Numerical Simulation of the Dynamic Behavior of a LaNi5 Water Pumping System

Miled Amel, Ben Maad Hatem, Askri Faouzi, Ben Nasrallah Sassi

Abstract**—**Metal hydride water pumping system uses hydrogen as working fluid to pump water for low head and high discharge. The principal operation of this pump is based on the desorption of hydrogen at high pressure and its absorption at low pressure by a metal hydride. This work is devoted to study a concept of the dynamic behavior of a metal hydride pump using unsteady model and LaNi5 as hydriding alloy. This study shows that with MHP, it is possible to pump 340l/kg-cycle of water in 15 000s using 1 Kg of LaNi5 at a desorption temperature of 360 K, a pumping head equal to 5 m and a desorption gear ratio equal to 33. This study reveals also that the error given by the steady model, using LaNi5 is about 2%.A dimensional mathematical model and the governing equations of the pump were presented to predict the coupled heat and mass transfer within the MHP. Then, a numerical simulation is carried out to present the time evolution of the specific water discharge and to test the effect of different parameters (desorption temperature, absorption temperature, desorption gear ratio) on the performance of the water pumping system (specific water discharge, pumping efficiency and pumping time). In addition, a comparison between results obtained with steady and unsteady model is performed with different hydride mass. Finally, a geometric configuration of the reactor is simulated to optimize the pumping time.

Keywords**—**Dynamic behavior, unsteady model, LaNi5, performance of the water pumping system.

I. Introduction

METAL hydrides are promising materials for many hydrogen-based applications such as heat pumps; hydrogen storage, thermal sorption compressor and water pump systems. The metal hydride pump is one of the unconventional pump systems which use hydrogen as a working fluid to convert thermal energy into mechanical energy.

Studies have shown that many alloys ($LaNi_{4.9}Ge_{0.1,}$ $MmNi_4Al$, $LaNi_{4.8}Sn_{0.2}MmNi_{4.2}Al_{0.8}$, $La_{0.8}Ce_{0.2}Ni_{4.25}C_{0.5}Sn_{0.25}$) and also many of AB5 type alloys are used in water pumping application [1], [2].

A recent study by Miled Amel discusses the dynamic behavior of metal hydride pumping (MHP) using Mg_2Ni, the results obtained appear to be promising [3]. For example, using 1 Kg of Mg_2Ni, it is possible to pump 1375 l of water in 10.000 s at a heating temperature of 623K and for pumping head of 5m. Furthermore, Prasad has shown that high pressure alloys are suitable for high head and low discharge application [4], then, he discusses the performance of a metal hydride pump using $LaNi_5$ and a steady model [5]. They suppose that the interior temperature of the reactor is constant and equal to the heating temperature. However, based on this steady model, the pumping time and the time evolution of specific water discharge are not mentioned.

To our knowledge, dynamic behavior of water pumping system using $LaNi_5$ has not been studied yet. Therefore, the principle objective of the present work is to extend results obtained by Prasad [5] using an unsteady model and taking into consideration the time space evolution of hydrogen concentration, pressure and temperature within the reactor. In the following sections, the mathematical model is developed. Afterwards, a numerical simulation presents the time evolution of the specific water discharge and evaluates the effect of different parameters (desorption temperature, absorption temperature, desorption gear ratio on the dynamic behavior of water pumping system. Also, a comparison between steady and unsteady model is carried out with different hydride mass. Finally, different geometric configurations are compared.

II. Operating Concept of Metal Hydride Pump

Fig. 1 presents the metal hydride water pump used in this study. The principal operation of this pump is based on the movement of hydrogen and pump piston during desorption process (hydride heating). Such a device comprises: the hydride module and the pumping module. These two modules are connected by a gear system which adjust the ratio between the displacement and the force of hydrogen and pump piston.

The first one consists of a metal hydride reactor (MHR) with heating and cooling coils, a frictionless piston cylinder and dead weight. This hydride module converts the heat input into mechanical energy. The second module consists of a frictionless piston cylinder, dead weights, and two tanks: one for suction and the other for delivery joined by connecting pipes and check valves. Initially, the reactor is full of hydrogen and the gear system has an appropriate gear ratio Gde. Then, heat is supplied to desorb hydrogen from the reactor causing the increase of hydrogen concentration; therefore, the rise of average temperature and pressure inside the reactor. Then, if the interior pressure exceeds the required pressure fixed by the gear ratio, the hydrogen piston starts moving outward. Therefore, the pumping piston moves inwards which causes the pumping of water to the delivery tank.

