

# Heat management on rectangular metal hydride tanks for green building applications

Gkanas, E., Statheros, T. & Khzouz, M.

Author post-print (accepted) deposited by Coventry University's Repository

## Original citation & hyperlink:

Gkanas, E, Statheros, T & Khzouz, M 2018, 'Heat management on rectangular metal hydride tanks for green building applications' *International Journal of Hydrogen Energy*, vol (In-Press), pp. (In-Press).

<https://dx.doi.org/10.1016/j.ijhydene.2018.06.030>

DOI 10.1016/j.ijhydene.2018.06.030

ISSN 0360-3199

Publisher: Elsevier

**NOTICE: this is the author's version of a work that was accepted for publication in *International Journal of Hydrogen Energy*. Changes resulting from the publishing process, such as peer review, editing, corrections, structural formatting, and other quality control mechanisms may not be reflected in this document. Changes may have been made to this work since it was submitted for publication. A definitive version was subsequently published in *International Journal of Hydrogen Energy*, Vol. (In-Press), pp. (In-Press), 2018. DOI: 10.1016/j.ijhydene.2018.06.030**

© 2017, Elsevier. Licensed under the Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International

<http://creativecommons.org/licenses/by-nc-nd/4.0/>

Copyright © and Moral Rights are retained by the author(s) and/ or other copyright owners. A copy can be downloaded for personal non-commercial research or study, without prior permission or charge. This item cannot be reproduced or quoted extensively from without first obtaining permission in writing from the copyright holder(s). The content must not be changed in any way or sold commercially in any format or medium without the formal permission of the copyright holders.

This document is the author's post-print version, incorporating any revisions agreed during the peer-review process. Some differences between the published version and this version may remain and you are advised to consult the published version if you wish to cite from it.

# Heat Management on Rectangular Metal Hydride Tanks for Green Building Applications

Evangelos I. Gkanas\*, Thomas Statheros and Martin Khzouz

*Hydrogen for Mobility Lab, Institute for Future Transport and Cities, Coventry University, Coventry University, Priory Street, Coventry, CV1 5FB, United Kingdom*

\*Email: [ac1029@coventry.ac.uk](mailto:ac1029@coventry.ac.uk)

## Abstract

A numerical study fully validated with solid experimental results is presented and analysed, regarding the hydrogenation process of rectangular metal hydride tanks for green building applications. Based on a previous study conducted by the authors, where the effective heat management of rectangular tanks by using plain embedded cooling tubes was analysed, in the current work the importance of using extended surfaces to enhance the thermal properties and the hydrogenation kinetics is analysed. The studied extended surfaces (fins) were of rectangular shape; and several combinations regarding the number of fins and the fin thickness were examined and analysed. The values for fin thickness were 2-3-5 and 8mm and the number of fins studied were 10-14-18 and 20. To evaluate the effect of the heat management process, a modified version of a variable named as Non-Dimensional Conductance (NDC) is introduced and studied. A novel AB<sub>2</sub>-Laves phase intermetallic was considered as the metal hydride for the study. The results of the hydrogenation behaviour for the introduced parameters (fin number and thickness) showed that the rectangular tank equipped with the cooling tubes in combination with 14 fins of 5mm fin thickness has the capability of storing hydrogen over 90% of its theoretical capacity in less than 30min.

*Keywords: Hydrogen storage; Heat management; Extended surfaces; Heat and Mass transfer; Green Buildings*

## 1. Introduction

The environmental negative impact of buildings is majorly connected to energy consumption and gas emissions [1, 2]; thus, the necessity for promoting novel approaches for mitigation of CO<sub>2</sub> is of major importance [3]. The energy consumption in buildings at both USA and EU has exceeded the energy consumption of the industrial and transportation sectors [4]. The usage of hydrogen technologies might be a powerful

technique to enhance the sustainability in the building sector and to promote the green technology [5]. Hydrogen technologies can be used for grid stabilization; as secondary reserves for grid frequency and voltage regulation [6]. One of the major drawbacks that prevent the full implementation of hydrogen technologies in the market is the effective storage of hydrogen [7]. The solid-state storage of atomic hydrogen in metallic materials with the formation of metal hydrides is an effective way to store hydrogen, as it is a safe and reliable technique during the operation at moderate temperature and pressure ranges [8-11]. Some of the parameters governing the thermodynamic performance of metal hydrides are the (specific) enthalpy of formation (during the hydrogenation process) or the deformation (during the dehydrogenation process)  $\Delta H$  [kJ/kmol], the specific heat capacity of the hydride  $C_p$  [kJ/kmol/K], the thermal conductivity  $\lambda$  [W/mK], hysteresis and slope [12]. There are also several other parameters that affect the hydrogenation/dehydrogenation process related to the design of metal hydride beds such as the porosity of the metal hydride, the packing density, the supply pressure and the heat management techniques [13]. The storage of atomic hydrogen in the metal lattice is an exothermic process, where enormous quantities of heat are produced, forcing the reaction kinetics to slow down [14]. The produced amount of heat has to be removed to maintain the kinetics of the reaction; thus, the effective heat management of the metal hydride tanks is of major importance [15]. There are mainly two heat management techniques that have been applied to enhance the heat transfer to/from the metal hydride tank; internal heat management and external heat transfer [16-18]. The major focus to improve the heat transfer in a metal hydride bed should be the reduction of the metal hydride thickness [19, 20], the increase of the thermal conductivity [21, 22] and the introduction of a large temperature difference [23, 24]. On a recent study [25], the authors investigated the usage of embedded plain tubes on rectangular metal hydride beds and used a parameter named as Non-Dimensional Conductance (NDC) to evaluate the effectiveness of the heat management in three different materials convenient for hydrogen storage and the optimum conditions were identified.

