DOI: 10.51984/SUCP.V3I3.3751

المؤتمر السادس للعلوم الهندسية والتقنية
The Sixth Conference for Engineering Sciences and Technology (CEST-6)
Conference Proceeding homepage: https://cest.org.ly

Dynamic Study of Hydrogen Absorption in Metal Hydride-based Storage Systems

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Keywords:
Metal hydride
Hydrogen Storage
Absorption,
Kinetics reaction
Heat pipe

ABSTRACT

The paper is described an analysis of using Metal Hydride (MH) in hydrogen storage systems during charging process . A 3-D partial differential equations algebraic model is employed to describing the kinetic reaction of hydrogen charging into different MH beds ($LaNi_{4.75}A_{l0.25}$, and $LaNi_5$). A software simulation is discussed and created for MH reactor configurations equipped with and without heat pipe. The COMSOL 5.2a Multi-physics software was used for this simulation by solving simultaneously the energy, mass-momentum, and kinetic differential equations of conservation. The reaction kinetic of hydrogen is analyzed depending on some parameters including: (reactor design, hydrogen inlet pressure, cooling temperature and convective heat transfer coefficient). The results showed a good compatibility between the software simulations and the experimental work for $LaNi_5$ previously published by the authors. This is sensibly where the value of error was less than 8%, this confirm the efficiency of model to captured the key experimental trends. The maximum charging capacity is recorded in case of $LaNi_5$, while the fastest charging duration time is recorded for $LaNi_{4.75}Al_{0.25}$. Each MH materials has different hydriding process depending on it's thermo-physical properties. The hydrogen charging into MH systems inside the visuals is exothermic reaction associated with a high inner temperature achieved, and high heat energy release.

دراسة ديناميكية امتصاص الهيدروجين في أنظمة التخزين المعتمدة على هيدريد المعدن

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الكلمات الرئيسية:
هيدريد المعدن
تخزين الهيدروجين
امتصاص
رد الفعل الحركي
اتبوب الحرارة

الملخص

تتناول هذه الورقة استخدام هيدريد المعدن (**MH**) في أنظمة تخزين الهيدروجين أثناء عملية الشحن. تم استخدام نموذج جبري للمعادلات التفاضلية الجزئية ثلاثية الأبعاد لوصف التفاعل الحركي لشحن الهيدروجين وذلك باستخدام أنواع مختلفة من هيدريد المعدن (**$LaNi_{4.75}Al_{0.25}$** و**$LaNi_5$**). تم تصميم و مناقشة محاكاة برمجية لتكوينات مفاعل هيدريد المعدن المجهز بأنابيب الحرارة وبدونها. تم استخدام برنامج **COMSOL 5a.** متعدد المهام لهذه المحاكاة من خلال حل معادلات الحفظ للطاقة وزخم الكتلة والمعادلات التفاضلية الحركية في نفس الوقت. تم تحليل ديناميكية أو حركية التفاعل للهيدروجين بالاعتماد على بعض العوامل منها: (تصميم المفاعل، ضغط الهيدروجين الداخل، درجة حرارة التبريد، معامل انتقال الحرارة بالحمل الحراري). أظهرت النتائج توافقًا جيدًا بين عمليات محاكاة للبرنامج والتجارب المعملية لهيدريد المعدن **($LaNi_5$)** والذي تم نشره بواسطة المؤلفون سبقًا، وهذا معقول حيث كانت قيمة الخطأ أقل من 8%، وهذا يؤكد كفاءة النموذج في محاكاة الواقع في التطبيقات العملية. يتم تسجيل أقصى سعة شحن في حالة استخدام **$LaNi_5$**، بينما يتم تسجيل أسرع مدة شحن في حالة استخدام **$LaNi_{4.75}Al_{0.25}$**. من الملاحظ أن عملية تخزين الهيدروجين بواسطة هيدريد المعدن هي تفاعل طارد للحرارة، يسبب في ارتفاع درجة حرارة وعاء التخزين، و أن لكل هيدريد معدن تفاعل خاص به معتمدا على خواصه الحرارية والفيزيائية.

