in the hydride bed is 0.2 bars.

### 4.2 Boundaries conditions

On the limit where r = 0

The symmetry of revolution makes it possible to write:

$$\frac{\partial T}{\partial r}(0\,,\,z\,,\,t) = 0$$

On the limit where r = $R_1$

$$\lambda_{eff}\frac{\partial T}{\partial r}(R_1\,,\,z\,,\,t) = \lambda_{acier}\frac{\partial T}{\partial r}(R_1\,,\,z,\,t)$$

On the limit where r = $R_2$

$$\frac{\partial T}{\partial r}(R_2\,,\,z\,,\,t) = 0$$

On the limit where r = $R_1$ + a

$$\lambda_{acier}\frac{\partial T}{\partial r}((R_1+a)\,,\,z\,,\,t) = \lambda_{MCP}\frac{\partial T}{\partial r}((R_1+a)\,,\,z\,,\,t)$$

On the limit where z = 0

$$\frac{\partial T}{\partial z}(r\,,\,0\,,\,t) = 0$$

On the limit where z = e

$$\lambda_{MCP}\frac{\partial T}{\partial z}(r\,,\,e\,,\,t) = \lambda_{acier}\frac{\partial T}{\partial z}(r\,,\,e\,,\,t)$$

On the limit where z = e

$$\lambda_{eff}\frac{\partial T}{\partial z}(r\,,\,(e+a)\,,\,t) = \lambda_{acier}\frac{\partial T}{\partial z}(r\,,\,(e+a)\,,\,t)$$

On the limit where z = $H_{PCM}$

$$\frac{\partial T}{\partial z}(r\,,\,H_{PCM}\,,\,t)=0$$

On the limit where z = L

$$\frac{\partial T}{\partial z}(r\,,\,L\,,\,t)=0$$

## 5. Numerical Method and Validation

In order to verify the results obtained by our code, we studied in a first step the problem of hydrogen storage in a hydride reactor of magnesium.

The numerical model developed was validated with the experimental results of Albin Chair et al. [11] under the same conditions. Figure 2 shows that the digital model can predict experimental results quite satisfactorily.

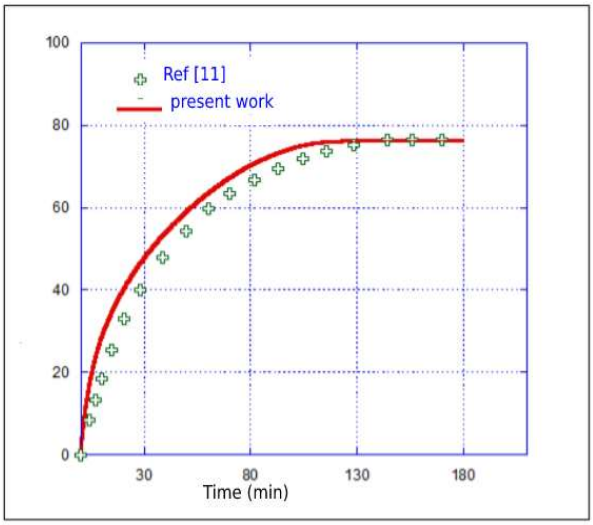


**Figure 2. Model validation**

## 6.Results and Discussion

### 6.1 Study of the feasibility of thermal coupling

The objective of this study is to store all of the heat released during the absorption of hydrogen in a phase change material "$Mg_{69}Zn_{28}Al_3$". A first loading was carried out by applying a pressure of 0.8 MPa. The settings geometric patterns of the reactor are grouped together in Table 1.

**Table 1: geometric patterns of the reactor**

| Parameter | Value |
|---|---|
| $H_{Mg}$ | 4 cm |
| $H_{PCM}$ | 5.45 cm |
| $R_1$ | 1.5 cm |
| $R_2$ | 2.35 cm |
| e | 0.75 cm |
| a | 0.1 cm |
| $L$ | 6.45 cm |
| Magnesium Mass $m_{Mg}$ | 12.65 g |
| $\frac{V_{PCM}}{V_{Mg}}$ | 1.85 |

In the following table 2 we present the different Parameters used for the Fluent simulation