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After the desorption process, the gear system is reset to a lower ratio (Ge), the valve Vh is closed and heat is no longer supplied. Now, less pressure in the hydrogen cylinder is sufficient to make the pump piston in movement further outwards, thus, more water is pumped. After expansion, gear system is disengaged and valve is opened. Then, absorption of hydrogen is caused by the circulation of cold water, then gas pressure drops and dead weight on the piston pushes it inwards. Consequently, dead weight pulls the pump piston outward sucking water from suction tank. At the end, piston returns to its initial position, gear system is reset to higher ratio, heat is supplied.

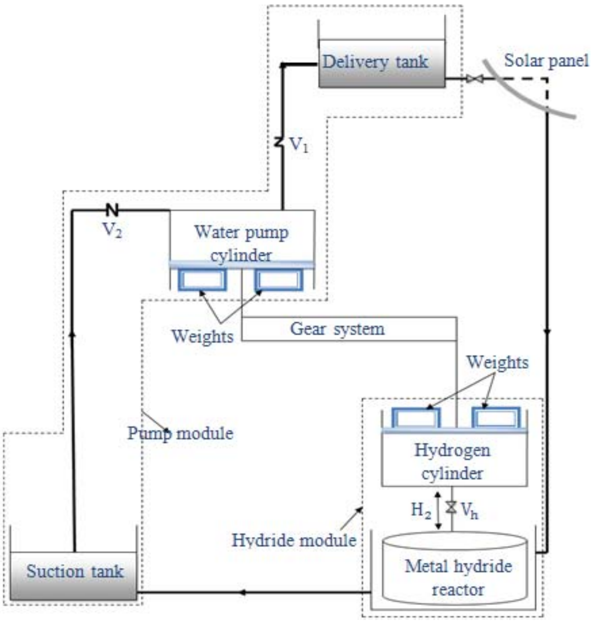


Fig. 1 Schematic of metal hydride water pumping system

III. Mathematical Model

The dynamic behavior of metal hydride pump and the determination of time space evolution of hydrogen concentration, pressure and temperature depend on the successful heat transfers and kinetic reaction of the metal hydride bed. The used MHR related to the pump is shown in Fig. 2. The reactor contains 1 kg of $LaNi_5$ and exchanges heat through lateral and base areas at a constant temperature T_f. It has a volume of V= 2.439 *$10^{-4}$$m^3$, with a radius R = 3.59 cm and a height H =6 cm.

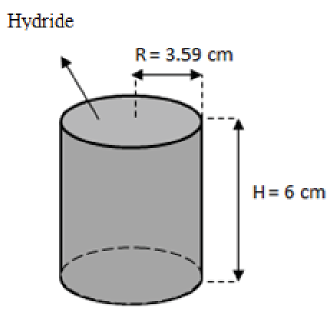


Fig. 2 Schematic of MHR

A. Governing Equations for the Metal Hydride Bed

1. Energy Equation

$$(\rho C_p)_e \frac{\partial T}{\partial t} = \lambda_e \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \lambda_e \frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right) + \dot{m}\left[\Delta H + T\left(C_{pg} - C_{ps}\right)\right] \quad (1)$$

where

$$(\rho C_p)_e = \varepsilon \rho_g C_{pg} + (1-\varepsilon)\rho_s C_{ps} \quad (2)$$

$$\lambda_e = \varepsilon \lambda_g + (1-\varepsilon)\lambda_s \quad (3)$$

ε, ρ_e, λ_e and C_{pe} are respectively the porosity of the metal hydride bed [6], the effective density, the specific heat and the effective thermal conductivity.

