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Numerical Heat and Mass Transfer Investigation of Hydrogen Absorption in an Annulus-Disc Reactor

Ali Boukhari[#,*1], Rachid Bessaïh[#2], Merouane Zedayria[#3]

[#]*LEAP Laboratory, Constantine 1 Univ., Constantine 25000, Algeria*
[1]fibonali2379@gmail.com
[2]bessaih.rachid@gmail.com
[3]merwane.zedayria@gmail.com
[*]*Department of Mechanical Engineering, El-Oued Univ., El-Oued 39000, Algeria*

***Abstract*— This work presents a numerical investigation of two-dimensional coupled heat and mass transfer process in a $LaNi_5$-based annulus-disc reactor, during hydrogen absorption using the commercial software FLUENT 6. Temperature and amount of hydrogen absorbed profiles inside the metal hydride bed, variation of average bed temperature and hydrogen storage capacity are presented for different reactor design configurations and different cooling tube radii, respectively. Numerical simulations revealed that the hydriding process time for the $LaNi_5$ alloy depends on the configuration and geometrical dimensions of the tubular heat exchange device, and moreover on the overall hydride formation. The question of minimizing the hydriding time is reduced to the accommodation of the amount of heat removed from the bed reactor. A good agreement was found between the present computational results and the experimental data reported in the literature.**

***Keywords*— Numerical Simulation, Metal hydride, Absorption, Coupled heat and mass transfer.**

I. INTRODUCTION

In many practical applications, the use of hydrogen as a fuel in the framework of renewable energies is limited by the constraints issued from the problems of storage and transport. The automotive industry must deal with many on-board hydrogen storage techniques or methods including compressed hydrogen, solid state systems (for instance metal hydrides, surface adsorption of hydrogen molecules) and liquid hydrogen, to appreciate a hydrogen-powered vehicle as an economical and sustainable surrogate for existing vehicles. The techniques of metal-hydrides-based hydrogen storage offer high volumetric density compared to that of liquid hydrogen, but unfortunately has low hydrogen absorption capacity [1]. The storage technique and requirements can be adapted to the application. Some applications require a lower quantity of hydrogen compared to others. However more to their disadvantages of weight and cost, metal hydrides have another disadvantage which is their limited kinetics because they release/absorb huge amounts of heat whereas hydriding/dehydriding process, thus the rate of hydrogen absorption/desorption process is restricted by the hydride's thermal properties mainly thermal conductivity and related cooling or heating techniques respectively. This causes serious challenges to the thermal management of the hydriding/dehydriding process [2]. The performances of metal-hydrides-based storage systems are measured by the rates of hydrogen absorption or desorption whose depend on the rate at which the amount of heat is removed or furnished to the metal hydride managed system.

Research on the design and performance optimization of the metal hydride (MH) reactors is essential for the efficient operation of corresponding systems in many industrial applications beside the hydrogen storage, notably heat pumps and thermal compression, etc., thus the configuration is the extremely imperative part in the design of a MH reactor[3-5].

In the light of the above, the present work involves a numerical study of an annulus-disc reactor (ADR) unit where the metal hydride alloy is packed in. In which the mass transfer takes place between the hydrogen gas supplied by the inner tube and the alloy or metal hydride packed inside the disc unit. At the same time, heat transfer occurs between the annulus-disc unit on one hand, and the cooling fluid outside it and the tubes inside it, on the other hand. In MH applications there are a plethora of bed reactors. Computations of this numerical investigation are performed by using the commercial CFD software FLUENT 6, while adopting the two-dimensional mathematical model of Jemni and coworkers [3] to show and analyse the influence of heat exchange devices and their geometrical dimensions on hydriding temperature fields of the metal-hydrogen bed reactor, and on the overall hydride formation too.

II. MATHEMATICAL MODEL

The mathematical model for the annulus-disc reactor (exposed schematically in Fig. 1) considered in the present work is similar to that of Jemni and Ben Nasrallah [3], with $LaNi_5$ as metal hydride alloy. The unit disc reactor considered is composed of a solid phase (metal-powder) and a gaseous phase (hydrogen), thus forming a porous medium.