In the current study, the optimum conditions from [25] are considered and the introduction of extended surfaces for effective heat management is discussed and analysed; the optimum metal hydride thickness was 10.39 mm and the optimum heat transfer coefficient was 2000 [W/m<sup>2</sup>K]. A three-dimensional, fully validated with experimental results numerical model describing the solid-state hydrogen storage is

introduced and applied on a commercial software (COMSOL Multiphysics 5.3). The metal hydride beds used in the current work are of rectangular shape and an effective heat management analysis is presented in terms of the number of fins and fin thickness. Also, a novel AB<sub>2</sub>-Laves phase intermetallic (Ti-Zr based) is used for the simulation. To evaluate the effect of the heat management process, a modified variable named as Non-Dimensional Conductance (NDC) is analysed and studied.

## **2. Methodology**

In the current study the heat, mass and momentum conservation equations were solved simultaneously using a commercial Multiphysics package (COMSOL Multiphysics 5.3). The proposed numerical model was validated with solid experimental data extracted from a lab-scale Sievert's type apparatus for both the hydrogen storage capacity and the temperature distribution. The expansion of the packed beds during the hydrogenation can introduce additional stress to the vessel walls; therefore, the hydride beds are assumed 50% full at the beginning of the hydrogenation process. The optimum values for the metal hydride thickness (10.39 mm) and the heat transfer coefficient (2000 W/m<sup>2</sup>/K) were adopted from a previous study [25] and the simulations were conducted for several fin geometries regarding the number of fins and the fin thickness; the optimised heat management scenario was identified. In the current work, four different values of fin thickness (2-3-5-8 mm) and four different number of fins (10-14-18-20) were introduced and studied.

### **2.1 Tank and Fin Designs**

The metal hydride tanks were selected to have rectangular shape [25]. The properties of the metal hydride beds were selected to be similar with the properties of stainless steel (316 SS) with wall thickness of 3mm. The dimensions of the bed were 30cm (Length)×15cm (Width)×12.63cm (Height) resulting on a net volume of 5683.5 cm<sup>3</sup>. The cooling tubes were placed along the 15-cm side of the bed and covered the total length of the tank (30 cm). The optimum metal hydride thickness was selected (10.39 mm) from [25] and thus 17 cooling tubes were considered. The cooling tubes were selected to have the dimensions of commercially available 316 SS, ¼ inch (external diameter) tubes. The extended surfaces were selected to be of rectangular shape. Fig. 1 presents the arrangement of the cooling tubes and the extended surfaces in the metal hydride bed. At the upper left corner, the geometry of the fins is explained. The fins are

perforated to fit with the cooling tubes and, in order to avoid the expansion impact and to ensure homogeneous distribution of the metal hydride powder during the packing, several open spaces have been considered on the fins (three under the cooling tubes and three over the cooling tubes).

*Fig. 1. Studied geometry and the arrangement of the cooling tubes and the extended surfaces in the metal hydride beds.*

## 2.2 Assumptions of the numerical model

Several assumptions were made to simplify the numerical description of the solid-state hydrogen storage and listed as follows:

- a) The medium is in local thermal equilibrium which implies that there is no heat transfer between solid and gas phases.
- b) Initially uniform temperature and pressure profiles.
- c) Hydrogen is treated as an ideal gas from a thermodynamic point of view.
- d) Thermal conductivity and specific heat capacity are assumed constant.
- e) The porosity remains constant and uniform during the hydrogenation.
- f) The characteristics (the kinetics and thermal properties) of the bed are unaffected by the number of loading and unloading cycles. Thus, the bed aging is neglected.
- g) The metal hydride bed fills the entire space between the cooling tubes and the fins (perfect packing condition).

