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Prediction of hydrogen absorption performance of $LaNi_5$ hydride reactors using the unstructured Lattice Boltzmann Method

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***Abstract*— In this paper, a new approach was adopted to numerically study the hydrogen absorption process in an $LaNi_5$ Hydrogen Reactor. The energy equation was solved using the Control Volume Lattice Boltzmann Method (CVLBM) with unstructured grids. In order to verify the computational efficiency of the considered approach, obtained results were compared to those of the unstructured Control Volume Finite Element Method (CVFEM). We found that the CVLBM correctly predicts hydrogen absorption phenomena and has less CPU time compared to the CVFEM. Furthermore, two different tank geometries were studied and we found that the proposed modification enhances the dynamic behavior of the reactor and reduces the charging time by 56% compared to the basic configuration.**

***Keywords*— Lattice Boltzmann Method, unstructured grids, metal hydride, LaNi5, hydrogen storage, heat transfer.**

I. INTRODUCTION

The study of heat and mass transfer within Metal Hydrogen Reactors (MHRs) was the field of interest of many researchers. Several numerical studies have been reported to investigate and enhance heat transfer rates in MH beds. Some researchers were interested to improve the hydride powder properties [1-3] and other aimed to increase the heat transfer area of the bed [4-10] by integrating heat exchangers, fins, heat fluid pipes… Also, adding a Phase Change Material (PCM) to MHRs shows a significant improvement of the bed performance [11-17]. Various mathematical and numerical models are proposed by authors to describe, solve and predict heat transfer in an MHR. Using the Finite Volume Method (FVM), Askri et al. [18] studied coupled heat and mass transfers in a MHR filled with different alloys. They concluded that the radiative effects are not important in the reactor filled with the LaNi5-H_2 alloy while they affect the transfer in the Mg-H2 system. Using the Control Volume Finite Element Method (CVFEM), Askri et al. [19] performed a two-dimensional study of heat and mass transfers within a closed MHR. The authors carried out a parametric study of the geometric characteristics and the expansion zone volume. The obtained results showed that the reactor that has a form factor equal to 2 has the least hydrogen storage capacity. Later, in another work [20], they analyzed primarily the tank behavior during the hydriding process and then they investigated the effect of some parameters such as the reactor size, the expansion volume, the hydrogen tank volume and the pressure inlet on the hydriding process. Kumar et al. [21] studied the absorption hydrogen process using the Fluent software. They indicate that at the beginning of the process, the speed of the hydrogen absorption is so high and by time, due to the increase of the temperature inside the reactor, the absorption speed decreases. Freni et al. [22] developed a three dimensional model of metal hydride beds filled with an $LaNi_5$ alloy and equipped with various types of exchangers. The simulation by "COMSOL Multiphysics" showed that a reactor design depends on the permeability as well as on the thermal conductivity of hydrides. Using the structured Lattice Boltzmann Method (LBM), Askri et al. [23] studied the discharge process of an MHR. They concluded that the developed model could be used as a part of a larger numerical model aimed to simulate a whole energy system including metal hydride bed. Garrison et al. [24] studied different designs of transverse and longitudinal fins incorporated into a combined Sodium alanate complex metal reactor and heat exchanger by employing COMSOL Multiphysics software. They concluded that the optimal longitudinal fin design appears to be slightly, but likely negligibly, more efficient than the transverse fin design. Ben Mâad et al. [25] applied the CVFEM to predict heat and mass transfers in an MHR filled with a magnesium alloy. They studied the sensitivity of the thermo-physical parameters, the radiative source and the effect of geometric parameters using three different geometrical configurations. Singh et al. [26] presented a model to predict heat and mass transfers in a metal hydride bed equipped with an annular heat exchanger tube with radial circular copper fins. This model is based on the Comsol Multiphysics software. Mellouli et al. [27] studied the hydrogen storage in cylindrical and spherical metal hydride beds equipped with a phase change material. They determined the effect of the PCM integration as well as the quality of the tank insulation on the system performance. Also, M. Valizadeh [28] investigated heat and mass transfers during hydrogen desorption in a metal hydride storage tank

