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Numerical Study of Metal Hydride Beds with LaNi4.88Al0.12 Alloy for Hydrogen Compression

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Abstract

The adsorption of hydrogen energy as a renewable energy carrier is particularly attractive because of the enormous demand for energy and the accelerated depletion of fossil fuel resources, so the development of an efficient technique for its storage is essentially essential. In the future, hydrogen energy appears to be an attractive substitute for fossil fuels like coal and oil. Because of its energy value, hydrogen energy is advantageous because it is renewable and its use would reduce the emission of pollutants into the environment. However, the problem of storing and transporting hydrogen efficiently and safely prevents its wide use and commercialization.

The LaNi4.88Al0.12 data show that heat transfer to and from the hydride bed significantly affects the hydrogen reaction duration in metal-hydride reactors (MHRs). In this work, the operational parameters of the heat exchanger were evaluated numerically to ascertain their impact on the MHR charging process's performance. The reactor's charge time is greatly shortened when the effects of various parameters (cooling fluid (T_F) temperature, applied hydrogen (P_{H2}) pressure in absorption and desorption cases) are examined and the results indicate that careful selection of these parameters is critical.

Keywords : Hydrogen; Metal-hydrogen reactor, hydrogen storage, $LaNi_{4.88}Al_{0.12}$, absorption, adsorption

1.INTRODUCTION

Heat transmission to/from the hydride bed has a significant impact on the reaction time of hydrogen in metal hydride tanks. To enable renewable energies to become a regular part of our lives, hydrogen as an energy vector is also an option that is being carefully explored globally. different methods are being investigated for hydrogen production Numerous obstacles remain to be addressed, including those related to production, storage, and operation. Alloys that absorb hydrogen have industrial uses, such as chemical heat pumps, chemical compressors, and hydrogen storage. High volumetric density, reversibility, and significant heat generation during the absorption process are the key requirements for these alloys [1,23]. The design and energy conversion of the metal hydride system depends heavily on the dynamic response of such a hydrogen storage system. Nevertheless, in the case of metal hydrides, the efficiency of hydrogen absorption and desorption is dependent on the heat transport in the metal hydride bed as well as the type of material being investigated for various elements of hydrogen storage. Using a one-dimensional mathematical model, Gopal et al. [2, 3] Mayer et al. [4] and S. Belkhiria et al [24] investigated transient heat and mass transfers in the reactor. In order to study absorption and desorption processes, Jemni and Ben Nasrallah [5,6] looked at two-dimensional heat and mass transfer in a metal-hydrogen reactor. Shmalkov et al. [7] examined the sorption process for combinations including inactive or weakly active impurities for the hydride-forming substance. Numerical studies of three-dimensional heat and mass transfers in a metal hydride bed during absorption were conducted by Mat et al. [8] and Aldas et al. [9]. To ascertain the metal-hydrogen reactor's effective thermal conductivity, equilibrium pressure, and reaction kinetics, Jemni et al. [10] conducted an experimental and numerical investigation. Hydrogen absorption was experimentally investigated in two LaNi5-H2 reactors by Demircan et al. [11].

In addition to studying two innovative cooling designs that involved adding more heat exchangers to an annular ring and a concentric inner tube inside the tank, Eustathios et al. [21] optimized hydrogen storage in metal hydride beds. Kaplan [12] conducted research recently on how different charge pressures affect the way heat transfer mechanisms affect metal hydride reactor charging. Three distinct cylindrical reactors are designed and produced, all sharing the same fundamental dimensions. According to experimental findings, heat transfer is the primary factor in metal-hydrogen reactor charge, and reactors with superior cooling have faster charging rates. A novel kind of metal hydride tank with a spiral heat exchanger was devised and produced by Mellouli et al. [13], who also reported a considerable reduction in the charging and discharging periods. Dhaou et al. [14] studied and modeled the hydrogen sorption kinetics by LaNi5 and two related pseudobinary compounds in a recent study. For a hydrogen storage tank containing LaNi5, Melnichuk et al. [15] adjusted the heat transmission fins' aluminum fraction at various absorption times and reactor diameters. A model was developed by Askri et al. [16] to examine the dynamic behavior of several reactor models.