## 2.3 Heat Equation

Assuming thermal equilibrium between the hydride powder and hydrogen gas, a single heat equation can be solved instead of separate equations for solid and gas phases:

$$(\rho \cdot Cp)_{eff} \cdot \frac{\partial T}{\partial t} + (\rho_g \cdot C_{p_g} \cdot \bar{v}_g) \cdot \nabla T + \nabla \cdot (k_{eff} \cdot \nabla T) = Q_H \quad (1)$$

The term  $Q_H$  ( $W/m^3$ ) in Eq. 1 represents the heat that has been generated during the hydrogenation process or the amount of heat that is necessary for the dehydrogenation process. The amount of heat that is been produced during the hydrogenation process depends on several thermophysical properties of the materials such as the enthalpy of formation  $\Delta H$  ( $J/mol$ ), the porosity of the material  $\varepsilon$ , the density changes during the reaction ( $kg/m^3$ ), the reaction rate ( $1/s$ ) and the molecular mass of the stored gas

(kg/mol) [26]. The enthalpy of the hydride formation was measured experimentally from the isotherm curves during the hydrogenation of the AB<sub>2</sub>-Laves phase intermetallic, while the density change was calculated and updated with time from the concentration of the species using the Transport of Diluted Species Module in COMSOL Multiphysics.

The effective heat capacity is given by;

$$(\rho \cdot Cp)_e = \varepsilon \cdot \rho_g \cdot C_{pg} + (1 - \varepsilon) \cdot \rho_s \cdot C_{ps} \quad (2)$$

and the effective thermal conductivity is updated by;

$$k_e = \varepsilon \cdot k_g + (1 - \varepsilon) \cdot k_s \quad (3)$$

The terms  $\rho_g$ ,  $C_{pg}$ ,  $C_{ps}$  and  $m$  refer to the density of the gas phase (kg/m<sup>3</sup>), the specific heat capacity of the gas phase (J/kg/K), the heat capacity of the solid phase and the kinetic term for the reaction respectively. The parameter that represents the void fraction is symbolized with  $\varepsilon$ . The values for  $k_g$  (W/m/K) and  $k_s$  (W/m/K) represent the thermal conductivity for the gas and the solid state respectively.  $M_{H2}$  represents the molecular mass of hydrogen (kg/mol) and  $T$  represents the temperature (K).

#### 2.4 Hydrogen Mass Balance

The diffusion of hydrogen gas within the metallic matrix is described by;

$$\varepsilon \cdot \frac{\partial(\rho_g)}{\partial t} + \text{div}(\rho_g \cdot \vec{v}_g) = \pm Q \quad (4)$$

Where  $v_g$  is the velocity of gas during diffusion within the metal lattice (described in section 2.5) and  $Q$  (kg/m<sup>3</sup>s) is the mass source term describing the amount of hydrogen mass diffused per unit time and unit volume in the metal lattice.

#### 2.5 Momentum Equation

By neglecting the gravitational effect, the equation which describes the velocity of gas inside the metal matrix is;

$$\vec{v}_g = -\frac{K}{\mu_g} \cdot \text{grad}(\vec{P}_g) \quad (5)$$

Where  $K$  (m<sup>2</sup>) is the permeability of the solid and  $\mu_g$  (Pa s) is the dynamic viscosity of gas and  $P_g$  (kPa) is the pressure of gas within the metal matrix.

#### 2.6 Hydrogenation Kinetic Expression

The kinetic description for the hydrogenation process per unit time and volume is updated by:

$$m_a = C_a \cdot \exp\left[-\frac{E_a}{R_g \cdot T}\right] \cdot \ln\left[\frac{P_g}{P_{eq}}\right] \quad (6)$$

Where  $E_a$  (J/mol) is the activation energy for the hydrogenation process and  $C_a$  (l/s) is the pre-exponential constant. Finally,  $P_g$  (Pa) is the pressure of hydrogen during the hydrogenation and  $P_{eq}$  (Pa) is the equilibrium pressure (presented on section 2.7).

## 2.7 Equilibrium Pressure

To incorporate and consider the effect of hysteresis and the plateau slope for the calculation of the plateau pressure  $P_{eq}$ , the following equation was used [27, 28]:

$$\ln \frac{P_{eq}}{10^5} = \left\{ \left[ \frac{\Delta H}{RT} - \frac{\Delta S}{R} \right] + (\varphi_s \pm \varphi_0) \cdot \tan \left[ \pi \cdot \left( \frac{x}{x_{sat}} - \frac{1}{2} \right) \right] \pm \frac{S}{2} \right\} \quad (7)$$

The plateau slope is given by the flatness factors  $\varphi_s$  and  $\varphi_0$  and  $S$  represents the hysteresis effect which is given by  $(\ln P_{abs}/P_{des})$  designated ‘+’ for the hydrogenation and ‘-’ for the dehydrogenation, while  $x$  and  $x_{sat}$  are the local hydride concentration at any given time and at saturation respectively. For all the studied materials, the flatness factors and the hysteresis effects were measured experimentally by using the data collected from the hydrogenation kinetics and isotherms.