1. Introduction

The reduction of fossil fuel resources and its energy consumption contamination have make a obvious request for substitute of new clean energy sources [1]. Hydrogen (H_2) considered being the best alternative energy to fossil fuels due to its great calorific worth and

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Article History: Received 00 December 00 - Received in revised form 00 January 00 - Accepted 00 February 00

being economically. However, all the studies on hydrogen energy have shown storage problem. Recently, H_2 stored in different forms (including: compressed gas, cooling liquid, and solid in porous medium of metal hydrides). Charging of H_2 in a porous media of MH is a complex multi-physics problem concern heat transfer and reaction kinetics, conjugated with compressible gas flow. Therefore, reducing thermal resistance of the storage system becomes a crucial issue for the vessel design. AB_5 inter-metallic compounds including $LaNi_5$, is well-advised very likely for these applications [2]. Experiments showed that hydrogen reaction can be improved intensively by enhancing the heat transfer of canisters [3-6]. There
are several numerical works on different aspects and designing parameters of the Metal Hydride Reactors (MHRs) [6-10]. In H_2 charging process into MH materials, different cooling systems are employed to increase the charging capacity. Recently, heat pipe is employed in H_2 charging process to over come the leak damage at heat exchange pipes, which caused to spoilage MH [4, 5, 10].
Heat pipe cooling system is used in present study to investigate, and comparison of H_2 storage into different MH beds ($LaNi_{4.75}Al_{0.25}$, and $LaNi_5$). A 3-D partial differential equations model is employed to describing the kinetic reaction of H_2 charging in the specific MH beds. A software simulation is created for MH reactor configurations equipped with and without heat pipe. The COMSOL 5.2a Multi-physics software is used for this simulation by solving simultaneously the energy, mass-momentum, and kinetic differential equations of conservation.

2. Numerical model

3-D axis-symmetrical and time dependent algebraic model are used for two MHRs configurations (see figure 1 and table 1). The model assumptions are:

- Gas/solid thermal equilibrium,
- H_2 is considered as an ideal gas,
- The solid phase is isotropic and has a uniform porosity,
- Natural convection is effected onto vessel walls,
- Radiation is negligible.
- Van't Hoff Law is considered for the reaction process.

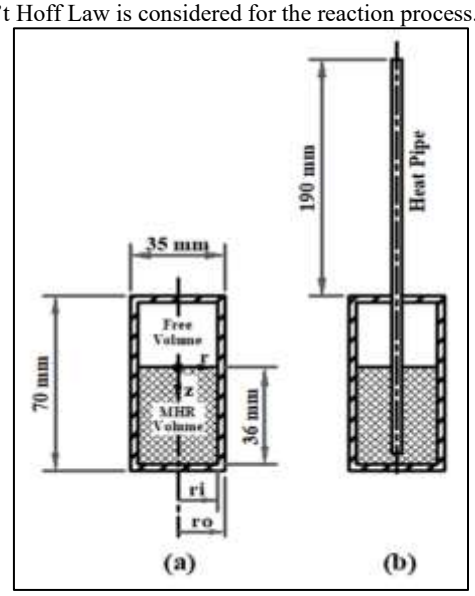

Fig. 1. Schematic diagram of MHRs
a) without heat pipe b) with heat pipe

In this study, consider $LaNi_5$ and/or $LaNi_{4.75}Al_{0.25}$ in MHR for numerical study on hydrogen absorption which that has been expressed below:

$$LaNi_5 + 3H_2 \overset{20\,^{\circ}C}{\longleftrightarrow} LaNi_5H_6 + Q$$

$$\mathrm{LaNi4.75Al0.25} + 3H_2 \overset{20\,^{\circ}C}{\longleftrightarrow} \mathrm{LaNi4.75Al0.25}H_6 + Q$$

The heat generated during the H_2 charging process is removed from the reactor by heat pipe. The cooling level has substantial impact on charging because hydrogen absorption takes place depending on the vessel temperature. Cooler vessels have higher absorption rate and shorter filling time. Table 1 shows important geometrical parameters for designated MH reactor configurations which have been applied in the simulation. Table 2 shows the physical properties used for algebraic model simulation.