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using the LBM. In a previous work, Bouzgarrou et al. [29] used the structured LBM to analyze heat and mass transfer within a closed $LaNi_5$-H_2 reactor. They found that, the LBM algorithm presents a simple implementation on a computer and has an accurate CPU time compared to FVM. Shaji et al. [30] reported numerical studies on the sorption performance of an MHR embedded with aluminium foam. The Comsol Multiphysics software was used. The effect of integrating foam within the hydride bed on the thermal behavior and walls strain was investigated. Chibani et al. [31] studied the charge and discharge processes in an $LaNi_5$ tank. They used a concentric triple-tube heat exchanger. In this study, the authors determined the diameters of the heat exchanger. Also, they compared the performance of the Lanthanume Nickel with the $MmNi_{4.6}Fe_{0.4}$ hydride and the activated charbon. The hydride thermal and mass behavior was integrated in the CFD Fluent with software (C++). A numerical model of a metal hydride reservoir, equipped with phase change material, has been developed on Comsol platform by Tong et al. [32]. In their study, the phase change materials were composited with various metal foams (copper and aluminium foams) to enhance the hydrogen storage efficiency. T.Alqahtani et al. [33] studied a new configuration which consists of an MH reactor encircled by a cylindrical sandwich bed packed with PCM. Results were obtained using the ANSYS Fluent software. Despite the stability and the precision of all the numerical methods, they remain restricted to dealing with simple geometries. Indeed, in the case of complex geometrical configurations, the structured technique of meshing requires not only the treatment of each case subjected to different boundary conditions and even the development of a numerical code for each geometry, but also extra effort and more computation time. Therefore, in this work, we aim to apply the unstructured Control Volume Lattice Boltzmann Method (CVLBM) [34], promoting both good accuracy with less computing time, to predict heat and mass transfer in an $LaNi_5$-H_2 reactor. In addition, a new geometrical configuration of the bed was proposed and compared to the basic configuration. The remainder of this paper is divided into three sections. We first describe the procedure of the discretization of equations governing transfer in metal hydrogen tanks. Then, the developed numerical tool is used to simulate transfer in the considered closed reactor. Simulation results performed are presented in the last section.

II. Formulation

A. Mathematical model

The considered reactor is filled with an $LaNi_5$ alloy and exchanges heat through the base and lateral areas with a heating fluid maintained at a constant temperature T_f.

In the absence of convective and radiative heat transfers, equations describing heat and mass transfers in an MH reactor, when transfers are two-dimensional, are as follow:

$$\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t}=\lambda_{eff}\left(\frac{\partial^2 T}{\partial z^2}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right)+\dot{m}\Delta H+\dot{m}\left(C_{pg}-C_{ps}\right)T \quad (1)$$

Where $\left(\rho C_p\right)_{eff}=\varepsilon\rho_g C_{pg}+\left(1-\varepsilon\right)\rho_s C_{ps}$ and $\lambda_{eff}=\varepsilon\ \lambda_g+\left(1-\varepsilon\right)\lambda_s$

ε, C_{pg} and C_{ps} are, respectively, the porosity of the hydride and the specific capacities of the gas and the solid.

ρ_g and ρ_s are the densities of the gas and the hydride. ΔH is the enthalpy of the formation and m is the hydrogen mass absorbed per unit time and volume.

The Boltzmann equation is written as follows:

$$\frac{\partial f_i}{\partial t}(r,t)+c_i.\nabla f_i(r,t)=\frac{1}{\tau}\left(f_i^{eq}(r,t)-f_i(r,t)\right)+\frac{w_i S}{\left(\rho C_p\right)_{eff}};i=0...n \quad (2)$$

Where f_i is the particle distribution function and S is defined by the following expression:

$$S=\frac{\lambda}{r}\frac{\partial T}{\partial r}+\dot{m}\left(C_{pg}-C_{ps}\right)T+\dot{m}\Delta H \quad (3)$$