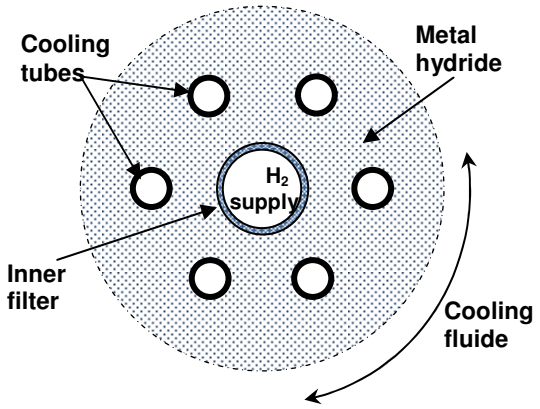

Fig. 1 Schematic of the studied metal hydride reactor.

A. Volume-Averaged Continuity Equation for Hydrogen Gas

$$\varepsilon \frac{\partial \rho_g}{\partial t} + \frac{\partial}{\partial x}(\rho_g u) + \frac{\partial}{\partial y}(\rho_g\ v) = -\dot{m} \tag{1}$$

The gas density ρ_g is deduced from the perfect gas model

$$\rho_g = \frac{P_g M_{H2}}{R_g T} \tag{2}$$

where M_{H2} and R_g denote the molecular mass of hydrogen and the universal gas constant respectively.

B. Volume-Averaged Mass Balance Equation for Metal Alloy

$$(1-\varepsilon)\frac{\partial \rho_s}{\partial t} = \dot{m} \tag{3}$$

C. Volume-Averaged Momentum Equations for The Gas

In the x-direction,

$$\rho_g \frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \rho_g\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) + S_{Dx} \tag{4}$$

In the y-direction,

$$\rho_g \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) - \rho_g\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) + S_{Dy} \tag{5}$$

D. Volume-Averaged Energy Equation

$$\begin{aligned}(\rho C_p)_e \frac{\partial T}{\partial t} = {} & \frac{\partial}{\partial x}\left(\lambda_e \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_e \frac{\partial T}{\partial y}\right) - (\rho_g C_{pg} u)\frac{\partial T}{\partial x} \\ & - (\rho_g C_{pg} v)\frac{\partial T}{\partial y} - \dot{m}(\Delta H - T(C_{pg} - C_{ps}))\end{aligned} \tag{6}$$

with the effective volumetric heat capacity :

$$(\rho C_p)_e = \varepsilon \rho_g C_{pg} + (1-\varepsilon)\rho_s C_{ps} \tag{7}$$

and the effective thermal conductivity is taken as :

$$\lambda_e = \varepsilon \lambda_g + (1-\varepsilon)\lambda_s \tag{8}$$

E. Reaction Kinetics

$$\dot{m} = -C_a \exp\left(-\frac{E_a}{R_g T}\right)\ln\left(\frac{P_g}{P_{eq}}\right)(\rho_{sat} - \rho_s) \tag{9}$$

P_{eq} is the equilibrium pressure calculated using the van't Hoff relationship

$$\ln\left(\frac{P_{eq}}{P_0}\right) = A - \frac{B}{T} + \varphi_{slp}(\xi - \xi_0)) + \varphi_{hys} \tag{10}$$

F. Initial and Boundary Conditions

At $t = 0$; $P(x,y,0) = P_0$, $T(x,y,t) = T_0$, *and* $\rho_s(x,y,t) = \rho_0$.

For $t > 0$;

- At the hydrogen inlet (the inner central tube) :
$$P(x,y,0) = P_0, \quad T(x,y,t) = T_0 \tag{11}$$
- The lateral cooling wall :
$$-\lambda_e \frac{\partial T}{\partial \vec{n}}(x,y,t) = h(T - T_f) \tag{12}$$
where h is the wall heat transfer coefficient taken from [4], and T_f is the temperature of the cooling fluid.
- The isothermal cooling tubes :
$$T(x,y,t) = T_f \tag{13}$$
- The other boundary conditions are assumed to have the symmetry condition type.

