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Study of the hydrogen absorption process in a Metal Hydrogen Reactor: Application of the unstructured Lattice Boltzmann Method

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***Abstract*— In this paper, the hydrogen absorption process in an $LaNi_5$ Hydrogen Reactor was studied. The energy equation was solved using the Control Volume Lattice Boltzmann Method by considering unstructured grids. To check the validity of the numerical approach, computational results were compared with those of the unstructured Control Volume Finite Element Method (CVFEM).We found that the new approach correctly predicts hydrogen absorption phenomena and has less CPU time compared to the CVFEM (about 8 times faster).**

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

I. INTRODUCTION

The study of heat and mass transfers within Metal Hydrogen Reactors (MHRs) were the field of interest of many researchers. Several numerical researches have been reported to study and intensify the heat transfer rates in MH beds. In these studies, various mathematical and numerical models are used. Using the Finite Volume Method (FVM), Askri et al. [1] 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-H2 alloy while they affect the transfer in the Mg-H2 system. Using the Control Volume Finite Element Method (CVFEM), Askri et al. [2] 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's 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 [3], 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. [4] studied the absorption hydrogen process using the Fluent software. In their study, they indicate that at the beginning of the process, the speed of the hydrogen absorption is so higher and by time, due to the increase of the temperature inside the reactor, the absorption speed decreases. Freni et al. [5] developed a three dimensional model of metal hydride beds filled with $LaNi_5$ alloy 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. [6] studied the discharge process of a 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 MHR. Garrison et al. [7] simulated a transverse and longitudinal fin designs of 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. [8] applied the CVFEM to predict heat and mass transfers in a 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. [9] presented a model to predict heat and mass transfers in a MHR equipped with an annular heat exchanger tube with radial circular copper fins. This model is based on the Comsol Multiphysics software. Mellouli et al. [10] 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 [11] investigated heat and mass transfer during hydrogen desorption in a metal hydride storage tank using the LBM. In a previous work, Bouzgarrou et al. [12] 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. [13] 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

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walls strain was investigated. Chibani et al. [14] studied the charge and discharge processes in a LaNi5 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 MmNi4.6Fe0.4 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. [15]. 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. [16] 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 geometries' configurations, the structured technique of mesh 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) [17], promoting both good accuracy with less computing time, to predict heat and mass transfer in a $LaNi_5$-H_2 reactor. The remainder of this paper is divided into three sections. We first describe the procedure of the discretization of the 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 reactor is filled with a $LaNi_5$ 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:

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

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

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 aborbed 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:

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

B. Numerical approach

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

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

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

Where the Control volume ΔV_N is expressed as follows [17]:

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

The calculation of the terms Q_1, Q_2, Q_3, Q_4 and Q_5 are detailed in a previous work [17].

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.

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 $(\rho_s, \rho_g, (\rho C_p)_{eff})$.
4- Compute the relaxation time τ.
5- Calculate the coefficients $CL_{i,N}^{i'}$ and γ_{i,N_j}.

6- Given the initial temperature field, compute the equilibrium distribution function, f_i^{eq}.
7- Calculate the first source term, Q4.
8- Calculate the hydrogen mass absorbed or desorbed.
9- Compute the second source term, Q5.
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, we consider a cylindrical Metal Hydrogen Reactor of a radius R = 2.5 cm and a height H = 6 cm that exchanges heat through its walls with a cooling fluid (Fig. 1).

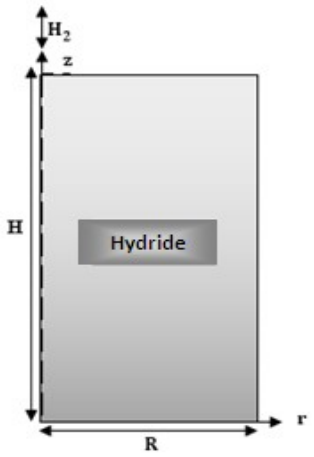

Fig. 1 Metal Hydrogen Reactor considered

Coupled heat and mass transfer was simulated numerically by the "CVLBM" approach and the results are compared with those of the unstructured CVFEM.

We investigated at first the effect of spatial grids on the temporal evolution of the hydrogen mass absorbed. The number of nodes is increased from 502 to 1874 and as shown in Fig.2, on 1560 nodes and beyond the maximum variation of the mass is less than 10^{-3}.