## 3. Validation of the numerical model

The validation of the numerical model has been done by extracting the experimental data from a 0.65 g sample of the AB<sub>2</sub>-Laves phase intermetallic. The pressure-composition-isotherm (PCI) hydrogenation measurements were performed on a commercial Sievert type apparatus provided by HIDEN Isochema (IMI Instruments). Both the hydrogenation and temperature behaviour of the material were extracted during the charging process at an initial hydrogen supply pressure of 15 bar and at temperature 20°C. Fig. 2a shows the geometry of the bed used for the validation of the numerical model and the position of the thermocouple. Fig. 2b shows the comparison of the temperature profile during the hydrogenation process and Fig. 2c shows the hydrogenation profile for the material. The results of the numerical work compared to

the experimental data present good agreement with a maximum deviation of no more than 5%.

*Fig. 2. Geometry used for the validation (2a). Validation of the predicted temperature distribution within the metal hydride with the temperature recorder from the thermocouple (2b) and validation of the predicted hydrogenation fraction with the actual fraction recorded experimentally (2c).*

#### 4. Non-Dimensional Conductance (NDC)

When using heat exchangers, there are several parameters that influence the rate of heat transfer such as the coolant temperature, coolant flow rate, contact resistance, metal hydride thickness and the thermal conductivity of the metal hydride bed. To monitor the influences of the above parameters on the heat transfer performance a Non-Dimensional Conductance (NDC) parameter has been used [20, 25]. The NDC was defined as the ratio of the maximum heating rate that can be removed from the metal hydride to the heat rate that would be generated for a specified thickness of the hydride to store hydrogen up to 90% of its maximum theoretical performance during a desirable time and its given by the following expression. In the current study, besides the effect of the cooling tubes on the heat management of the total metal hydride tank, the effect of the extended surfaces will be taken into account. If the NDC will be utilised to monitor and evaluate the total heat management of the tank, the fin volume, the material of the fin and the number of fins must be taken into account as the major factors that will affect the hydrogenation reaction. Thus, in the current work, a modified expression of the NDC will be used that takes into account the contribution of the fins and the cooling tubes and is presented in Eq. 8.

$$NDC = \frac{\left( \frac{T_{MH,max} - T_{cool}}{\left( K \cdot \left\{ \frac{1}{h_t} + R_{tc} + \frac{L}{\lambda_{MH}} \right\} + N \cdot \left\{ R_{Fin} + \frac{L}{\lambda_{Fin}} \right\} \right)} \right)}{\left( \frac{\Delta H \cdot (\text{wt } \% ) \cdot \rho \cdot L}{MW_{H_2} \cdot t_{des}} \right)} \quad (8)$$

In the above expression, the term  $T_{MH,max}(K)$  is the temperature of the metal hydride at the end of the pressure increase process and it's an indirect measurement of the pressure.  $T_{cool}(K)$  is the temperature of the coolant that flows within the cooling tubes and a higher NDC number can be achieved by reducing the coolant temperature. The term  $K(1/h_t + R_{tc} + L/\lambda_{MH})$  represents the contribution of the cooling tubes on the heat

management of the reaction tank. To describe the total effect of the cooling tubes, the term  $K$  represent the number of cooling tubes. The heat transfer coefficient is represented by  $h_t$  ( $W/m^2K$ ) and is directly related to the effect of the coolant flow rate. The thermal contact resistant is  $R_{tc}$  ( $mm^2K/W$ ) and appears when different metallic materials are in contact; only a small fraction of the surface are in actual contact, thus; forming the thermal resistant and it depends on the hydride powder properties (grain size and packing density).  $L$  ( $mm$ ) is the hydride layer thickness, which in the current work is defined as the distance between the centers of two adjacent coolant tubes and consists of the metal hydride, the contact resistance and the wall of the coolant tube. The term  $N(T/\lambda_{fin}+R_{fin})$  corresponds to the contribution of the extended surfaces on the heat management of the tank. The number of fins is represented by  $N$ , where  $T$  is the fin thickness ( $mm$ ) and it is an indirect relation to the fin volume. The thermal conductivity of the fins is given by  $\lambda_{Fin}$  ( $W/mK$ ) and the thermal resistance between the fins and the metal hydride is given by  $R_{Fin}$  ( $mm^2K/W$ ). The denominator in Eq. 8 is the average heat generation rate if the metal hydride of thickness  $L$  is hydrided within a desired filling time  $t_{des}$ . In the current analysis, the desired time  $t_{des}$  is selected 2000s.