2. Kinetic Reaction

The hydrogen mass desorbed per unit time and unit volume is given by:

$$\dot{m} = \rho_s C_d \exp\left(-\frac{E_d}{RT}\right)\left(\frac{P_g - P_{eq}}{P_{eq}}\right) \quad (4)$$

where C_d and Ed are, respectively, the desorption rate constant (C_d= 9.57) and the desorption activation energy (E_d= 16473.59). Peq is the equilibrium pressure. It is calculated from the P-X-T relation [7]:

$$P_{eq} = \exp[\frac{-\Delta H}{RT_{ab}} + \frac{\Delta S}{R} + f_s \tan\left(\pi\left(\frac{X_i - \left(\frac{X_s}{2}\right)}{X_s}\right) - 0.5\right) \quad (5)$$

B. Governing Equations for Pumping System

1. Initial Pressure (P_i) and Initial Number of Mole of Hydrogen

The initial pressure of the metal hydride bed is equal to the equilibrium pressure at the end of the absorption process. The initial hydrogen number of moles present in the hydrogen cylinder is as:

$$n_0 = \frac{p_i A_h Z_0}{R_g T_i} \quad (6)$$

2. Bed Pressure Equation

During desorption process, heat supplied to the reactor causes the rise of number of moles of hydrogen and consequently the increase of the pressure inside the MHR. Infact, hydrogen concentration, pressure and temperature of the hydrogen gas in the hydrogen tank are assumed to vary only with time. The bed pressure after any time interval (dt) is as:

$$P(t) = \frac{(n(t) + n_0)RT_{moy}}{V_0} \quad (7)$$

where V_0, n(t) and T_{moy} are respectively the initial volume of the hydrogen cylinder, the number of moles of hydrogen gas in the tank and the average temperature during desorption process.

3. Number of Moles of Hydrogen Desorbed:

The number of moles of hydrogen gas in the cylinder is:

$$n(t) = \frac{1000(H/M)_{\max}(X_i - X(t))}{2M_m} \quad (8)$$

where X(t) is the dimensionless hydrogen concentration in the metal which defined as:

$$X = \frac{\frac{H}{M}}{\left(\frac{H}{M}\right)_{\max}} \quad (9)$$

Xi is the dimensionless hydrogen concentration at the end of the absorption process.

4. Volume of Pumped Water During Desorption

Total forces exerted by the hydrogen and pump piston are given by:

$$F_{pd} = \rho g h_t A_p \quad (10)$$

$$F_{hde} = F_{pd} G_{de} = \rho g h_t A_p G_{de} \quad (11)$$

where A_p, ht represent respectively the pump piston base area, the total head and the gear ratio. G_{de} is the ratio of force exerted by the hydrogen piston to the force required at the pump piston. Then, for the given parameters and the set gear ratio (G_{de}) there existsa unique desorption pressure which decides the operation of the pump.

$$P_{de} = P_i + \rho g h_t G_{de} \frac{A_p}{A_h} \quad (12)$$

When the pressure P(t) within the reactor tends to exceed the pressure set by the gear ratio (P_{de}) the hydrogen piston starts moving outwards and the pump process begins.

The outward movement and the volume of hydrogen cylinder during desorption can be calculated by:

$$Z_{hde}(t) = \left(\frac{V_{hde}(t)}{A_h} = \frac{n(t)R_g T_{moy}}{P_{de} A_h} \right) \quad (13)$$

$$V_{hde} = \frac{n(t)R_g T_{moy}}{P_{de}} \quad (14)$$

Thus, the corresponding inward movement of pump piston is:

$$Z_{pde} = G_{de} Z_{hde}(t) \quad (15)$$

Consequently, the volume of water pumped during the movement of the pump piston is as:

$$V_{pd}(t) = G_{de} V_{hde}(t) \frac{A_p}{A_h} \quad (16)$$

5. Volume of Pumped Water during the Expansion Process

After the desorption process the gear ratio is reset to a lower value G_e. Then, the net force exerted by the hydrogen piston during expansion is given by:

$$F_{he} = G_e F_{pd} \quad (17)$$

So, the volume of extra water pumped during the expansion of hydrogen piston is:

$$V_{pe}(t) = G_e \frac{A_p}{A_h} V_{hde}(t) \left[\left(\frac{P_{de}}{P_{he}} \right)^{\frac{1}{\gamma}} - 1 \right] \quad (18)$$

where P_{he} is the hydrogen pressure in the hydrogen cylinder during expansion. In fact, during this process, hydrogen expands adiabatically from P_{de} to P_{he}. This pressure is sufficient to have a further movement of hydrogen and pump piston, therefore further volume pumped.