B. Numerical approach

The integration of equation (2) on the control volume ΔV_N and the time interval Δt gives:

$$\underbrace{\int_t^{t+\Delta t}\int_{\Delta V_N}\frac{\partial f_i}{\partial t}dtdV}_{Q_1}+\underbrace{\int_t^{t+\Delta t}\int_{\Delta V_N}\vec{\nabla}.(\vec{c}_i f_i)dtdV}_{Q_2}=\underbrace{\int_t^{t+\Delta t}\int_{\Delta V_N}\frac{f_i^{eq}-f_i}{\tau}dtdV}_{Q_3}+ \quad (4)$$

$$\underbrace{\int_t^{t+\Delta t}\int_{\Delta V_N}\frac{w_i\dot{m}\alpha_{eff}}{r}\frac{\partial T}{\partial r}dtdV}_{Q_4}+\underbrace{\int_t^{t+\Delta t}\int_{\Delta V_N}\frac{w_i\dot{m}}{(\rho C_p)_{eff}}\left(\Delta H+\left(C_{pg}-C_{ps}\right)T\right)dtdV}_{Q_5},i=0...n$$

Where the Control volume ΔV_N is expressed as follows [34]:

$$\Delta V_{N,j}=2\ \pi\ r_j\ A_{N,j} \quad (5)$$

The calculation of terms Q_1, Q_2, Q_3, Q_4 and Q_5 are detailed in a previous work [34].

C. Boundary conditions

The reactor exchanges heat by convection through its different areas, we can consider the convective boundary condition given by:

$$-\lambda_{eff}\ \vec{grad}\ T.\vec{n}=h\ \left(T-T_f\right) \quad (6)$$

And by using this equation and considering a linear interpolation, we can calculate the temperature at the node N as follows:

$$T_N=\frac{h\ T_f-\lambda_{eff}\left(M_{12}n_r+M_{22}n_z\right)T_{N_j}-\lambda_{eff}\left(M_{13}n_r+M_{23}n_z\right)T_{N_j}}{h+\lambda_{eff}\left(M_{11}n_r+M_{21}n_z\right)} \quad (7)$$

And the temperature at the corners of the enclosure is calculated by adopting the Finite Difference scheme.

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III. SOLUTION PROCEDURE

After dividing the domain of interest into the desired number of nodes, a computer code was developed on Fortran 90 according to the following steps:

1- Calculate the geometrical parameters (control volumes, surfaces…) in cylindrical coordinates.
2- Define the thermo-physical and geometrical parameters of the reactor.
3- Initialize the input parameters (ρ_s, ρ_g, $(\rho C_p)_{eff}$).
4- Compute the relaxation time τ.
5- Calculate the coefficients $CL^{i'}_{i,N}$ and $\gamma_{i,Nj}$.
6- Given the initial temperature field, compute the equilibrium distribution function, f_i^{eq}.
7- Calculate the first source term, Q_4.
8- Calculate the hydrogen mass absorbed or desorbed.
9- Compute the second source term, Q_5.
10- Calculate the coefficients $\alpha_{i,N}$ and $\beta_{i,N}$.
11- Calculate the distribution function,$f_{i,N}$.
12- Compute the temperature field T.
13- Calculate f_i^{eq}.
14- Obtain the convergence when the steady state is achieved.

IV. RESULTS AND DISCUSSION

In this study, different geometrical models of MH containers are investigated to optimize the hydrogen storage capacity (Fig.1). Heat and mass transfers within considered reactors were studied by using the unstructured CVLBM and computational results were compared with those of the CVFEM.