## 5. Results and Discussion

### 5.1 Hydrogenation Characteristics of the AB<sub>2</sub>-Laves Phase Intermetallic

For the purposes of the current study, the initial temperature of the powder at the beginning of the hydrogenation process was selected 20 °C; same as the temperature of the coolant. The initial pressure of hydrogen was selected 15 bar; similar to the pressure that a commercial electrolyser can supply. The properties of an AB<sub>2</sub>-Laves phase intermetallic were introduced to the model. The extended surfaces were of rectangular shape and several number of fins were selected (10-14-18 and 20). Furthermore, several values for fin thickness were considered and studied (2-3-5 and 8 mm). Fig. 3 presents the hydrogenation behaviour of the selected material in terms of the necessary time that the material needs to reach the hydrogenation fraction of 90% ( $X=0.9$ ) with the modified NDC for all the number of fins considered. Furthermore, the effect of the different fin thickness is presented.

*Fig. 3. Hydrogenation response of the AB<sub>2</sub>-Laves phase intermetallic. The time that the material needs to be hydrogenated up to 90% ( $X=0.9$ ) is plotted with the NDC for all the values of fin thickness and fin number*

For all the cases considered, the evolution of the hydrogenation time presents an almost parabolic dependency with the NDC. Initially, when the number of fins increases from 10 to 14, the difference in the time to reach  $X=0.9$  drops intensively for all the cases of fin thickness. While the number of fins increases even more (18), the decrease on the hydrogenation time continues but the drop is not as massive as on the previous case. Finally, by increasing even more the fin number (20), it will result to another small drop on the hydrogenation time. This behaviour indicates a limitation mechanism on the hydrogenation time (and thus to the effectiveness of the heat management). After a certain number of fins (14) the further increase on the fin number will not result on a significant drop of the charging time. This phenomenon might be related to the total amount of material between two adjacent fins and the amount of heat that is able to be removed during the exothermic process. The modified NDC, as described on Eq. 8, incorporates both the contribution of the fins and the cooling tubes on the heat management of the metal hydride tank. The number of the cooling tubes in the current study has been kept constant (17) as extracted from [25]. Thus, the contribution of the cooling tubes does not change and it has a certain value on the numerator of Eq. 8, while the contribution of the fins on the denominator is in terms of fin number and thickness. From Fig. 3, it seems that an almost parabolic behaviour between the time to  $X=0.9$  and the NDC appears, where, as the fin number increases ( $N$ ) the NDC also increases; the decrease of hydrogenation time is not sufficient after a certain value of fin number, indicating that after that point the fin thickness dominates.

## **5.2 Effect of the Fin Thickness and Number of Fins on the Hydrogenation Performance**

As extracted from Fig. 3, the usage of 14 fins seems to provide an effective heat management during the hydrogenation process. As also explained, from the modified NDC, the fin thickness appears to dominate on the heat management after a certain number of fins. The next step will be the study of the effect of the fin thickness on the hydrogenation time. Fig. 4a presents the relation between the hydrogenation performance of the selected material with the fin thickness. For the case of using 10 fins, the increase on the fin thickness does not significantly enhance the hydrogenation process. The increase of the fin thickness from 2 to 8 mm can reduce the time for  $X=0.9$

only by 3 min (175 s) indicating that for a fin number lower than 14, the fin thickness is not the dominant factor for the heat management. On the contrary, when the fin number increases, the dependency of the hydrogenation time on the fin thickness becomes more significant and dominant. For the case of using 14 fins, the increase of the fin thickness even by 1mm (from 2 to 3 mm) can reduce the hydrogenation time by more than 8 min (531 s). A further increase to 5 mm can cause a drop of another 4.5 min and finally, when the thickness is 8 mm, can cause a reduction of 5.5 min, causing a total decrease by 19 min when the fin thickness increases from 2 to 8 mm. For the case of 18 fins, the increase of the fin thickness can also significantly reduce the charging time by a total of more than 14 min (from 2mm to 8mm). The same behaviour was observed for the case of 20 fins with a total decrease on the hydrogenation time of more than 13min (from 2mm to 8mm). For almost all the cases, the maximum reduction on the hydrogenation time was observed during the transition of the thickness from 3mm to 5mm. Furthermore, according to Fig. 4b, for the thickness of 2mm, an increase on the fin number can influence on a positive way the hydrogenation time by almost 19min when the fin number increases from 10 to 14, by more than 12min for an increase from 14 to 18 and only 4min for a further increase to 20 fins. The same behaviour was observed for the rest cases of fin thickness (3, 5 and 8mm). These results indicate that there is a limitation on the reduction of hydrogenation time when the fin number increases more than 14 that is might related to the minimum amount of the hydride between two adjacent fins. From the above analysis, the optimum number of fins for the current material was 14.