III. Results and Discussion

Firstly, before showing and discussing the obtained results, we have carried out some simulations for the validation of the considered model in comparison with the experimental data present in literature, especially those from the work of Jemni *et al*. [4], in which a cylindrical $LaNi_5$–H_2 reactor was investigated. Fig. 2 shows the temperature evolution in the metal bed in three different points within the reactor.

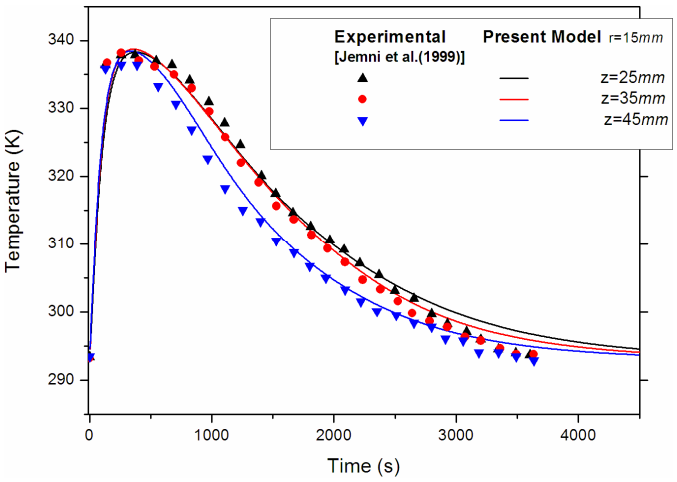

Fig. 2 Temperature evolution at three points within the cylindrical MH tank experimented by Jemni et al. [4] in the hydriding case with the cooling fluid temperature at 20°C.

The temperature of the cooling fluid and the pressure are $T_f = 20°C$ and $P=8bars$ for the absorption case. The temperatures show a rushed rise in the metal bed at the beginning, because the hydrogen-metal reaction is exothermic then decrease gradually with the reaction kinetics decay. The simulation results are in good agreement with the experiments, conceding that the model can be used for further investigations of the transient thermal–fluid behavior in MH reactors.

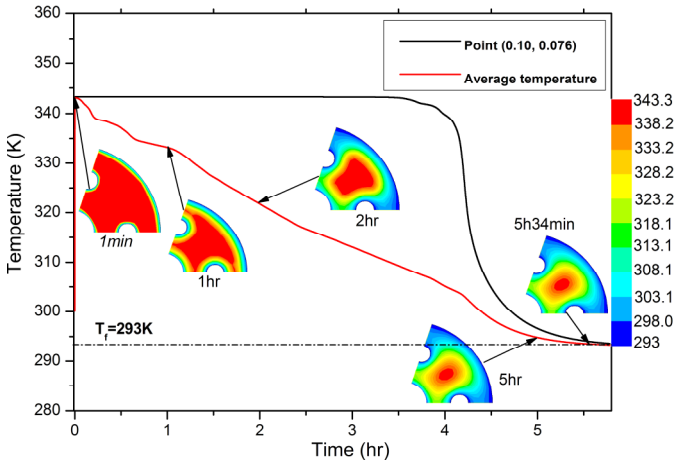

Fig. 3 Temperature evolution at the point x= 0.10, y= 0.076 within the reactor, plotted with the averaged bed temperature and contours of temperature.

Fig. 3 shows the temperature evolution at the monitoring point $(x, y) \equiv (0.10, 0.076)$, and the average bed temperature inside a selected five tubes-cooled reactor. Initially, the temperature of the bed is assumed to be the same as the cooling fluid ($T_0 = 293K$). From the temperature contours thumbnails presented on top of the Fig. 3 we can see easily that the maximum temperature value is quickly reached over the bulk of the bed, this is due to the abrupt heat release in the metal bed, and then decrease progressively beneath the work of the cooling process. The temperature history of the monitored point (0.10, 0.076) let us see that the maximum values of temperature stand for a long periods of time before decreasing to reach the cooling fluid temperature.

TABLE I
COORDINATES OF THE MONITORING POINTS WITHIN THE MH BED REACTOR.