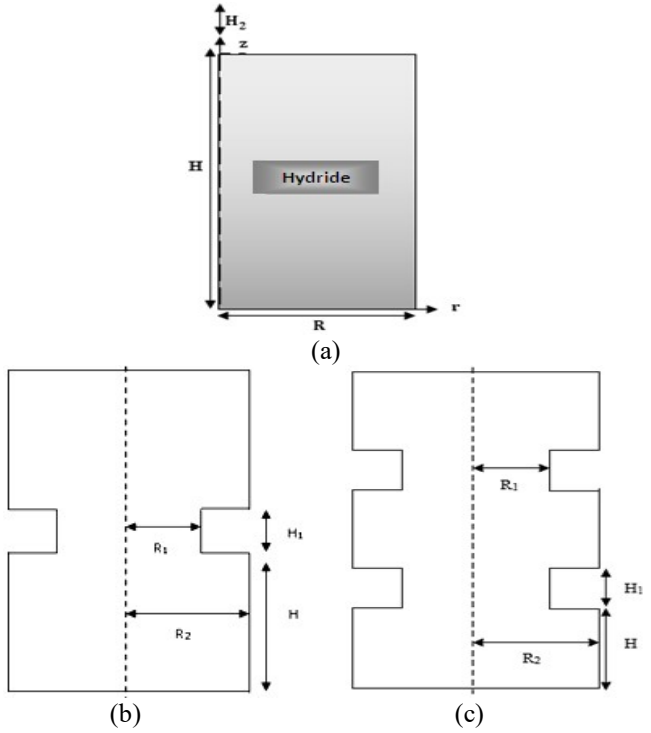

Fig. 1 Various designs of reactors studied: (a) basic reactor (configuration 1), (b) modified MHR (configuration 2), (c) modified MHR (configuration 3)

To verify the computational accuracy of the numerical model, we consider a basic cylindrical Metal Hydrogen Reactor of a radius R=2.5cm and a height H=6cm that exchanges heat through its walls with a cooling fluid maintained at a constant temperature T_f (Fig. 1a).

In fig.2 a-b we present, respectively, the time evolution of the hydride temperature and the hydrogen mass absorbed. Fig.2a shows an increase of the temperature at the beginning due to the exothermic aspect of the hydrogenation process. Then, it decreases with the increase of the kinetic reaction. In addition, the comparison of results with those of the CVFEM showed a good concordance, with a relative difference of 0.46% and 2.5%, respectively, for the temperature and the hydrogen mass stored. Consequently, we can assert the applicability of the CVLBM to simulate the hydriding process within an MHR.

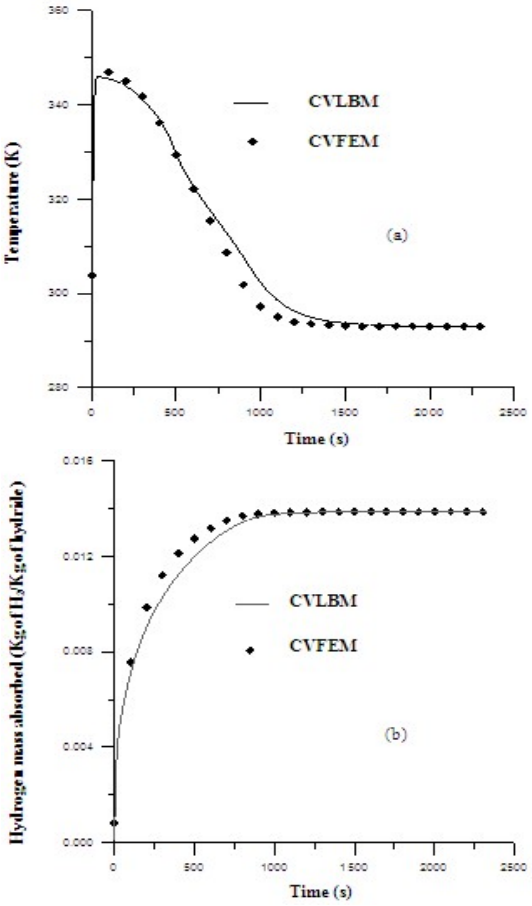

Fig. 2 Temporal evolution of (a) the hydride temperature and (b) the hydrogen mass absorbed

Fig.3 illustrates the evolution of isotherms at selective times (tt=60, 360, 540, 720s and the steady state). It is seen that the temperature increases in the reactor since the absorption process in metals is exothermic. The temperature of the central region is high, while walls are slightly colder due to the external cooling fluid. By time, the temperature progressively decreases until reaching the temperature of the