*Fig.4. Effect of the fin thickness on the hydrogenation behaviour of the AB<sub>2</sub>-Laves phase intermetallic (4a) and the effect of the fin number on the hydrogenation behaviour of the AB<sub>2</sub>-Laves phase intermetallic (4b)*

For the case of utilising 14 fins in the hydride tank, as the thickness increases from 2 to 3mm a significant reduction on the charging time is observed, by almost 11min. A further increase on the fin thickness to 5mm leads to the reduction of the hydrogenation time by 3min and finally, for a thickness of 8mm, the hydrogenation time drops by 1.5min. Furthermore, it is observed that the hydrogenation time follows an almost parabolical trend, by reaching a plateau for thicknesses over 5mm; the hydrogenation time for further thickness increase remains almost the same. The reason for this

phenomenon can be explained from the fact that the term  $T_{MH,max}-T_{cool}$  on the NDC reaches an almost constant value; as a result of the small pressure ramp that is achieved during the hydrogenation for thickness over 5mm.

A further investigation on the effect of the fin thickness on the effective heat management of the hydride tank is presented in Fig. 5, where the reaction progress at the end of the desired time ( $t_d=2000s$ ) with the modified NDC is considered for all the fin thicknesses and fin numbers. It can be observed that the hydrogenation fraction of  $X=0.9$  at 2000s is not achieved for all the studied cases; especially for the case of 2 mm thickness, the target can be achieved only when 20 fins are utilised. For the fin thickness of 3mm, the hydride can store more than  $X=0.9$  in the desired time when using 18 and 20 fins, but for the case of 10 and 14 fins this target can't be achieved. On the contrary, for the fin thickness of 5mm, except the case of using 10 fins, all the rest cases can achieve a charging more than  $X=0.9$  within the desired time and finally, the same behaviour is extracted for the case of fin thickness 8mm.

*Fig.5. The reaction progress at the end of the desired time (2000s) for all the studied fin thicknesses and fin numbers*

### **5.3 Hydrogenation Kinetics and Temperature Profile**

Fig. 6a presents the bed average temperature evolution of the hydride during the hydrogenation process for the case of using 14 fins and considering all the fin thicknesses (2, 3, 5 and 8mm). The temperature at the beginning of the hydrogenation increases due to the highly exothermic process and reaches a maximum point. After that, due to the heat management process the temperature drops and tends to reach the temperature of the coolant. The maximum temperature achieved during the hydrogenation process was 64.65°C for 2mm thickness, 63.72°C for 3mm thickness, 61.78°C for 5mm thickness and 59.1°C for 8mm thickness. The temperature behaviour of the hydride affects the hydrogenation kinetics as presented in Fig. 6b. The hydrogenation process can be divided in two steps. During the first step, the hydrogenation rate increases rapidly due to the large pressure difference between the pressure of the gas and the equilibrium pressure which acts as the driving potential for the hydrogenation process. For the case of fin thickness 5mm, the temperature at the first step reaches the maximum value (61.78°C) during the first 80 s of the reaction due to the low thermal conductivity of the hydride powders that restrict to the effective heat removal, and at that time the hydride stores an amount of hydrogen at a hydrogenation

fraction  $X = 0.21$  (21% of the theoretical maximum amount of hydrogen that can be stored). During the first step, the pressure difference is the major factor for the storage. The temperature increase though, results on the increase of the equilibrium pressure; thus, the driving potential for the hydrogenation decreases. During the second stage of the hydrogenation, the circulating coolant removes the produced heat from the tank and reduces the temperature. As a result, the driving potential increases and further storage takes place; this process continues until the maximum capacity achieved.

*Fig.6. Bed average temperature distribution during the hydrogenation process for the case of 14 fins, when all the thicknesses are considered (6a) and the bed average hydrogenation capacity (6b).*

## **6. Conclusions**

The work presented in this paper discusses the heat management of rectangular metal hydride tanks when using extended surfaces in combination with cooling heat exchangers. A mathematical model, including the heat, mass and momentum conservation equations was proposed. Validation with solid experimental results took place. For the validation needs, the storage behaviour, the temperature distribution and the heat transfer during the hydrogenation were considered. Parameters such as the fin thickness and the fin number were considered and studied in terms of influencing the temperature distribution and the hydrogenation capacity during the hydrogenation. Additionally, a modified Non-Dimensional Conductance parameter was introduced for the evaluation of the heat management. The results of the hydrogenation behaviour for the introduced parameters (fin number and thickness) showed that the rectangular tank equipped with the cooling tubes in combination with 14 fins with 5mm fin thickness has the capability of storing hydrogen over 90% of its theoretical capacity in less than 30min. Furthermore, a novel  $AB_2$ -Laves phase intermetallic used for the study. Therefore, in this work, the importance of the effective heat management in terms of using extended surfaces was highlighted to enhance the internal thermal conductivity of the system and the importance that the fin thickness and the number of fins in the thermal behaviour and therefore on the hydrogen storage.