According to optimization results, incorporating a concentric heat exchanger tube with fins and a cooling fluid fill can result in an approximate 80% improvement in reaction time. All of these investigations have demonstrated that heat transport from and to the hydride bed has a significant influence on the charge/discharge timings of metal-hydrogen reactors. Therefore, by incorporating the copper wire network structure [17] into the hydride bed with a multilayer corrugated sheet structure, several attempts have been made to increase the effective heat conductivity of metal hydride beds. Additional research looks at compact metal hydride powder with expanded graphite [19], compact metal hydride microencapsulated metal hydrides [18], and inserting aluminum foam [20]. One significant way to enhance the absorption and desorption processes is by incorporating fins into the hydride bed. All this provides a broad overview of solid-state hydrogen storage alloys based on absorption and their salient characteristics, which can help the scientific community gain valuable understanding [25].

SoThe present research presents a numerical study of a metal-hydrogen reactor at various pressures and temperatures during absorption and desorption .to investigate the effect of operating factors on hydrogen sorption performance in a metal hydride reactor process and can offer insight into how they can be improved.

2. Mathematical model

The equations governing the transfer of heat and mass in the tank (fig. 13) are given as follows:

$$(\rho C_p)_{ef}\frac{\partial T}{\partial t}=\frac{\lambda_{ef}}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\lambda_{ef}\frac{\partial^2 T}{\partial z^2}+m\Delta H+\dot{m}T(Cp_g-Cp_s) \tag{1}$$

Or:

$$(\rho C_P)_{ef}=\varepsilon\rho_g C_{pg}+(1-\varepsilon)\rho_s C_{ps} \tag{2}$$

$$\lambda_{ef}=\varepsilon\lambda_g+(1-\varepsilon)\lambda_s \tag{3}$$

Absorption case

$$\dot{m}=C_a\exp\left(-\frac{E_a}{RT}\right)\ln\left(\frac{P}{P_e}\right)\frac{\rho_s}{M_s}\left\{\left(\frac{H}{M}\right)_{SS}-\frac{H}{M}\right\} \tag{4}$$

Desorption case

$$\dot{m}=C_d\exp\left(-\frac{E_d}{RT}\right)\frac{P-P_e}{P_e}\frac{\rho_s}{M_s}\left(\frac{H}{M}\right) \tag{5}$$

The equilibrium pressure is given by:

$$P_e = f\left(\frac{H}{M}\right)\exp\left(\frac{\Delta H}{R_g}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right) \tag{6}$$

Where P_e is the equilibrium pressure at the reference temperature.

The coefficients (absorption/desorption) of the function f are given in table 1 [22].

Coefficients	**b$_0$**	**b$_1$**	**b$_2$**	**b$_3$**	**b$_4$**	**b$_5$**	**b$_6$**	**b$_7$**	**b$_8$**	**b$_9$**
Abs	0.0072	15.2	-33.579	40 .1	-25.882	10.89	-2.7541	0.412	-0.0421	0.0018
Des	-1.389	18.1	-41 .896	48.91	-32.96	14.43	-3.8632	0.654	-0.04563	0.0032

Table 1. The coefficients of the polynomial

The H_2 is supposed to be an ideal gas. The pressure of the hydride after an interval of time dt is given by:

$$P_{b,t+dt} = \frac{n_{t+dt} R T_{g,t+dt}}{V_r} \tag{7}$$

where, V_r, n_{t+dt} and $T_{g,t+dt}$, are the tank's volume, the number of moles of hydrogen, and the temperature of the hydrogen gas in the tank at time dt, respectively.

The number of the mole of hydrogen is obtained from the material balance.

Absorption case: $n_{t+dt} = n_t - \Delta n_{dt}$ (8)

Desorption case: : $n_{t+dt} = n_t + \Delta n_{dt}$ (9)

To solve these equations, we will consider the following hypotheses:

- Respectively turn is considered rotary.
- The tube has constant thermal conductivity.

Performing the energy balance for each turn on the control volume (Fig. 1) yields:

$$\dot{m}_w C_{p,w}(T_{water}(z+\Delta z) - T_{water}(z)) + h_i . A_i (T_{water,av} - T_{wall}) = 0 \tag{11}$$