	S_1	S_2	S_3	S_4	S_5
x	0.089	0.061	0.092	0.158	0.106
y	0.052	0.027	0.094	0.106	0.067

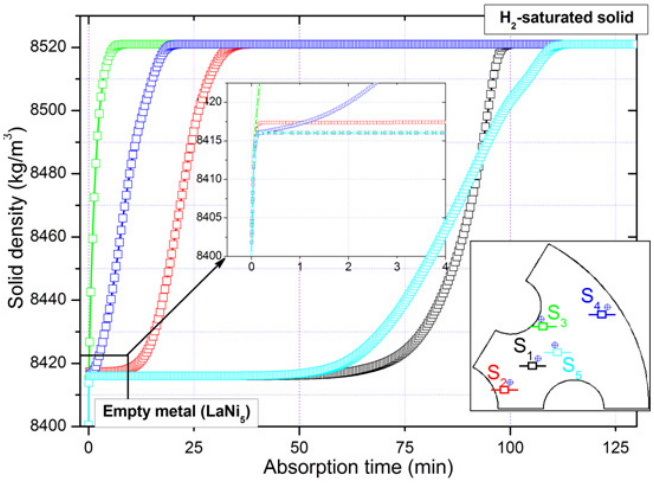

Fig. 4 Solid density history at selected monitoring points.

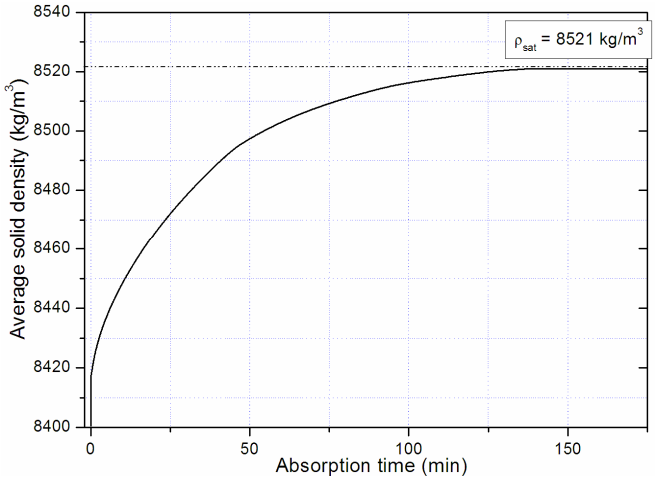

Fig. 5 Averaged solid density evolution.

From Figs. 4-5 we can observe that the solid density attains its maximum value $\rho_{sat} = 8521 kg/m^3$, and the metal alloy becomes a hydride (H_2-saturated solid, $LaNi_5H_6$) in almost the first 150 minutes after the beginning of the hydriding operation, besides the fact that the reaction kinetics differ for different regions inside the bed. An outstanding fact seen in all the monitoring data points (Fig. 4), is the abrupt

increase in solid density after few seconds from the reaction start, before it behave normally (obeying the reaction kinetics), this fact is due to the high reaction rate value $\dot{m}$, which is proportional to the difference $\rho_{sat} - \rho_s$, being maximum at the hydriding process start where $\rho_s - \rho_{emp} = 8400 kg/m^3$.

IV. Conclusion

In this study, hydrogen absorption in metal hydride bed is numerically investigated in an annulus-disc reactor. A two-dimensional mathematical model describing the transient coupled heat and mass transfer in the hydride bed during the absorption process of hydrogen has been adopted. The temperature of the bed rises during the hydriding operation, and a cooling device must be taken into consideration to remove the amount of heat released, as well as increasing the hydride formation rate. For that reason the system must be efficiently cooled for a quicker absorption process. The numerical results showed good accordance with the experimental data reported in the literature. By investigating the effects of the number and dimension of cooling tubes respectively on hydriding time and mass transfer, this study also revealed that the additions of more cooling tubes and/or increasing their radii enhance significantly the heat and mass transfer, and reduce the hydrogen absorption time by about 60% in an ADR configuration having 6 cooling tubes compared to a reactor equipped with 4 cooling tubes, and 50% of that using 5 tubes. Nevertheless, an optimization approach should be conceded in aim to efficiently design this metal-hydrogen reactor type.

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