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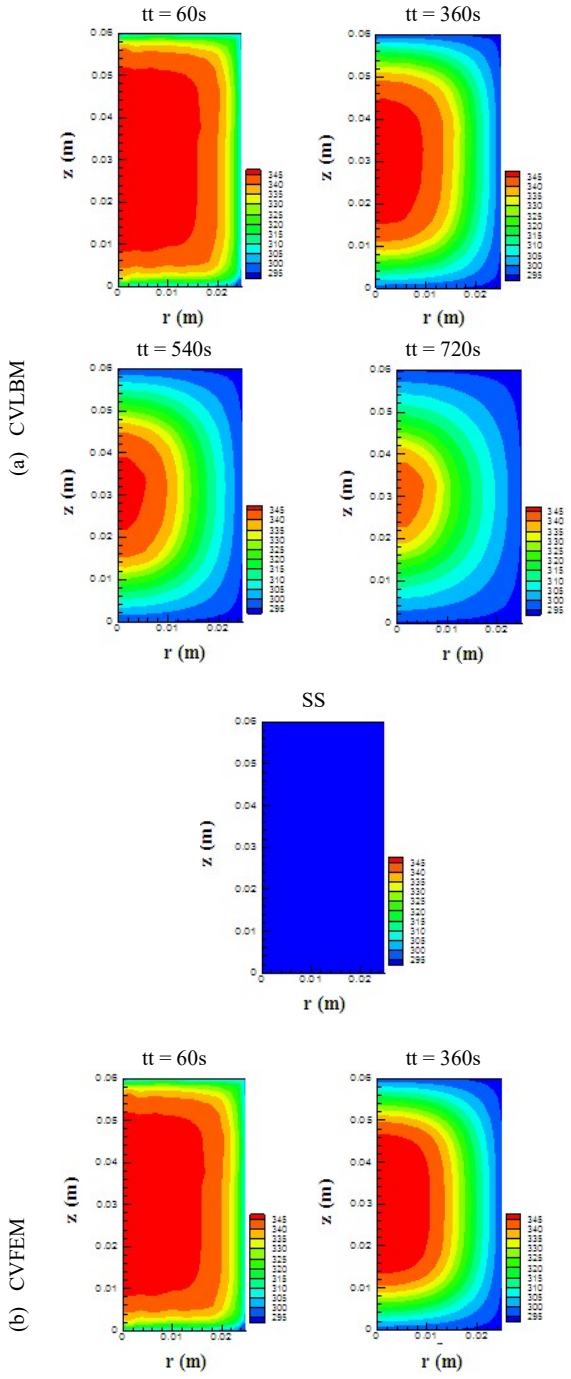
cooling fluid. Also, it is shown that the two plots match well which proves the efficiency of the new approach.

Furthermore, by comparing the CPU time required to reach the steady state for the CVLBM and the CVFEM (Table 1) using the same Intel® core (TM) i7 CPU 2.4 computer, we conclude that the CVLBM is faster than the CVFEM. Thus, it is important to adopt a numerical method presenting such an advantage.