Table 1. Geometrical parameters of the reactor [5]

Parameter	Value
Reactor diameter	29 mm
Tube height with metal hydride	36 mm
Tribune free height	24 mm
Heat pipe internal diameter	4 mm
Heat pipe external diameter	6 mm
Heat pipe section outside the reactor	190 mm
Total heat pipe length	250 mm
Reactor wall thickness	3 mm
TC1 thermocouple position	5.1 mm
TC2 thermocouple position	17.9 mm
TC3 thermocouple position	35.8 mm

Table 2. Constantly used parameter values in analyzes [10]

Parameter	$LaNi_5$ value
(ε) Metal hydride porosity	0.5
Diffusion coefficient (H_2) m^2/s	$50*10^{-9}$
H_2 initial concentration g	0
Storage tank initial pressure Bar	1
Reaction rate constant (Absorption) 1/s	59.187
Activation energy - Absorption J/mol	21179.6
Reaction enthalpy J/mol	30800
Reaction entropy J/mol	104.5
Reaction hysteresis	0.2
Metal hydride saturation density kg/m^3	8394
Metal hydride thermal conductivity W/(m-K)	1.32
Metal hydride specific heat value J/(kg-K)	419
Storage tank material density (steel) kg/m^3	7800
Storage tank material thermal conductivity (steel) W/(m-K)	80
Storage tank material specific heat value (steel) J/(kg-K)	2000
H_2 inlet temperature ^oC	20
H_2 system pressure (Bar)	3
Time step (s)	5
Total simulation time (s)	5000

A software simulation is created for MH reactor configurations equipped with and without heat pipe. The COMSOL 5.2a Multi-physics software is used for this simulation by solving simultaneously the energy, mass-momentum, and kinetic differential equations of conservation. The main equations used are:

Energy equation;
$$(\rho.C_p)_e.\frac{\partial T}{\partial t} + (\rho_g.Cp_g).\bar{v}_g.\nabla T = \nabla.(k_e.\nabla T) + m.[\Delta H - T.(Cp_g - Cp_s)] \quad (1)$$

Hydride mass balance;
$$(1-\varepsilon).\frac{\partial(\rho_s)}{\partial t} = -m \quad (2)$$

Hydrogen mass balance;
$$\varepsilon.\frac{\partial(\rho_g)}{\partial t} + div(\rho_g.\bar{v}_g) = -m \quad (3)$$

Darcy's law;
$$\vec{v}_g = -\frac{K}{\mu_g}.grad(\bar{P}_g) \quad (4)$$

Where:
$$K = \frac{dp^2\varepsilon^3}{180.(1-\varepsilon^2)} \quad (5)$$

Substituting equations (4) $\vec{v}_g$ and (5) K in Hydrogen mass balance equation
$$\left(\frac{\varepsilon M_g}{R_u T}\right)\frac{\partial P_g}{\partial t} + \left(\frac{\varepsilon M_g P_g}{R_u}\right)\frac{\partial}{\partial t}\left(\frac{1}{T}\right) - \frac{K}{\nu_g r}\frac{\partial}{\partial r}\left(r\frac{\partial P_g}{\partial r}\right) - \frac{K}{\nu_g}\frac{\partial}{\partial z}\left(\frac{\partial P_g}{\partial z}\right) = m \quad (6)$$

Vant't Hoff law;

$$lnP_{eq} = \frac{\Delta H}{R_g.T} - \frac{\Delta S}{R_g} \quad (7)$$

Absorption Kinetic equation

$$m = C_a.\exp\left[-\frac{E_a}{R_g.T}\right].\ln\left[\frac{P_g}{P_{eq}}\right].(\rho_{ss} - \rho_s) \quad (8)$$