Then, considering 1560 nodes, we plot in fig.3 a-b, respectively, the time evolution of the hydride temperature and the hydrogen mass absorbed. The comparison of the 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.

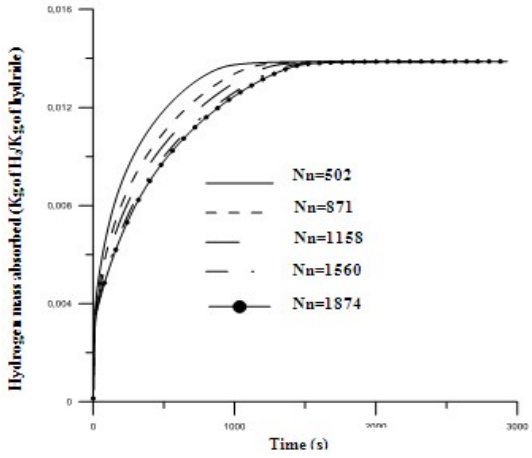

Fig. 2 Temporal evolution of the hydrogen mass absorbed for different number of nodes

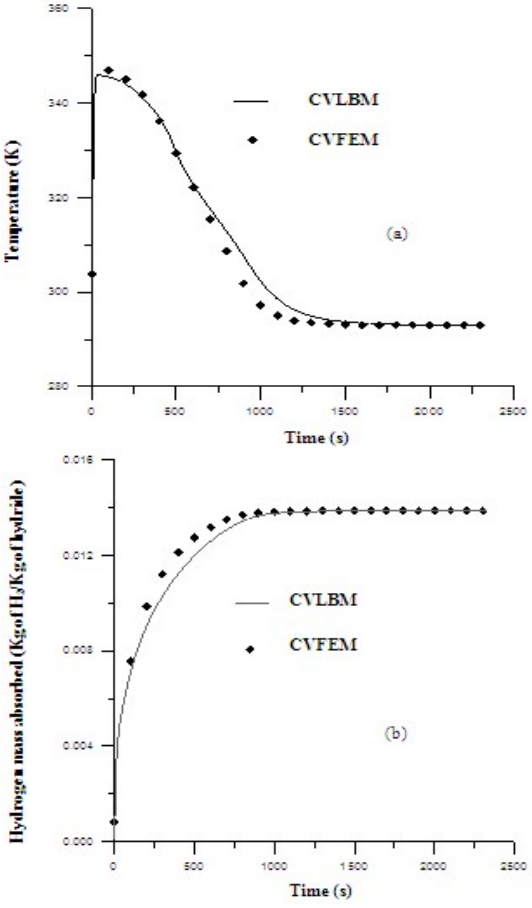

Fig. 3 Temporal evolution of (a) the hydride temperature and (b) the hydrogen mass absorbed

The evolution of temperature along the axis of symmetry (r = 0) and at different times is also plotted in Fig.4. The profiles obtained by the CVLBM and the CVFEM are in a good agreement. This agreement is well proven in Fig. 5 corresponding to the evolution of isotherms at different representative times. It is seen that temperature increases in the reactor since the absorption process in metals is

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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 cooling fluid.

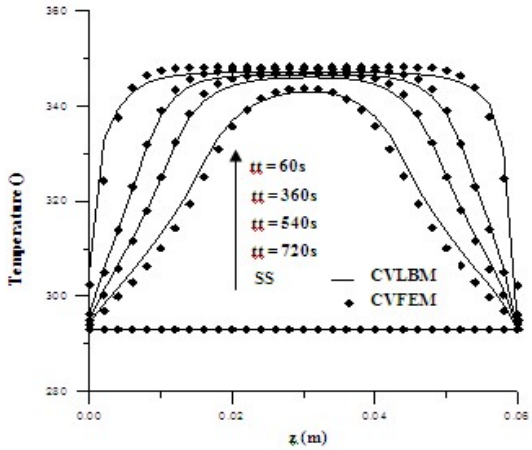
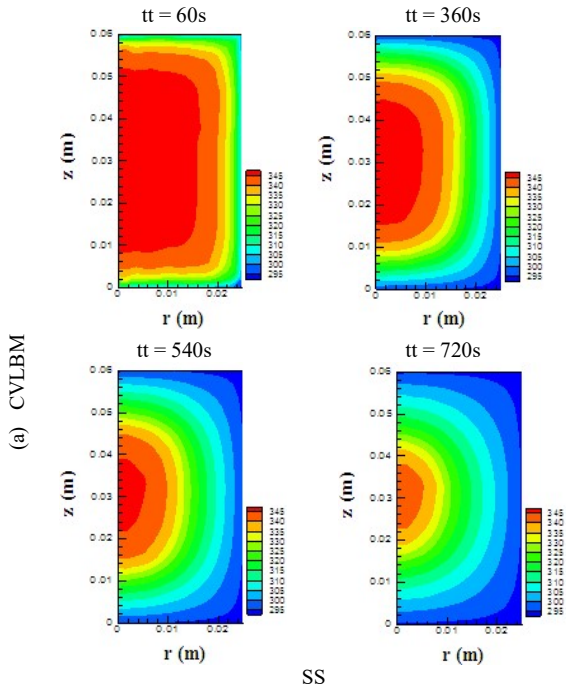