**Table 2: different Parameters used for the Fluent simulation**

| Parameter | Value |
|---|---|
| $Cp_{PCM}$ | 1100 J $Kg^{-1}K^{-1}$ |
| $Cp_{MgH2}$ | 1945 J $Kg^{-1}K^{-1}$ |
| $E_a$ | 130000 J $mol^{-1}H_2$ |
| $K_0$ | $10^9 s^{-1}$ |
| $K_{01}$ | $10^{10} s^{-1}$ |
| $K_{02}$ | 4.3 $10^9 s^{-1}$ |
| $M_{H2}$ | 0.002 Kg $mol^{-1}$ |
| $T_{Soildus}$ | 607 K |
| $T_{liquidus}$ | 610 K |
| $\rho_{PCM}$ | 2900 Kg $m^{-3}$ |
| $\rho_{MgH2}$ | 1945 Kg $m^{-3}$ |
| $\lambda_{PCM}$ | 100 W $m^{-1}K^{-1}$ |
| $\lambda_{MgH2}$ | 0.48 W $m^{-1}K^{-1}$ |
| ε | 0.77 |
| $\omega_t$ | 5.8 $\omega t$ % |
| $\Delta H_{MgH2}$ | -75000 J $mol^{-1}$ |
| $\Delta S_{MgH2}$ | 135.6 J $K^{-1}mol^{-1}H_2$ |
| $\Delta H_{PCM}$ | 142 J / g |

## 6.2 Change in heat flux density

The process of hydrogen absorption is limited by the capacity of the domain hydride to remove the heat of reaction. Figure 3 shows the temporal evolution the density of heat flux transferred through the intermediate wall of the reactor. At onset, the heat flow density increases with increasing temperature in the hydride bed. This amount of heat is dissipated first in the form of sensible heat in magnesium hydride, then as the latent heat of fusion of PCM. At as time goes by, the heat evacuated by the hydriding reaction decreases until it is canceled out.

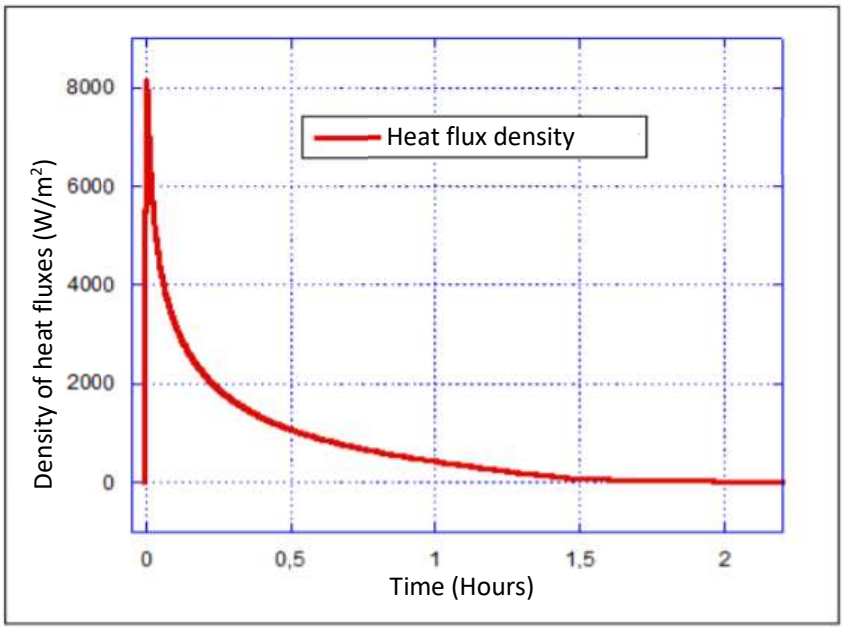


**Figure .3 Temporal evolution of the density of heat fluxes transferred through the intermediate wall**

## 6.3 Variation of hydriding rate and melting titer

Figure 4 shows the temporal evolution of the hydriding rate of magnesium and the fusion title of PCM. At the start of absorption, the hydriding curve of magnesium exhibits a high rate of diffusion of hydrogen atoms in the solid matrix of magnesium, which gives a heat dissipation to the area of the Phase Change Material. The PCM fusion phenomenon begins and the title melting triggers in the vicinity of the hydriding rate of magnesium. Then, from 1800 seconds, the hydride formation kinetics show a slow change in speed reaction, which slows down the fusion reaction of the PCM. Finally, when we approach

saturation, the speed decreases rapidly until it is canceled and the whole heat evacuated by the hydrogen absorption reaction is stored as latent heat by the Phase Change Material.