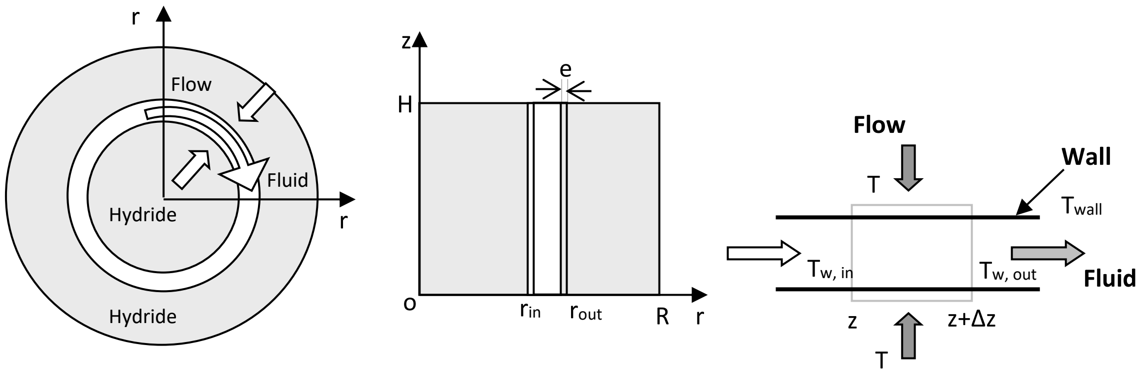

Figure 1. Calculation of domain and volume elements

Where $\dot{m}_w$ is the flow amount of heat transfer liquid, C_{pw} is the specific heat of the liquid, h_i is the internal heat transmission coefficient on the tube side, A_i is the interior surface zone, T_w and T_{wall} are the cooling temperatures of heat transfer fluid and wall respectively, $T_{w,_{av}}$ is the middling temperature.

$$T_{w,av} = \frac{T_{water}(z+\Delta z)+T_w(z)}{2} \tag{12}$$

The heat transfer rate transferred from the hydride can be calculated by:

$$h_i A_i \left(T_{water,av} - T_{wall}\right) = \frac{T_{wall\_}T(z,r_{in})}{R_{tube}} \tag{13}$$

Where $T(z,r_{in})$ is the hydride temperature on the surface of the exchanger and is the thermal resistance of the spiral tube:

$$R_{tube} = \frac{Ln\left(\frac{r_{out}-r_{in}}{r_{out}-in-2e}\right)}{2\pi^2\lambda_{tube}(r_{in}+r_{out})} \tag{14}$$

The interior surface A_i, is:

$$A_i = 2\pi^2(r_{out} - r_{in} - 2e)(r_{in} + r_{out}) \tag{15}$$

The wall temperature is obtained using eqs (12) and (13):

$$T_{wall} = \frac{T(z,r_{in})}{h_i A_i R_{tube}+1} + h_i A_i R_{tube}\left(\frac{T_w(z+\Delta z)+T_w(z)}{2(h_i A_i R_{tube}+1)}\right) \tag{16}$$

Substituting Eq. (16) in Eq. (11) we obtain:

$$T_{water}(z + \Delta z) = \alpha T_{water}(z) + \beta T(z, r_{in}) \tag{17}$$

Where $\alpha = \dfrac{2\dot{m}_w C_{P_w}\left(h_i A_i R_{tube}+1\right) - h_i A_i}{2\dot{m}_w C_{P_w}\left(h_i A_i R_{tube}+1\right) + h_i A_i}$ and $\beta = \dfrac{2h_i A_i}{\dot{m}_w C_{P_w} 2\left(h_i A_i R_{tube}+1\right) + h_i A_i}$ (18)

3. Initial and boundary conditions

We initially consider that the temperature and pressure are constant:

$$P(r,z,0)=P_0\ ,\ T(r,z,0)=T_0 \tag{19}$$

The boundary conditions depend on the heat exchanger configuration. In our study the boundary conditions are as follows:

For r = 0 $$\frac{\partial T}{\partial r}(0,z,t)=0 \tag{20}$$

For z = 0 $$\lambda_e \frac{\partial T}{\partial z}(0,r,t)=h_0.(T-T_\infty) \tag{21}$$

For r = R $$-\lambda_e \frac{\partial T}{\partial r}(z,R,t)=h_w.(T-T_{w,c}) \tag{22}$$

For z = H $$-\lambda_e \frac{\partial T}{\partial z}(H,r,t)=h_1.(T-T_\infty) \tag{23}$$

3. Numerical validation of the model

The finite volume method (MVF) is used to solve the system of equations numerically. This approach has the benefit of guaranteeing flow conservation. To validate our calculation code, we compared the results obtained numerically to experience. Good agreement between numerical and experimental results (Fig.2).