3. Results and Model Validation

The resulting simulation findings and the experiments findings are compatible with using the same methodology as in simulation and presented in a previous work by the authors [5, 10]. Figure (2)demonstrated a strong correlation between the software simulations and the experimental work, this is a clearly observed in temperature vs. time maps from the thermo-couple (TC3) placed at the reactor bottom (35.8mm). For both experimental and algebraic model, the temperature variables yield results that are almost identical. But then, it is found that the getting charge time is longer in experimental work than in modeling work. It is envisaged that some losses will occur at the hoses during the suction and charging procedures in the experimental work. Figure 3 illustrates the measured and projected hydrogen capacities. Evidently, the numerical results are in satisfactory accord with the experimental data.

As illustrated in Fig. 4b, the $LaNi_5$ material achieves the largest quantity of hydrogen mass to be held under the specified working conditions, while the $LaNi_{4.75}Al_{0.25}$ material achieves the minimum values. In general, the $LaNi_5$. material has the longest hydrogen absorption period, while the $LaNi_{4.75}Al_{0.25}$ material has the lowest.

It is evident from analyzing the modeling study's results that $LaNi_5$ material should be chosen in order to store the greatest possible amount of hydrogen mass. In this instance, you should be aware that it will take longer to obtain the maximum mass of hydrogen. However, if you require the mass of hydrogen in a short amount time, and the quantity is not important you should use $LaNi_{4.75}Al_{0.25}$.

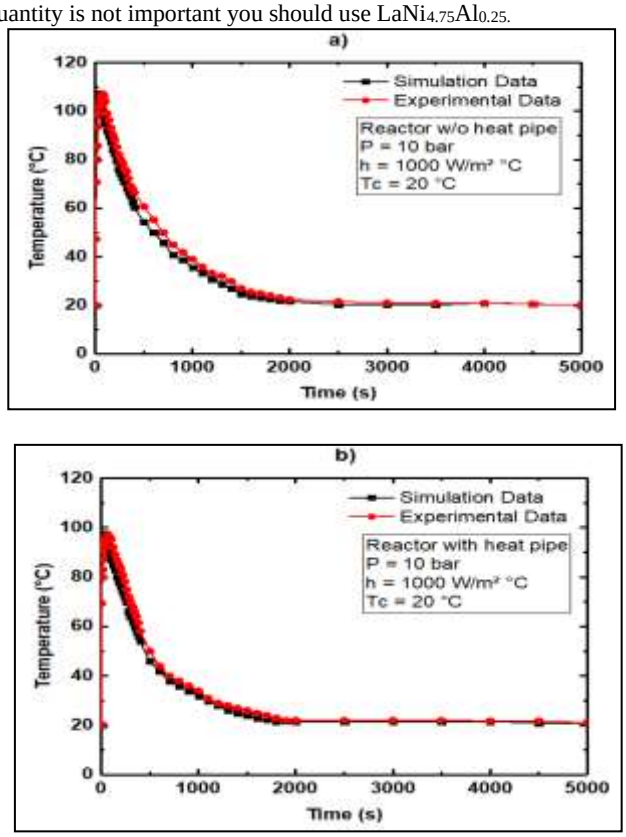

Fig. - 2. The temperature histories at 35.8mm from the bottom. a) With no heat pipe, b) with a heat pipe.