6. The Total Volume

The total amount of water pumped during desorption and expansion is given by:

$$V_t(t) = V_{pd}(t) + V_{pe}(t) \quad (19)$$

7. Total Heat Input

During the sensible heating and desorption process, total heat input per kilogram of $LaNi_5$ is as:

$$Q_t = m_{LaNi_5} C_p (T_{de} - T_{ab}) + n_{H_2} \Delta H \quad (20)$$

where Cp is the specific heat of hydride bed.

8. Pump Efficiency

$$\eta = \frac{\rho V_t g . h_t}{Q_t} \quad (21)$$

IV. Results and Discussion

The numerical simulation is carried out using a desorption temperature (T_{de}) from 348K to 365K, absorption temperature from 298K to 308 K and desorption gear ratio from 8 to 33. The values of constant parameters are presented in Table I.

TABLE I
Constant Parameters

Parameter	Value
Enthalpy of formation	30 932 J/mol
Entropy of formation	108 J/mol K
Slope factor (f_s) [8]	0.13
Initial concentration Xi	0.91
Molar mass of metal	432 g/mol
Specific heat of hydrogen	14500 J/Kg K
Specific heat of LaNi5 [9], [10]	600 J/Kg k

A. Effect of Desorption Temperature

The effect of desorption temperature on the performance of the pump system is presented. Three simulations have been considered (T_f= 348, K, T_f= 355 K, T_f = 365K).

Fig. 3 (a) shows the effect of the desorption temperature on the trigger of pumping process. It is seen that high desorption temperature allows triggering quickly the pumping process. Also, the specific water discharge is null for first instants. In fact, at the beginning of hydrogen desorption, the pressure inside the reactor is still lower than the required pressure set by the gear ratio. So, hydrogen and pump piston are in their initial position and the volume pumped is null.

Fig 3 (b) shows that a higher volume of water can be pumped when high desorption temperature is used. Similarly, we observed that the time required for pumping water decreases for higher temperatures. By comparing the two temperatures 348 K and 365 K, an improvement in the pumping time of about 86% is noted.

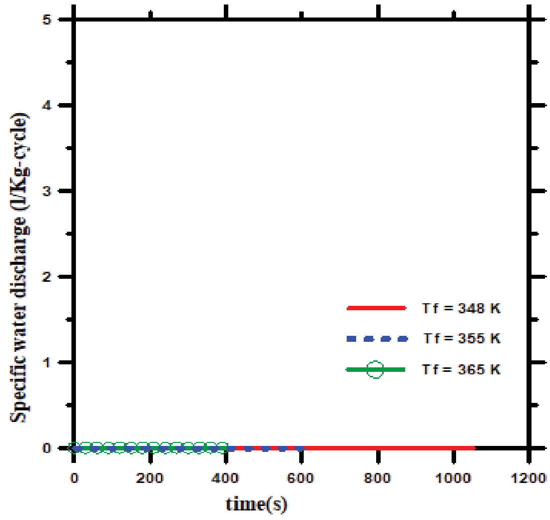
B. Effect of Desorption Gear Ratio

In order to test the effect of the desorption gear ratio on the performance of metal hydride pump, three cases are considered in this study (Gde=8, Gde=19, Gde=33).

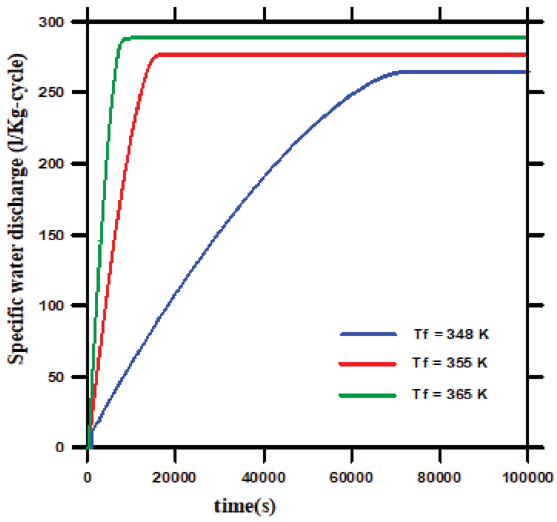
It is seen from Fig.4 (a) that the time required to start pumping process decreases for low values of desorption gear ratio.