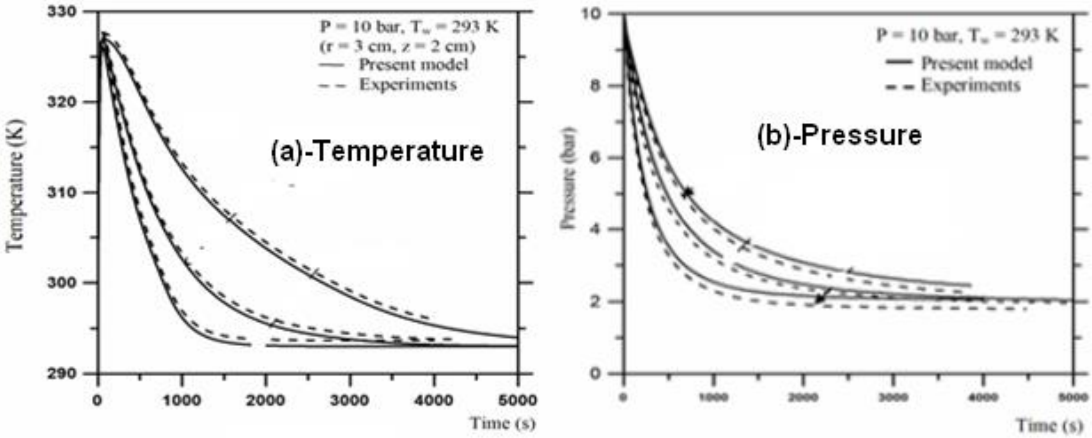

Figure 2. Model validation

4. Results and discussions

This section aims to investigate the effects of hydrogen injection pressure (P_{H2}) and cooling fluid temperature (T_F) on the rate of hydrogen absorption and desorption. The proposed mathematical model was initially validated by simulations, and only after that was it compared to the experimental results. The findings show the mass evolution contours in the cylindrical bed for various hydrogen absorption times.

4.1 Absorption Case

4.1.1 Variation of fluid temperature on absorption kinetic

For temperature (290K, 320K ,330K and 340K), together with the same operational parameters in each case, are taken into consideration to evaluate the impact of refrigeration liquid temperature on the absorption case. The findings depicted in Figs. 3a and 3b illustrate that although the exothermic character of the reaction may be the cause of the decrease in the mass of hydrogen absorbed when the temperature rises. Heat release during absorption is hampered by the decrease in the temperature gradient between the hydride bed and the external environment caused by the initial temperature increase. As a result, the reaction rate drops. low temperature can speed up a process, but the overall mass absorbed is unaffected. It's also crucial to remember that lowering the cooling temperature below a particular point has no significant impact.

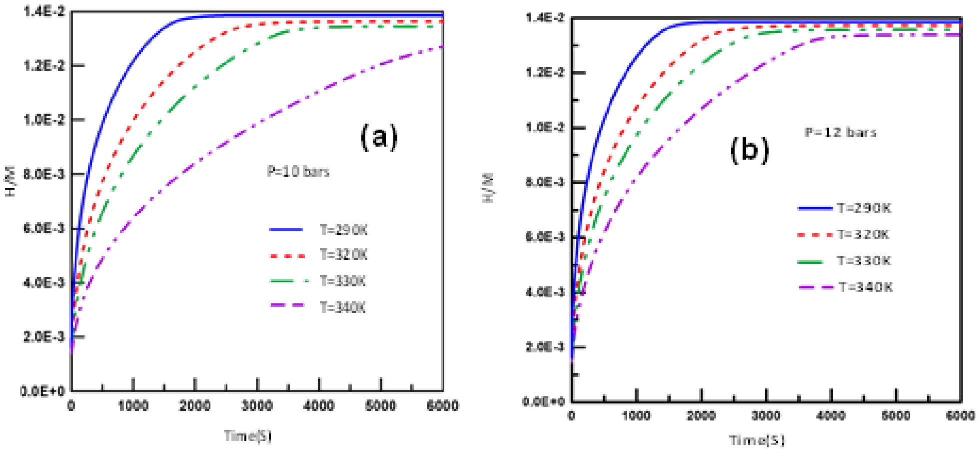

Figure 3. Effect of the cooling temperature on the absorption hydrogen kinetics, at (a) P=10bars and (b) P=12bars.