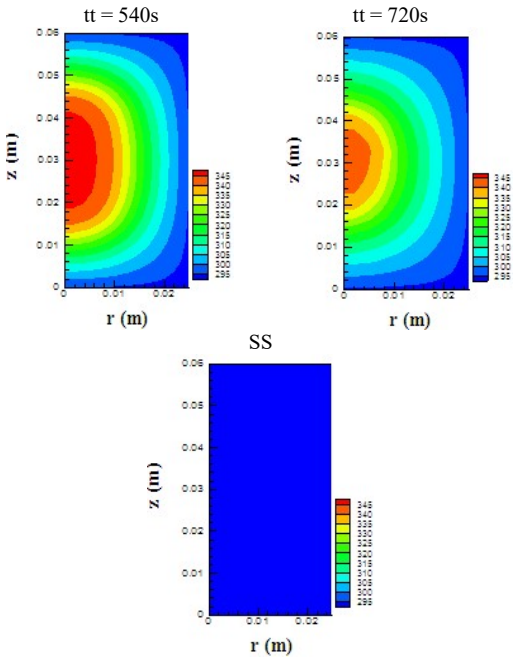


Fig.3 Contours of the temperature at different times (a) CVLBM, (b) CVFEM

For the three configurations, we compared the cycling time and the amount of hydrogen to be absorbed. Figures 4 and 5 illustrate, respectively, the effect of the geometrical modification on the time evolution of the temperature and the hydrogen mass absorbed. We note that by increasing the number of empty zones, the temperature inside the hydride medium decreases more rapidly. In fact, when the contact surface between the hydride and the cooling fluid increases, the kinetic of the reaction is improved which leads to store a more amount of hydrogen. And consequently, the charging time will be reduced. Fig.5 shows that 540, 300 and 200s are, respectively, required to absorb 86% of hydrogen for the first, second and third configurations. So, the proposed geometrical modification improved the cycling time by 34% and 56% for the second and third configurations compared to the first reactor.

All these results show that the CVLBM can predict heat and mass transfers in hydrogen tanks with complex geometries.

V. Conclusions

In this study, a numerical approach based on the unstructured Lattice Boltzmann Method "CVLBM" is adopted to simulate heat and mass transfer in a Metal Hydrogen Reactor during the absorption process.

The obtained results were compared with those of the unstructured CVFEM and a relative difference of about 0.46%, for the temperature, was obtained. We found that the new approach correctly predicts hydrogen absorption phenomena and has less CPU time compared to the CVFEM. In addition, two new configurations are proposed and it is shown that the configuration with two empty zones reduces

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the filling time by 56% and improves the dynamic behavior of the reactor.

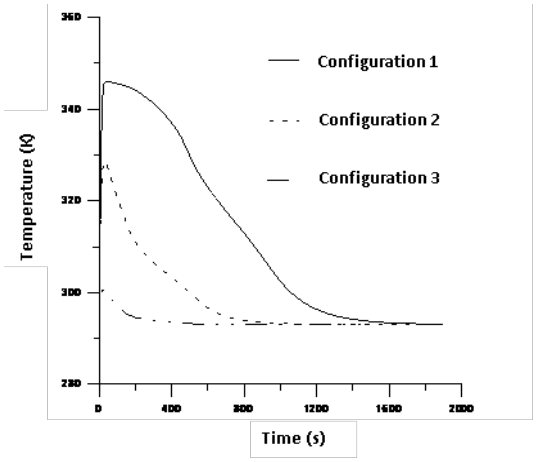

Fig.4 Time evolution of the temperature for the three configurations

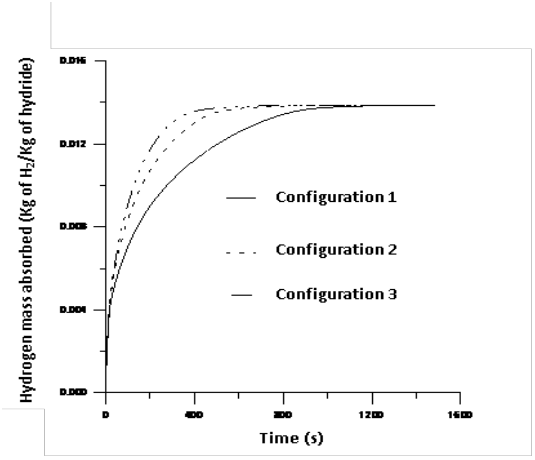

Fig.5 Time evolution of the hydrogen mass absorbed for the three configurations

VI. REFERENCES

[1] CHAISE A, DE RANGO P, MARTY PH, FRUCHART D, MIRAGLIA S, OLIVES R. ENHANCEMENT OF HYDROGEN SORPTION IN MAGNESIUM HYDRIDE USING EXPANDED NATURAL GRAPHITE. INT. J. HYDROGEN ENERGY 2009; 34:8589-8596.