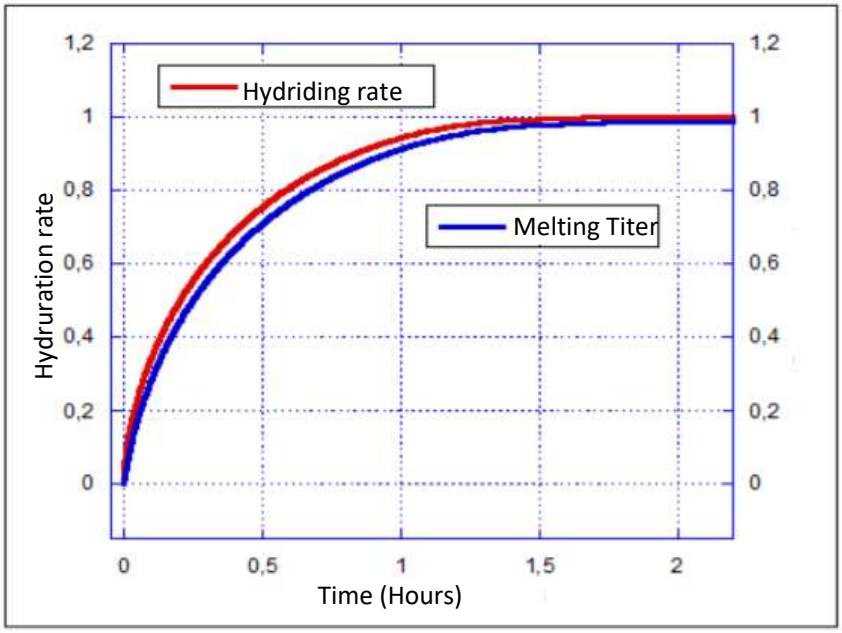


**Figure .4 Temporal evolution of the hydriding rate of magnesium and of the PCM melting**

The superposition of the melting titer and hydriding rate curves indicates that the sizing of one domain in relation to the other has been correctly carried out.

## 6.4 Effect of thermal conductivity of PCM

The thermal conductivity of phase change material is a parameter important for optimizing the thermal coupling between the hydride bed and the PCM.

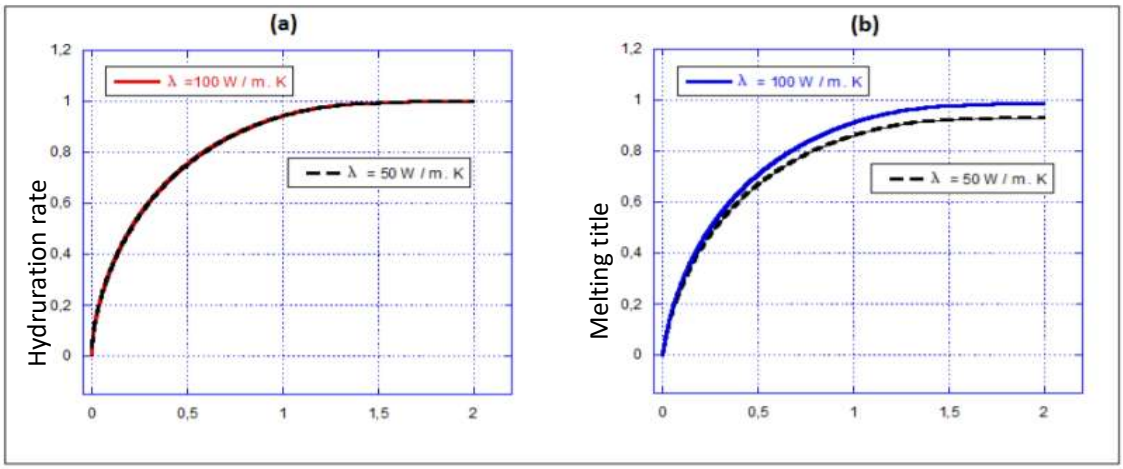


**Figure .5 Influence of thermal conductivity of PCM on thermal coupling**

Figure 5 (a) shows that the reaction kinetics do not depend on the conductivity PCM thermal. However, according to the curves of figure 5 (b), the decrease thermal conductivity increases the time required to melt the Material at Phase change. In conclusion, the thermal conductivity of phase change material influences on the time of fusion and is not on the time of hydriding of magnesium.