Regarding the time parameter (Fig 3.a and Fig 3.b), it can be concluded that time has a significant effect on the kinetics of the absorption and desorption reaction for a constant temperature and pressure. the storage time decreases if the temperature decreases and the pressure increases.

4.1.2 Effect of hydrogen pressure

The decrease in pressure gas (Figs. 4a and 4b) at constant temperature impacted the hydrogen (H/M) concentration. As a matter of fact, when pressure drops, so does the hydrogen concentration.

represents the effect of the applied initial pressure of hydrogen at constant temperature on the hydrogen absorption mass. The initial pressure influenced the absorbed hydrogen mass and the reaction's rate. If the pressure increases, the concentration of hydrogen and the reaction rate increase, too.

This is could be explained by the increase of the gradient of pressure between the equilibrium pressure and the initial pressure. In fact, in order to ensure sufficiently quick hydrogen charging, the charging pressure needs to be kept higher enough than the equilibrium pressure. This is made clear by the fact that mechanical pressures cause the interstitial sites' size to increase in response to an increase in pressure.

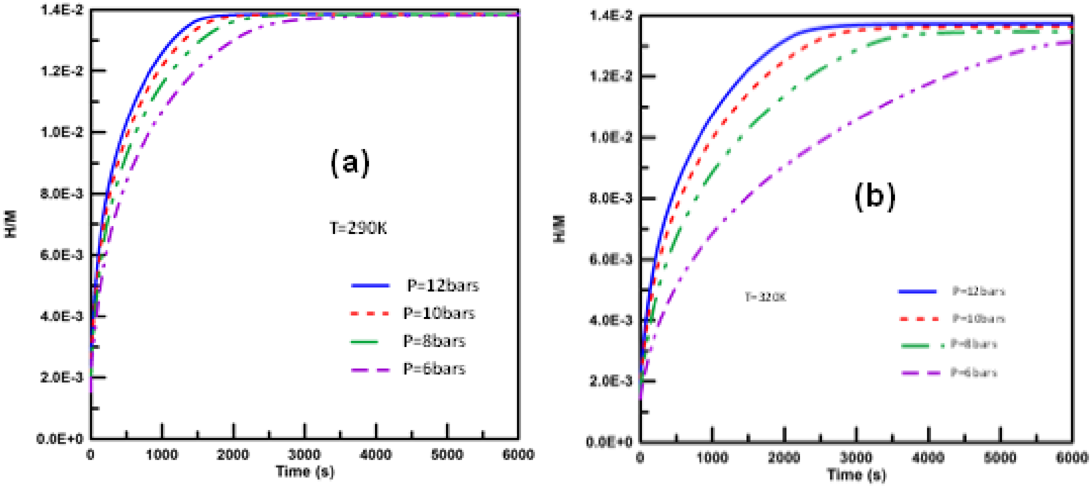

Figure 4. Effect of the gas pressure on the absorption hydrogen kinetics at (a) T=290K and (b) T=320 K.

4.1.3 Effect of hydrogen pressure and fluid temperature

Figures 5 and 6 show that upon increasing the hydrogen pressure and reducing the initial temperature, from now, its consequences in a debauched charging time for the entire to saturate, and this increases the speed of the absorption process.

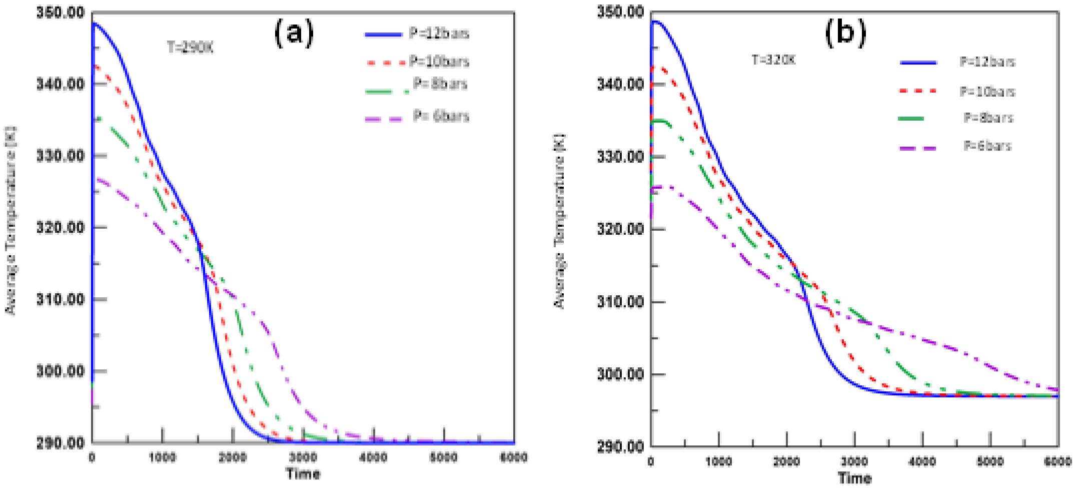

Figure 5. Effect of the hydrogen gas pressure on the absorption case, at (a) T=290K and (b) T=320K