**Acknowledgments:** The current research was partially funded by Coventry University ECR Funding Schemes.

---

---

## **Nomenclature**

---

**Subscripts**

<b>C<sub>a</sub></b>	<i>Absorption Reaction Constant, s<sup>-1</sup></i>	<b>a</b>	<i>Absorption</i>
<b>C<sub>p</sub></b>	<i>Specific Heat, J/kg-K</i>	<b>d</b>	<i>Desorption</i>
<b>E<sub>a</sub></b>	<i>Activation Energy for Absorption, J/molH<sub>2</sub></i>	<b>e</b>	<i>Effective</i>
<b>h</b>	<i>Heat Transfer Coefficient, W/m<sup>2</sup>K</i>	<b>eq</b>	<i>Equilibrium</i>
<b>k</b>	<i>Thermal Conductivity, W/m-K</i>	<b>f</b>	<i>External Cooler</i>
<b>K</b>	<i>Permeability, m<sup>2</sup></i>	<b>g</b>	<i>Gas</i>
<b>M</b>	<i>Molecular Weight, kg/mol</i>	<b>i</b>	<i>Initial</i>
<b>m</b>	<i>Kinetic Expression</i>	<b>s</b>	<i>Solid</i>
<b>n</b>	<i>Number of Hydrogen Moles</i>	<b>SS</b>	<i>Saturation</i>
<b>P</b>	<i>Pressure, bar</i>	<b>Greek Letters</b>	
<b>R</b>	<i>Gas Global Constant, J/mol-K</i>	<b>ε</b>	<i>Porosity</i>
<b>t</b>	<i>Time (s)</i>	<b>μ</b>	<i>Dynamic Viscosity, kg/ms</i>
<b>T</b>	<i>Temperature (K)</i>	<b>ρ</b>	<i>Density, kg/m<sup>3</sup></i>
<b>v</b>	<i>Gas Velocity, m/s</i>	<b>ΔH</b>	<i>Reaction Enthalpy, J/mol</i>
<b>V</b>	<i>Volume, m<sup>3</sup></i>	<b>ΔS</b>	<i>Reaction Entropy, J/mol-K</i>

---

## References

- [1] Levin H. Systematic evaluation and assessment of building environmental performance (SEABEP). Proc Second Int Conf Build 199:3–10.
- [2] Frazzica A, Briguglio N, Sapienza A, Freni A, Brunaccini G, Antonucci V, et al. Analysis of different heat pumping technologies integrating small scale solid oxide fuel cell system for more efficient building

heating systems. *Int. J. Hydrogen Energy*, vol. 40, 2015, p. 14746–56. doi:10.1016/j.ijhydene.2015.08.003.

[3] Gkanas EI, Steriotis TA, Stubos AK, Myler P, Makridis SS. A complete transport validated model on a zeolite membrane for carbon dioxide permeance and capture. *Appl Therm Eng* 2015;74:36–46. doi:10.1016/j.applthermaleng.2014.02.006.

[4] Bland A, Khzouz M, Statheros T, Gkanas EI. PCMs for residential building applications: A short review focused on disadvantages and proposals for future development. *Buildings*. 2017. p. 7.

[5] Wilberforce T, Alaswad A, Palumbo A, Dassisti M, Olabi AG. Advances in stationary and portable fuel cell applications. *Int J Hydrogen Energy* 2016;41:16509–22. doi:10.1016/j.ijhydene.2016.02.057.

[6] Verbecke F, Vesly B. Safety strategy for the first deployment of a hydrogen-based green public building in France. *Int J Hydrogen Energy* 2013;38:8053–60. doi:10.1016/j.ijhydene.2013.03.019.

[7] Makridis SS, Gkanas EI, Panagakos G, Kikkinides ES, Stubos AK, Wagener P, et al. Polymer-stable magnesium nanocomposites prepared by laser ablation for efficient hydrogen storage. *Int J Hydrogen Energy* 2013;38:11530–5. doi:10.1016/j.ijhydene.2013.04.031.

[8] Gkanas EI, Makridis SS. Effective thermal management of a cylindrical  $MgH_2$  tank including thermal coupling with an operating SOFC and the usage of extended surfaces during the dehydrogenation process. *Int J Hydrogen Energy* 2016;41:5693–708. doi:10.1016/j.ijhydene.2016.01.165.

[9] Gkanas EI, Makridis SS, Stubos AK. Modeling and simulation for absorption-desorption cyclic process on a three-stage metal hydride hydrogen compressor. *Comput Aided Chem Eng* 2013;32:379–84. doi:10.1016/B978-0-444-63234-0.50064-6.

[10] Rusman NAA, Dahari M. A review on the current progress of metal hydrides material for solid-state hydrogen storage applications. *Int J Hydrogen Energy* 2016;41:12108–26. doi:10.1016/j.ijhydene.2016.05.244.

[11] Shafiee S, McCay MH. Different reactor and heat exchanger configurations for metal hydride hydrogen storage systems - A review. *Int J Hydrogen Energy* 2016;41:9462–70. doi:10.1016/j.ijhydene.2016.03.133.