## 6.5 PCM volume effect

In order to study the effect of volume of the phase change material on the thermal coupling in the reactor. Two configurations, containing the same mass of magnesium (12.65 g) and different PCM volume were tested:

**Configuration 1**: The volume of the PCM domain is in default to store the whole heat of reaction.

**Configuration 2**: The volume of the PCM domain is in excess to absorb the totality thermal heat.

Figure 6 shows the evolution over time of the hydriding rate and the titer of merge for both configurations. From figure (6 (a)), the amount of heat to storing is then too large. Thus, from 1328 seconds, the PCM is totally melted while only 65% of the material is hydrated. It is then the sensitive energy of the PCM which allows the heat of reaction to be stored. The temperature difference between the hydride magnesium and PCM gradually decreases, (Figures 6 (a)), which slows the absorption reaction. At the end of the reaction, the system being adiabatic, the reaction is totally blocked (80% of the magnesium is hydrated) and the temperature of the whole magnesium hydride + PCM reaches the equilibrium temperature.

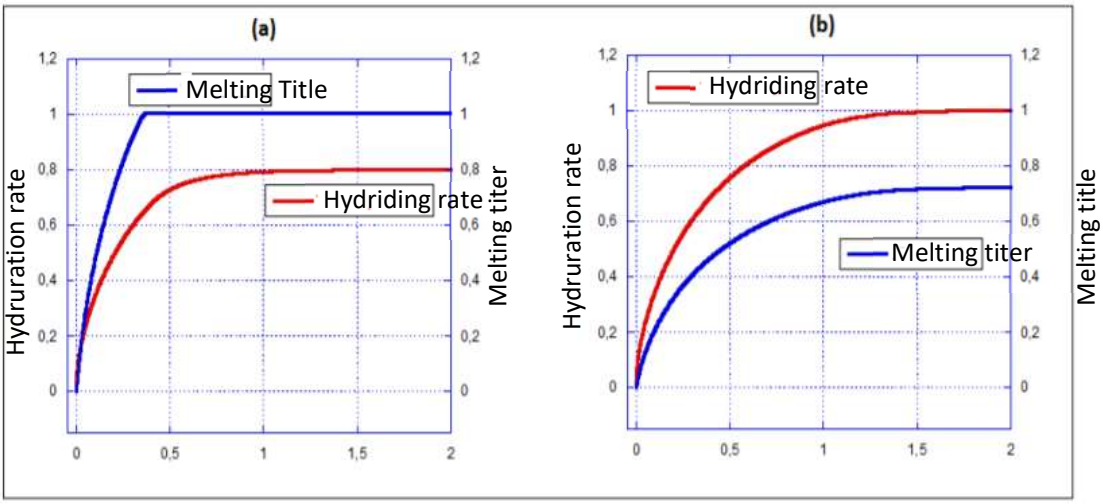


**Figure .6 Temporal evolution of hydriding rate and PCM melting titer: (a) configuration 1 and (b) configuration 2**

The second configuration was simulated under the same conditions as the first. According to figure (6 (b)), the magnesium domain is completely hydrated because the all of the heat released is stored by the melting of the PCM. The temperature difference between the hydride bed and the PCM is important during absorption, which explains why the all of the magnesium is hydrated (Fig. 7 (b) and Fig. 8 (b)).