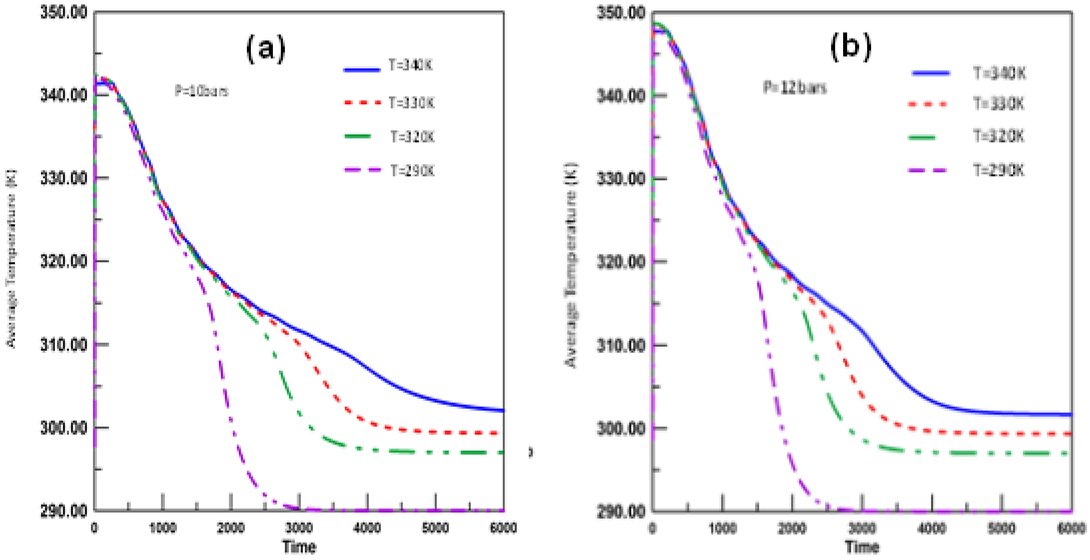

Figure 6. Effect of the fluid temperature on the absorption case, at (a) P=10 bars and (b) 12 bars.

4.2 Desorption case

4.2.1 Effect of the heating temperature

Due to the reaction's endothermic nature, the mass of hydrogen adsorbed increases as temperature rises. The release of heat during the adsorption reaction is made easier by increasing the starting temperature because it widens the temperature difference among the hydride layer and the surrounding air. The reaction rate then quickens. Figs 7 shows the impact at four values, 320, 330, 340 and 350 K, of initial temperature on the desorption rate.