[2] Mellouli S, Dhaou H, Askri F, Jemni A, Ben Nasrallah S. Hydrogen storage in metal hydride tanks equipped with metal foam heat exchanger. Int. J. Hydrogen Energy 2009; 34:9393-9401.

[3] Lewis SD, Chippar P. Analysis of heat and mass transfer during charging and discharging in a metal-hydride-phase change material reactor. J. Energy Storage 2021; 33:102108.

[4] Jincheng Ma, Yuqi W, Shaofei Sh, Fusheng Y, Zewei B, Zaoxiao Z. Optimization of heat transfer device and analysis of heat and mass transfer on the finned multi-tubular metal hydride tank. Int. J. Hydrogen Energy 2012; 37:14292-14299.

[5] Wang H, Prasad AK, Advani SG. Hydrogen storage system based on hydride materials incorporating a helical-coil heat exchanger. Int. J. Hydrogen Energy 2014; 39:13583-13595.

[6] Zhen W, Fusheng Y, Zaoxiao Z, Zewei B. Magnesium based metal hydride reactor incorporating helical coil heat exchanger: Simulation study and optimal design. App. Energy 2014; 130:712-722.

[7] Chung CA, Chen YZ, Chen YP, Chang M. CFD investigation on performance enhancement of metal hydride hydrogen storage vessels using heat pipes. Appl. Therm. Energy2015; 91:434-446.

[8] Yuzhu Liu, Wang Hui, Ajay Prasad K, G. Advani S. Role of heat pipes in improving the hydrogen charging rate in a metal hydride storage tank. Int. J. Hydrogen Energy 2014; 39:10552-10563.

[9] Sekhar BS, Lototskyy M, Kolesnikov A, Moropeng ML, Tarasov BP, Pollet BG. Performance analysis of cylindrical metal hydride beds with various heat exchange options. Journal OF alloys and compounds 2015; 645: 589-595.

[10] Bao Z. Performance investigation and optimization of metal hydride reactors for high temperature thermochemical heat storage. Int J Hydrogen Energy 2015; 40:5664-5676.

[11] Garrier S, Delhomme B, De Rango P, Marty P, Fruchart D, Miraglia S. A new MgH2 tank concept using a phase change material to store the heat of reaction. Int. J. Hydrogen Energy 2013; 38: 9766-9771.

[12] Mellouli S, Ben Khedher N, Askri F, Jemni A, Ben Nasrallah S. Numerical analysis of metal hydride tank with phase change material. Applied Thermal Engineering 2015; 90: 674-682.

[13] Ben Mâad H, Miled A, Askri F, Ben Nasrallah S. Numerical simulation of absorption-desorption cyclic processes for metal-hydrogen reactor with heat recovery using phase-change material. Appl. Therm. Eng 2016; 96:267-276.

[14] Melouli S, Askri F, Abhilash E, Ben Nasrallah S. Impact of using a heat transfer fluid pipe in a metal hydride-phase change material tank. Appl. Therm. Eng 2017; 113:554-565.

[15] Al Mghari H, Huot J, Xiao J. Analysis of hydrogen storage performance of metal hydride reactor with phase change materials. Int. J. Hydrogen Energ 2019; 44:28893-28908.

[16] Alqahtani T, Bamasag A, Mellouli S, Askri F, Phelan P E. Cyclic behaviors of a novel design of a metal hydride reactor encircled by cascaded phase change materials. Int. J. Hydrogen Energy 2020; 45:32285-32297.

[17] El Mghari H, Huot J, Tong L, Xiao J. Selection of phase change materials metal foams and geometries for improving metal hydride performance. Int. J. Hydrogen. En 2020; 45:14922-14939.

[18] F. Askri, A. Jemni, and S. Ben Nasrallah, "Study of two-dimensional and dynamic heat and mass transfer in a metal hydrogen reactor," *Int J Hydrogen Energy.*, vol. 28, pp. 537–557, 2003.

[19] F. Askri, A. Jemni, and S. Ben Nasrallah, "Prediction of transient heat and mass transfer in a closed metal-hydrogen reactor," *Int J Hydrogen Energy.*, vol. 29, pp. 195–208, 2004.