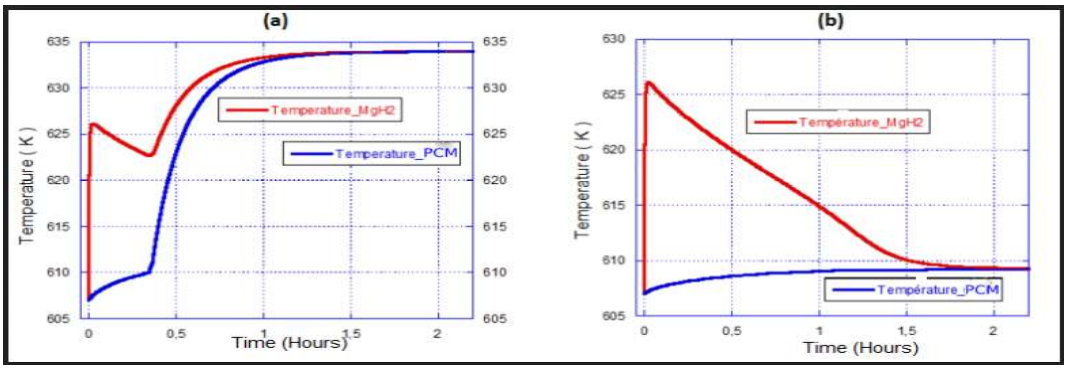


**Figure .7 Temporal evolution of the temperatures of different points of the domain of magnesium hydride: (a) configuration 1 and (b) configuration 2**

Numerically recording of temperatures at different points in the PCM domain, (Fig 8), shows that the temperature is uniform at all times in the material at phase change for both configurations.

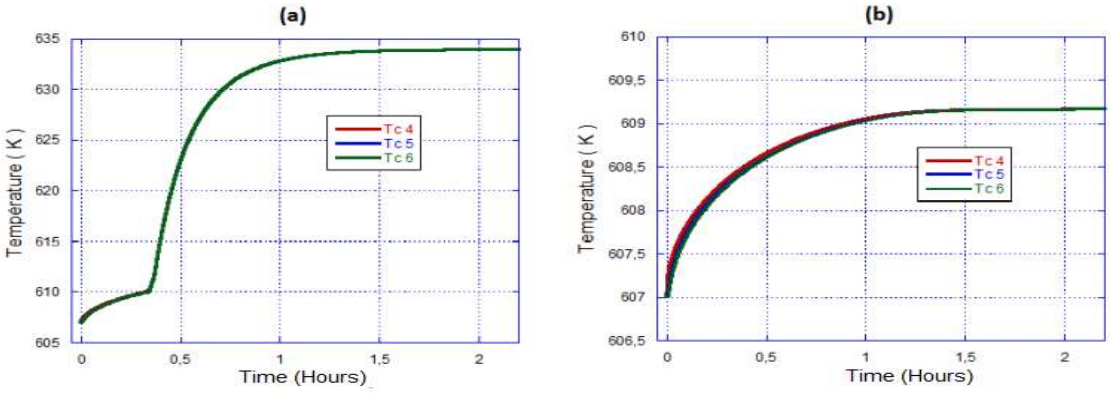


**Figure .8 Temporal evolution of the temperatures of different points of the domain** PCM**: (a) configuration 1 and (b) configuration 2**

According to figure (8 (a)), from 1278 seconds, the PCM is totally melted. The temperature of the domain increases over time to the equilibrium temperature of

magnesium hydride. The molten material behaves like a storage medium heat sensitive heat absorption of hydrogen.

## 7. Conclusion

In this manuscript, we have numerically simulated the thermal coupling between a magnesium hydride and a phase change material. A mathematical model unsteady two-dimensional is developed. A Fluent® calculation code has been developed, validated and applied to simulate the dynamic behavior of a hydride reservoir of magnesium with recovery of the heat of absorption by a Change Material of Phase (PCM).

In conclusion**:**

- The thermal conductivity of phase change material (PCM )influences on the time of fusion and is not on the time of hydriding of magnesium.
- The thermal conductivity of phase change material (PCM) is a parameter important for optimizing the thermal coupling between the hydride bed and the PCM.
- The speed decreases rapidly until it is canceled and the whole heat evacuated by the hydrogen absorption reaction is stored as latent heat by the phase change material (PCM).

We have shown that:

- The thermal conductivity of a phase change material (PCM) influences the melting and is not on the hydrogen absorption time.
- A good choice of the geometric parameters of the (PCM) domain, such as the volume, is necessary.

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