Fig. 4 (b) shows the time evolution of the volume pumped for different desorption gear ratio. It is found that higher desorption gear ratio allows to pump more water. In fact, higher desorption pressure requires higher desorption temperature, then, more water can be pumped. But, lower desorption gear ratio permits an acceleration of pumping process.

Fig. 4 (c) shows the effect of desorption gear ratio and desorption temperature on the pump efficiency. It is seen that, from a well-determined desorption gear ratio, the pump efficiency increases gradually and then tends to a constant. Also, this figure reveals that higher efficiency is obtained at higher gear ratio and higher desorption temperature.



(a)



(b)

Fig. 3 Effect of heating temperature on the (a) trigger of the pumping process and (b) specific water discharge

C. Comparison between Steady and Unsteady Models for Different Hydride Mass

Fig. 5 shows the comparison between steady and unsteady model for different masses of LaNi5. The steady model supposes that the hydrogen concentration, the interior pressure and temperature are constant and temperature is equal to the heating temperature. Unless the unsteady model takes into account the time space evolution of hydrogen concentration, temperature and pressure within the reactor.

It is shown that, for the different mass (m= 1Kg, 5Kg, 10Kg), the specific water discharge obtained by the steady model is slightly higher than that given by the unsteady model. In fact, for the unsteady model, the temporal and spatial variation of pressure and temperature inside the reactor causes heterogeneity of the hydrogen concentration in the metal.

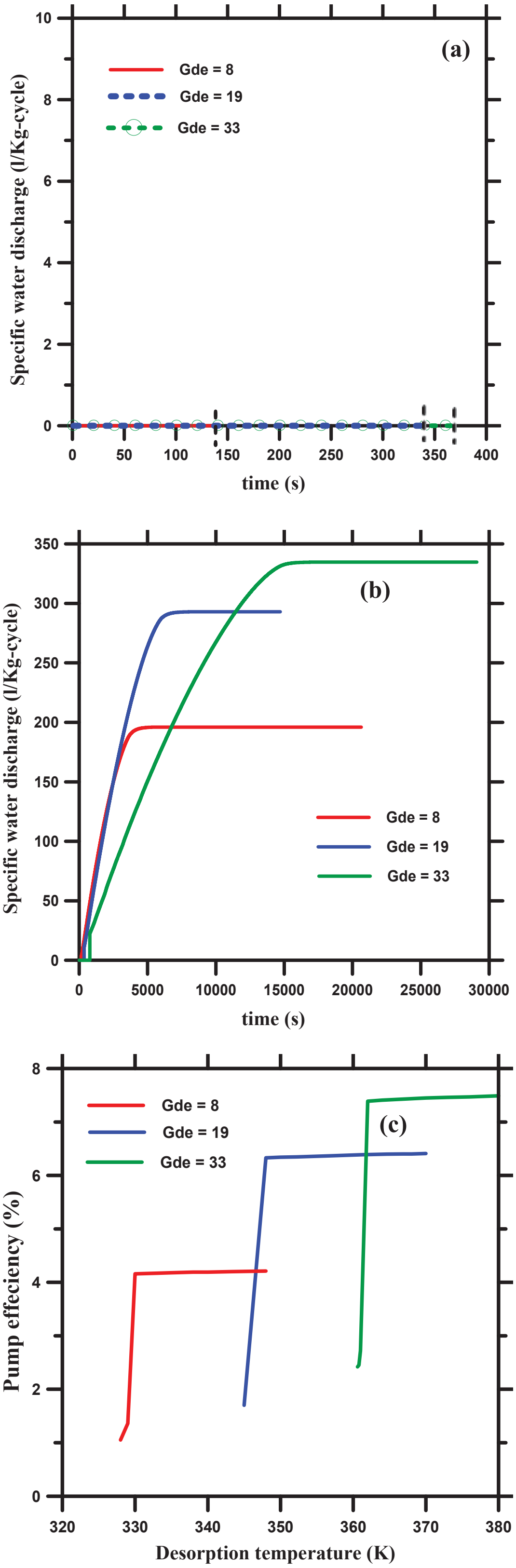


Fig. 4. Effect of desorption gear ratio on the: a) trigger of the pumping process b) specific water discharge and c) pump efficiency