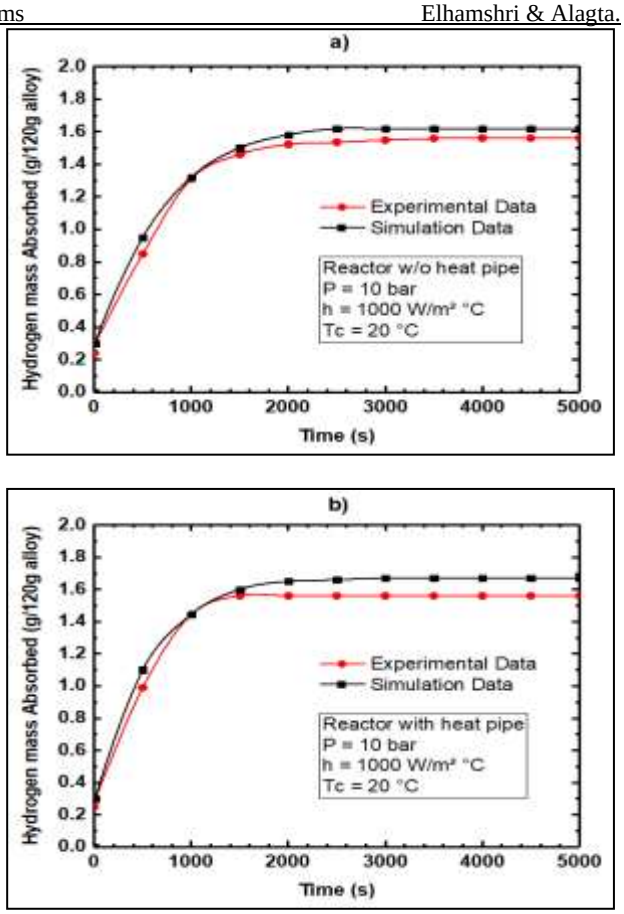

Fig. - 3. Time evolution's of the absorbed hydrogen amount under 10 bar hydrogen pressure supply by both experimental and simulation studies a) With no heat pipe, b) with a heat pipe.

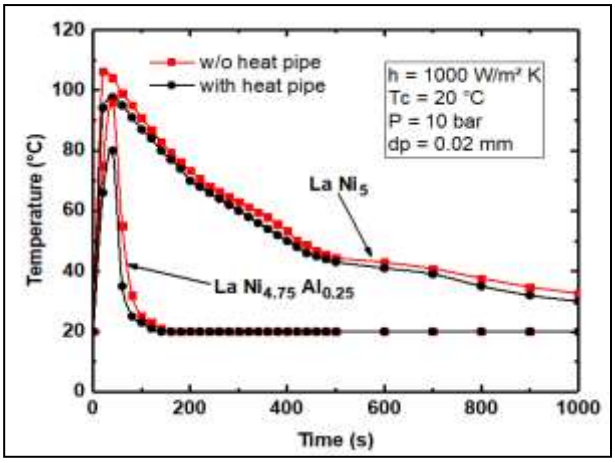

Fig. – 4. The fluctuation in interior temperatures over time in MHRs with or without heat pipes.

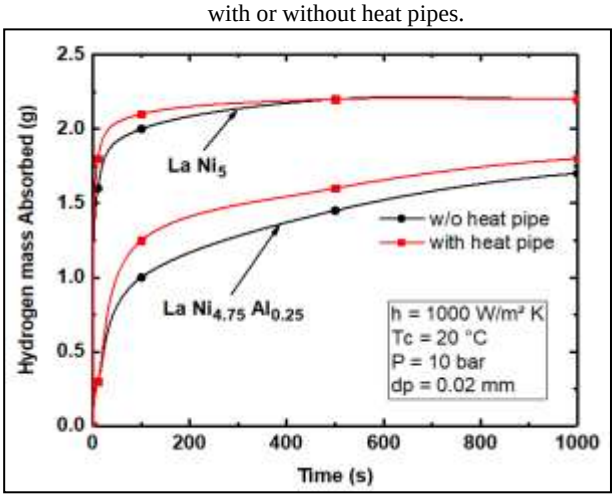

Fig. (5) The quantity of hydrogen mass varies time depending on whether the MHR contains a heat pipe or not.

4. Conclusion

In the Hydrogen charging process, a large amount of heat energy is released in a short period of time. To achieve an effective charging process, heat must be evacuated from the system efficiently and fast. Upon analyzing all of the results and graphs, the model was compatible with earlier experimental results provided by the authors. This is sensibly where the value of error was less than 8%, this confirm the efficiency of model to captured the key experimental trends. In contrast, the MHR design which has a heat pipe performs better than the other configuration that was tested in terms of both charging time and storage capacity. As a result, the model can be applied to improve the performance and designs of MHRs.

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