[20] F. Askri, A. Jemni, and S. Ben Nasrallah, "Dynamic behavior of metal-hydrogen reactor during hydriding process," Int.J.Hydrogen.Energy, vol. 29, pp. 635-647, May 2004.

[21] A. Kumar, MP. Maiya, SS. Murthy, "Simulation of transient heat and mass transfer during hydrogen sorption in cylindrical metal hydride beds," Int J Hydrogen Energy,vol. 32, pp. 1969-1981, August 2007.

[22] A. Freni, F. Cipiti, and G. Gacciola, "Finite element-based simulation of a metal hydride-based hydrogen storage tank," Int.J.Hydrogen.Energy, vol. 34, pp. 8574-8582, October 2009.

[23] F. Askri, M. Ben Salah, A. Jemni, and S. Ben Nasrallah, "A new algorithm for solving transient heat and mass transfer in metal hydrogen reactor," *Int J Hydrogen Energy.*, vol. 34, pp. 8315–8321, 2009.

[24] SL. Garrison, BJ. Hardy, MB. Gorbounov, DA. Tamburello, C. Corgnale, BA. VanHassel et al, "Optimization of internal heat exchangers for hydrogen storage tanks utilizing metal hydrides," Int.J.Hydrogen.Energy, vol. 37, pp. 2850-61, 2012.

[25] H. Ben Mâad, F. Askri, and S. Ben Nasrallah, "Numerical investigation of heat and mass transfer during the desorption process of an Mg2NiH2 reactor," *Int J Hydrogen Energy.*, vol. 38, pp. 4597–4610, 2013.

[26] A. Singh, M. P. Maiya, and S. Srinivasa Murthy, "Effects of heat exchanger design on the performance of a solid state hydrogen storage device," *Int J Hydrogen Energy.*, vol. 40, pp. 9733–9764, 2015.

[27] S. Mellouli, N. Ben Khedher, F. Askri, A. Jemni, and S. Ben Nasrallah, "Numerical analysis of metal hydride tank with phase change material," *Appl Therm Eng.*, vol. 90, pp. 674–682, 2015.

[28] M. Valizadeh, M. Aghajani Delavar and M. Farhadi, "Numerical simulation of heat and mass transfer during hydrogen desorption in

ISSN: 1737-9296

metal hydride storage tank by Lattice Boltzmann Method," Int.J.Hydrogen.Energy, vol. 41, pp. 413-424, 2016.

[29] F. Bouzgarrou, F. Askri, A. Jemni, and S. Ben Nasrallah, "Numerical investigation of heat and mass transfer during the desorption process of a LaNi5-H2 reactor," *J Heat Transf*, vol. 138, pp. 1-7, 2016.

[30] S. Shaji, and G. Mohan, "Numerical simulation of the effect of aluminium foam on sorption induced wall strain in vertical, metal hydride based hydrogen storage container," *J alloys and compounds*, vol. 735, pp. 2675-2684, 2017.

[31] A. Chibani and Ch.Bougriou, "Effect of the tank geometry on the storage and destocking of hydrogen on metal hydride (LaNi5- H2)," Int J Hydrogen Energy, vol.42, pp.23035-23044, 2017.

[32] L. Tong, J. Xiao, P. Bénard, and R. Chahine, "Thermal management of metal hydride hydrogen storage reservoir using phase change materials," *Int J Hydrogen Energy*, vol. 44, pp. 21055-21066, 2019.

[33] T.Alqahtani, S.Mellouli, A.Bamasag, F.Askri and PE.Phelan, "Thermal performance analysis of a metal hydride reactor encircled by a phase change material sandwich bed," Int.J.Hydrogen.Energy, vol. 45, pp. 23076-23092, 2020.

[34] F. Bouzgarrou, F. Askri, H. Belhaj Ali and S. Ben Nasrallah, "Analyses of unsteady conduction-radiation heat transfer using unstructured Lattice Boltzmann Method," Int.J.Therm Sc, vol. 116, pp. 287-309, 2017.

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