[12] Wenelska K, Michalkiewicz B, Chen X, Mijowska E. Pd nanoparticles with tunable diameter deposited on carbon nanotubes with enhanced hydrogen storage capacity. *Energy* 2014;75:549–54. doi:10.1016/j.energy.2014.08.016.

[13] Omer G, Yavuz AH, Ahiska R. Heat pipes thermoelectric solar collectors for energy applications. *Int J Hydrogen Energy* 2017;42:8310–3. doi:10.1016/j.ijhydene.2017.01.132.

[14] Madaria Y, Anil Kumar E. Effect of heat transfer enhancement on the performance of metal hydride based hydrogen compressor. *Int J Hydrogen Energy* 2016;41:3961–73. doi:10.1016/j.ijhydene.2016.01.011.

[15] Singh A, Maiya MP, Srinivasa Murthy S. Experiments on solid state hydrogen storage device with a finned tube heat exchanger. *Int J Hydrogen Energy* 2017;42:15226–35. doi:10.1016/j.ijhydene.2017.05.002.

[16] Anbarasu S, Muthukumar P, Mishra SC. Thermal modeling of  $LmNi_4.91Sn_{0.15}$  based solid state hydrogen storage device with embedded cooling tubes. *Int J Hydrogen Energy* 2014;39:15549–62. doi:10.1016/j.ijhydene.2014.07.088.

- [17] Mazzucco A, Dornheim M, Sloth M, Jensen TR, Jensen JO, Rokni M. Bed geometries, fueling strategies and optimization of heat exchanger designs in metal hydride storage systems for automotive applications: A review. *Int J Hydrogen Energy* 2014;39:17054–74. doi:10.1016/j.ijhydene.2014.08.047.
- [18] Gkanas EI, Grant DM, Stuart AD, Eastwick CN, Book D, Nayebossadri S, et al. Numerical study on a two-stage Metal Hydride Hydrogen Compression system. *J Alloys Compd* 2015;645:S18–22. doi:10.1016/j.jallcom.2015.03.123.
- [19] Jemni A, Nasrallah S Ben. Study of two-dimensional heat and mass transfer during absorption in a metal-hydrogen reactor. *Int J Hydrogen Energy* 1995;20:43–52. doi:10.1016/0360-3199(93)E0007-8.
- [20] Visaria M, Mudawar I, Pourpoint T, Kumar S. Study of heat transfer and kinetics parameters influencing the design of heat exchangers for hydrogen storage in high-pressure metal hydrides. *Int J Heat Mass Transf* 2010;53:2229–39. doi:10.1016/j.ijheatmasstransfer.2009.12.010.
- [21] Laurencelle F, Goyette J. Simulation of heat transfer in a metal hydride reactor with aluminium foam. *Int J Hydrogen Energy* 2007;32:2957–64. doi:10.1016/j.ijhydene.2006.12.007.
- [22] Kim KJ, Montoya B, Razani A, Lee K-H. Metal hydride compacts of improved thermal conductivity. *Int J Hydrogen Energy* 2001;26:609–13. doi:10.1016/S0360-3199(00)00115-4.
- [23] Gkanas EI, Khzouz M. Numerical analysis of candidate materials for multi-stage metal hydride hydrogen compression processes. *Renew Energy* 2017;111:484–93. doi:10.1016/j.renene.2017.04.037.
- [24] Gkanas EI, Grant DM, Khzouz M, Stuart AD, Manickam K, Walker GS. Efficient hydrogen storage in up-scale metal hydride tanks as possible metal hydride compression agents equipped with aluminium extended surfaces. *Int J Hydrogen Energy* 2016;41:10795–810. doi:10.1016/j.ijhydene.2016.04.035.
- [25] Gkanas EI, Khzouz M, Panagakos G, Statheros T, Mihalakakou G, Siasos GI, et al. Hydrogenation behavior in rectangular metal hydride tanks under effective heat management processes for green building applications. *Energy* 2018;142:518–30. doi:https://doi.org/10.1016/j.energy.2017.10.040.
- [26] Gambini M, Stilo T, Vellini M, Montanari R. High temperature metal hydrides for energy systems Part A: Numerical model validation and calibration. *Int J Hydrogen Energy* 2017;42. doi:10.1016/j.ijhydene.2017.05.062.
- [27] Nishizaki T, Miyamoto K, Yoshida K. Coefficients of performance of hydride heat pumps. *J Less Common Met* 1983;89:559–66. doi:10.1016/0022-5088(83)90372-7.
- [28] Bowman RC, Luo CH, Ahn CC, Witham CK, Fultz B. The effect of tin on the degradation of LaNi<sub>5</sub>-ySny metal hydrides during thermal cycling. *J Alloys Compd* 1995;217:185–92. doi:10.1016/0925-8388(94)01337-3.