Fig. 4 Temporal Evolution of temperature along the axis of symmetry

Besides the stability and the accuracy of the numerical approach, the CVLBM is eight times faster than the CVFEM (Table 1) using the same Intel® core (TM) i7 CPU 2.4 computer. We found that the obtained results are comparable with those of the CVFEM and this agreement proves that the CVLBM can correctly describe the physical phenomena in the reactor.



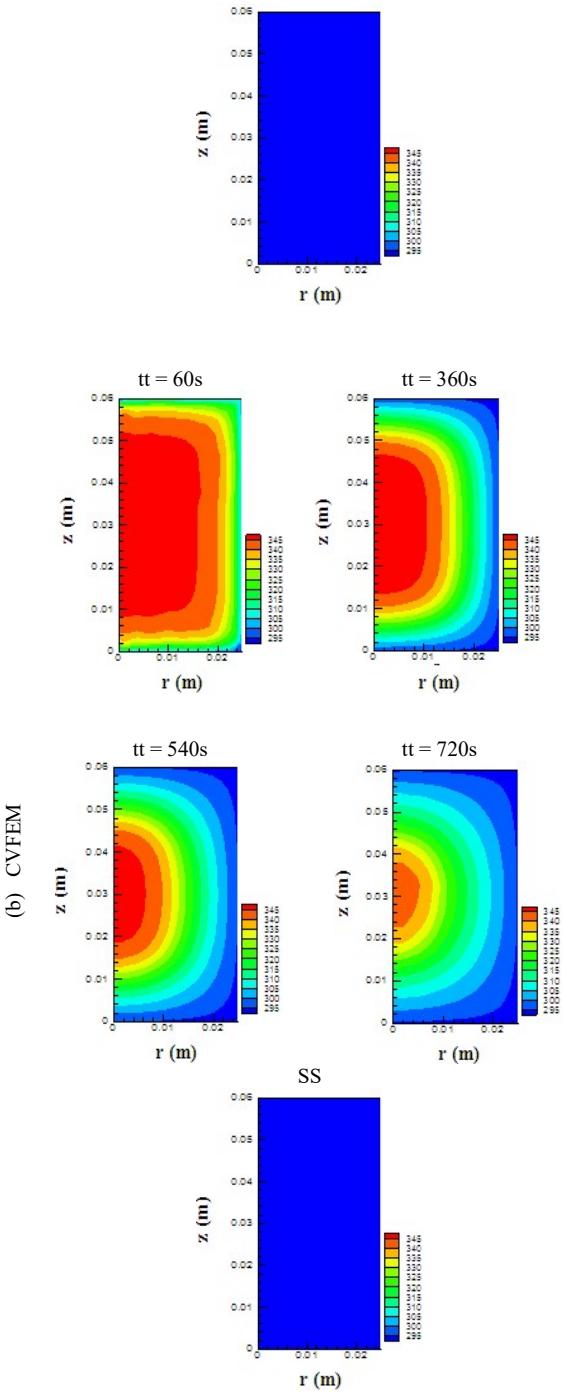


Fig. 5 Contours of the temperature at different times (a) CVLBM, (b) CVFEM

TABLE I
Comparison of CPU times

	CPU time (s)
CVLBM	12.57
CVFEM	97.03

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V. CONCLUSIONS

In this study, a numerical approach based on the unstructured Lattice Boltzmann Method "CVLBM" is applied 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 (8 times faster). In a following work, the CVLBM will be applied to simulate heat and mass transfers in MHRs of complex geometric shapes in order to check its computational efficiency.

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