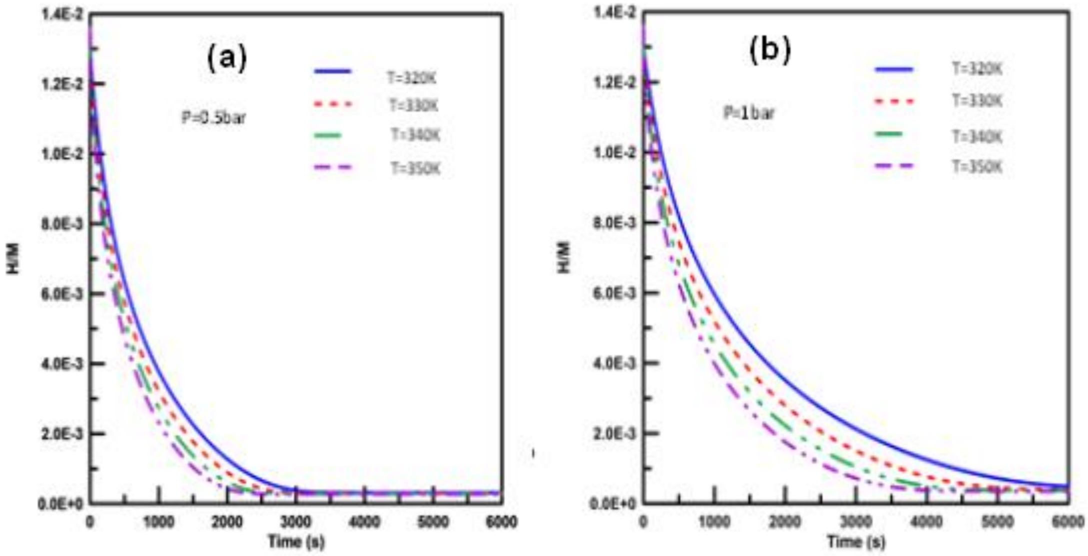

Figure7. Effect of the heating fluid temperature on the desorption hydrogen kinetics, at (a) P=0.5 bar and (b) P=1 bar.

4.2.2 Effect of the hydrogen pressure

Figures 8 demonstrates that when pressure decreases (0.5bar, 1bar,1.5bar and 2 bar) the process of desorption becomes more efficient. Because of the increased pressure gradient and hydrogen's propensity to desorb, the system's temperature decreases because the endothermic reaction is more effective.

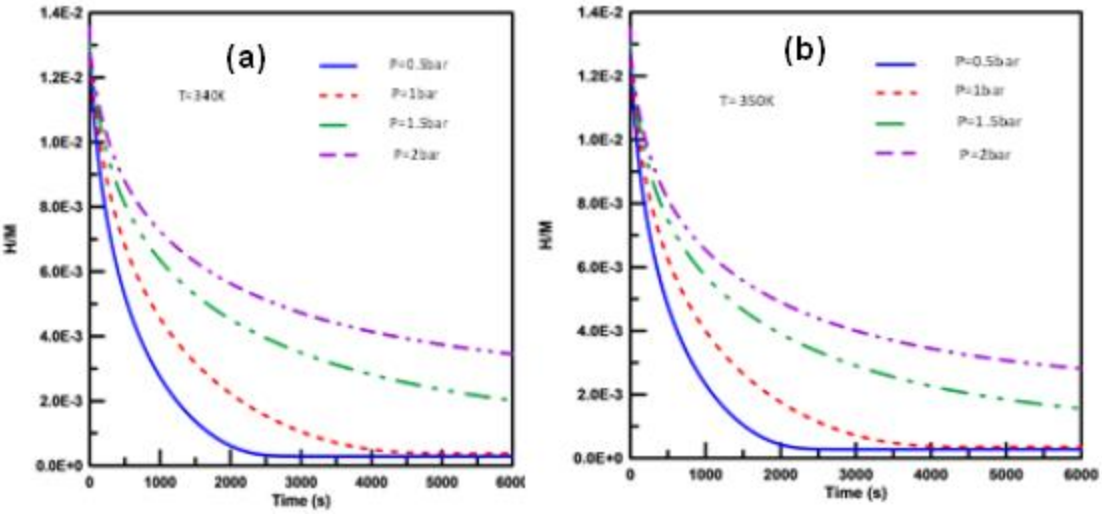

Figure 8. Effect of the hydrogen gas pressure on the desorption hydrogen kinetics at (a) T=340 K and (b) T=350 K.

4.2.3 Effect of hydrogen pressure and water temperature

Figures 9 and 10 indicate that upon decreasing the pressure and increasing the water temperature, Hence, it results in a fast-discharging time for the entire to dehydrated, and this increases the speed of the desorption process.