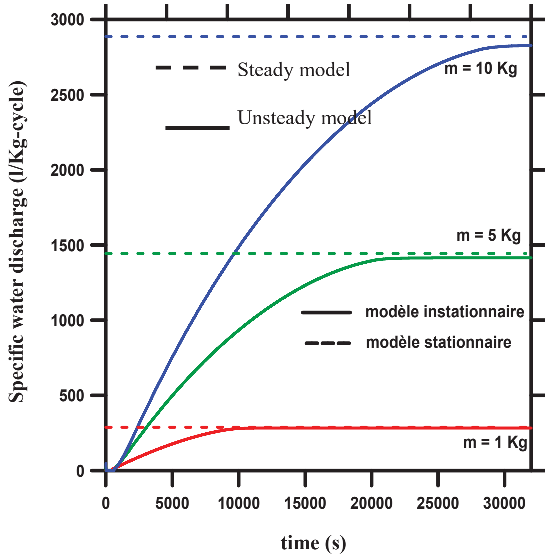


Fig. 5 Comparison between steady and unsteady models for different masses of LaNi5

As a result, the specific water discharge is slightly lower than that obtained when temperature is constant during the desorption process (steady model). Also, it is seen, from this figure, that the difference between the two pumped volumes becomes more and more remarkable when increasing the mass of metal used. For example, the difference between the two volumes is of 5.97 l/cycle, 28.94 l/cycle and 57.89 l/cycle, for respectively m=1Kg, 5Kg and 10 Kg. Then the error given by the steady mode, using LaNi5, is about 2%.

D.Effect of the Geometric Configuration and Absorption Temperature

In order to bring out the effect of the reactor geometry on performances of water pump system, three configurations are tested.

C1. A cylindrical reactor that exchanges heat through its lateral and base surfaces

C2. Similar to C1, with the addition of a concentric heat exchange

C3. A cylindrical reactor with aside surface of elliptic form, with the addition of a concentric heat exchange

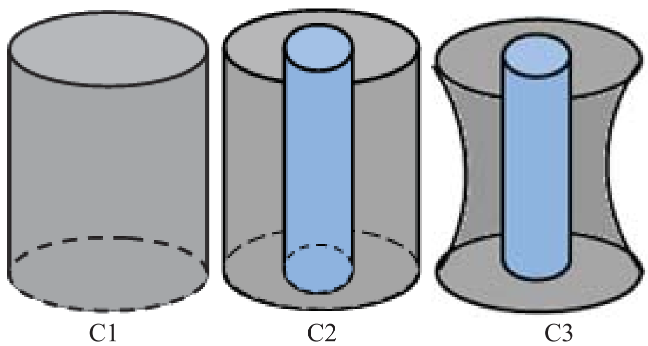


Fig. 6 Geometric configurations

Fig. 7 shows the effect of the geometric configuration on the specific water discharge, pumping time and pump efficiency for different absorption temperature.