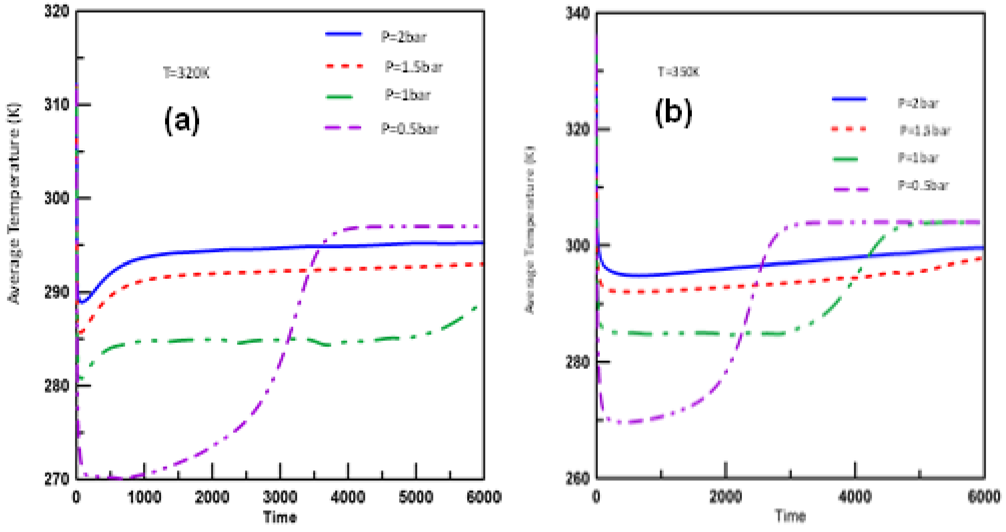

Figure 9. Effect of the hydrogen gas pressure on the desorption process, at (a) T=320 K and (b) T=350 K.

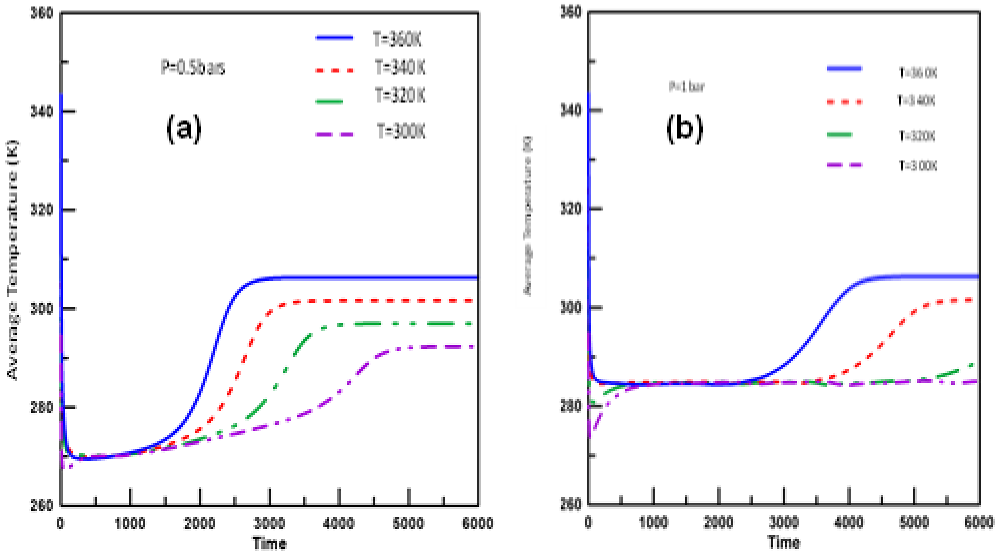

Figure 10. Effect of the heating fluid temperature on the desorption process, at (a) P=0.5 bar and (b) 1 bar.

5. **Conclusion**

The object of this numerical investigation is to investigate the outcome of operating factors on hydrogen sorption performance in a metal hydride reactor. The results show that a respectable optimal of these parameters is significant for governing the adsorption/desorption cases and can offer insight into how they can be enhanced.

The results of the numerical simulation show that:

1- The reaction kinetics during the absorption process increase as the initial hydrogen pressure increases and the temperature of the heat transfer fluid decreases.

2- The reaction kinetics during the desorption process decrease as the initial hydrogen pressure decreases and the temperature of the heat transfer fluid increases.

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الملخص باللغة العربية

تتناول هذه الرسالة دراسة محاكاة عددية لعمليات امتصاص وإزالة الهيدروجين في مفاعل أسطواني معدني-هيدروجيني لتخزين الهيدروجين. وتهدف الدراسة إلى تطوير نموذج رياضي ثنائي الأبعاد يُحاكي انتقال الحرارة والكتلة في وسائط مسامية داخل المفاعل. من خلال تطبيق الحلول العددية باستخدام برنامج فورتران، تم فحص أداء المفاعل باستخدام سبيكة **LaNi4.88Al0.12** ودراسة توزيع درجة الحرارة، الكثافة، الضغط، وسرعة الغاز الهيدروجيني أثناء عمليات الامتصاص والإزالة. تساهم هذه النتائج في تحسين تصميم المفاعلات ورفع كفاءة تخزين الهيدروجين، مما يعزز التوجه نحو استخدامه كحامل طاقة نظيف ومستدام.