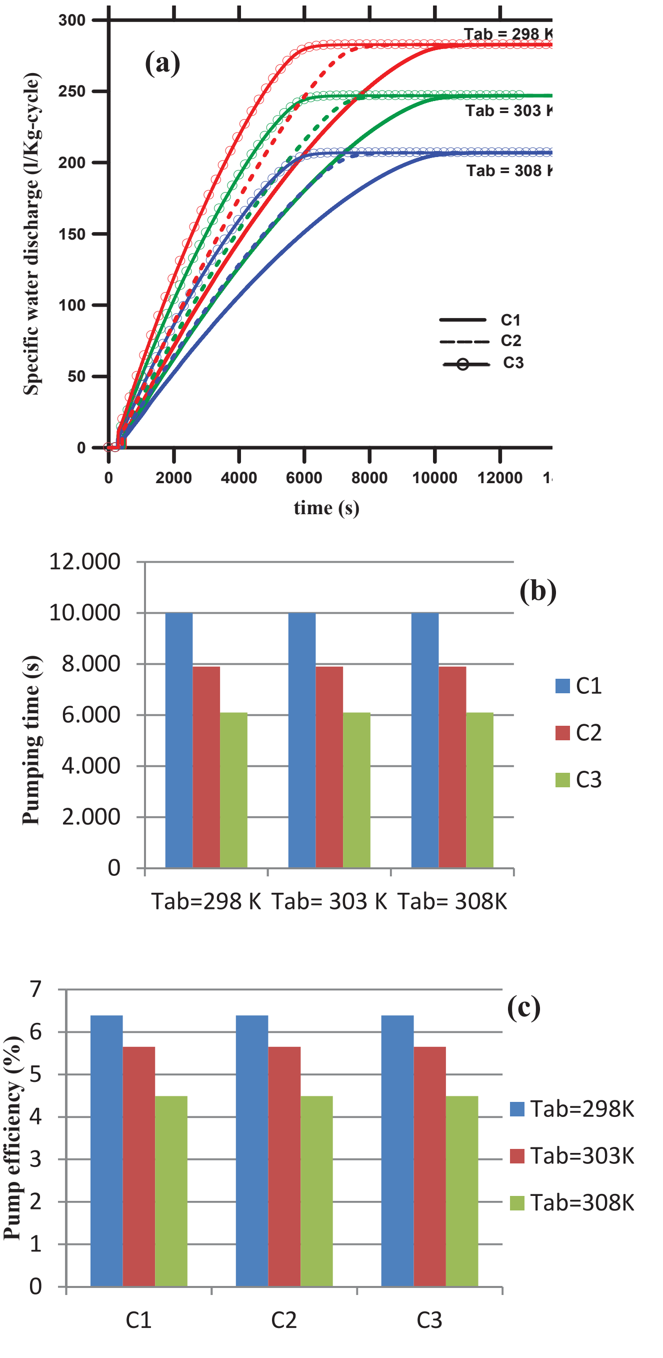


Fig. 7 Effect of geometric configuration and absorption temperature on the a) specific water discharge, b) pumping time and c) pump efficiency

It is seen from Fig. 7 (a) that higher absorption temperature results in lower volume pumped. In fact, higher absorption temperature leads to the increase of absorption pressure and then the increase of dead weight on the hydrogen piston. Thus, the force exerted by hydrogen piston decreases, so, a decrease in the volume pumped. From the same figure, we note that we obtain the same specific water discharge for the three configurations.

Fig. 7 (b) shows that absorption temperature has no effect on the pumping time. Therefore, we note that for the first configuration, the pumping process is very slow, because of the low heat transfer in the hydride bed and the limitation of kinetics of the chemical reaction. Similarly, we find that the integration of a concentric heat exchanger at the center of the reactor (C2) significantly improves the water pumping time. Also, we note that the third configuration, allow to get the best pumping time.

For example, for Tab =298K, we note that the required time to pump 282.4 l/Kg-cycle of water is 10 000s, 7 900s and 6 100s for respectively C1, C2 and C3. Then, the second and the third configuration allow respectively an improvement of about 21% and 39% compared to the first configuration.

Fig. 7 (c) shows that the geometric configuration has no effect on the pump efficiency. Also, it is seen that higher absorption temperature results in lower pump efficiency.

V. Conclusion

In this paper, a dynamic study of metal hydride pump using LaNi5 as hydriding allow is developed. The study shows that the increase of heating temperature and desorption gear ratio improve the volume of water pumped. However, absorption temperature has an adverse effect. This study reveals also that the error given by the steady mode, using LaNi5, is about 2%. Then, the steady model can give a good estimation of the specific water discharge, but no information about the pumping time.

To reduce the pumping time, two new configurations of the reactor were proposed. Using the developed numerical code, this pump has been successfully simulated and the results showed that these new configurations (C2 and C3) improve the pumping time respectively by 21% and 39% compared to the basic configuration (C1).

This study can be extended by studying the effect of other parameters (expansion gear ratio, pumping head, form factor, hydrogen and pump piston surfaces)

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