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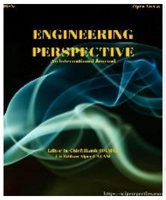

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Research Paper

# Thermal Modeling of Solid Hydrogen Storage in a LaNi5 Metal Hydrid Tank

Mohand-Ouyahia Bousseksou[1*], Yucai Lin[1]

[1]*Capgemini engineering, Ile de France, Division APA, 12 rue de la Verrerie, 92190 Meudon, France*

ABSTRACT

This paper presents a detailed 3D model of a solid hydrogen storage tank based on metal hydride LaNi5 technology, utilizing COMSOL Multiphysics 6.1 software. The model takes into account the coupling of momentum, heat, mass and energy transfer within the LaNi5 metal hydride during hydrogen absorption. The main objective of the study is to analyze the temporal evolution of temperature and pressure within the tank as hydrogen is absorbed. In addition, the paper investigates the effectiveness of a cooling strategy involving the integration of cooling tubes into the tank configuration. This approach aims to enhance the thermal management of the storage system by dissipating excess heat generated during hydrogen absorption.

Simulation results demonstrate the changes in temperature and pressure occurring within the LaNi5 metal during the process of hydrogen absorption. The implementation of an air-based cooling system emerges as an effective means of regulating the temperature of the storage tank, thus creating optimal conditions for hydrogen absorption processes. This understanding is essential to the development of efficient thermal management solutions for solid hydrogen storage technologies. By comprehensively analyzing the thermal behavior of the LaNi5 metal hydride tank, this numerical study suggests that the efficient design of storage system is very important for rapid absorption of hydrogen.

**Keywords:** COMSOL Multiphysics; Cooling strategy; Hydrogen; LaNi5; Storage tank.

| **History** | **Author Contacts** |
|---|---|
| Received: 07.01.2024 | **Corresponding Author* |
| Accepted: 14.03.2024 | e-mail addresses : mohand-ouyahia.bousseksou@capgemini.com, yucai.lin@capgemini.com |
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## 1. Introduction

Since the beginning of the 21st century, the entire world has shifted its interest towards searching for alternatives to traditional transport technologies due to the consequences of their impact on the climate [1]. All industrial sectors are aiming to overcome their dependence on fossil fuels, which are responsible for a substantial proportion of greenhouse gas emissions [2].

In the environmental context, hydrogen is a promising energy carrier in the face of current challenges. it is a solution that can be used to replace fossil fuels in various fields, notably in the automotive sector [3], where it is used as a fuel to power a hydrogen fuel cell [4, 5] or even internal combustion engines [6]. Thanks to its various production [7] and storage methods [8], it is considered a clean, renewable, and highly powerful energy source.

Currently, there are three main approaches for hydrogen storage. High-pressure hydrogen storage, which is realized by compressing hydrogen gas at pressures ranging from 300 to 700 bars. Low-temperature liquid storage, it involves cooling hydrogen gas to as low as -253 °C to condensate it to a liquid state and solid-state hydrogen storage that requires the use of metal hydrides to absorb hydrogen gas [8].

The use of metal hydride-based hydrogen storage offers a significant volume density (of the order of 120 kg/m$^3$) compared with the other two storage methods, liquid (71 kg/m$^3$), and gaseous (42 kg/m$^3$) [9]. However, the enormous amount of heat emitted during the hydriding process is a major drawback [10]. This poses a challenge to the thermal management of the storage tank [11].

The storage of hydrogen in solid form utilizing metal hydrides necessitates thorough consideration of the thermal challenges. In order to be enable to absorb the hydrogen the tank must be maintained at an appropriate temperature [12].

The main objective of this work is to study the absorption phenomenon of a metal hydride-based solid-state hydrogen storage system for powering a PEMFC (proton exchange membrane fuel cell) fuel cell used in vehicles.

To optimize the performance of metal hydride tanks, research into tank design and configuration is essential for efficient operation of stored hydrogen distribution. The present work implies a numerical study on the comparison of different techniques proposed to improve the thermal management of a solid-state hydrogen storage tank based on a LaNi5 metal hydride. In particular, the evolution of the temperature within hydride bed upon absorption.

## 2. Numerical model

This study, a numerical model was used to simulate the thermal behavior of a solid-state hydrogen storage tank. The physical model of the metal hydride tank studied is composed of a solide phase (metal: LaNi5) and a pure gaseous phase (hydrogen: $H_2$), thus forming a porous medium as showed in Figure 1. The choice of tank geometry is based on a 3D type is seen on Figure 2. The tank consists of a cylindrical of radius R = 0.25 m and height H = 1 m. The hydrogen is injected into the tank from the top at $P_{H2\_in}$ = 8 bars during the absorption of hydrogen. The lateral surface experiences cooling through natural convection, while the remaining orthogonal surfaces are presumed to exhibit adiabatic behaviour. The temperature is maintained constant at the extremities of the tank and set to the value of $T_0$ = 293 K.

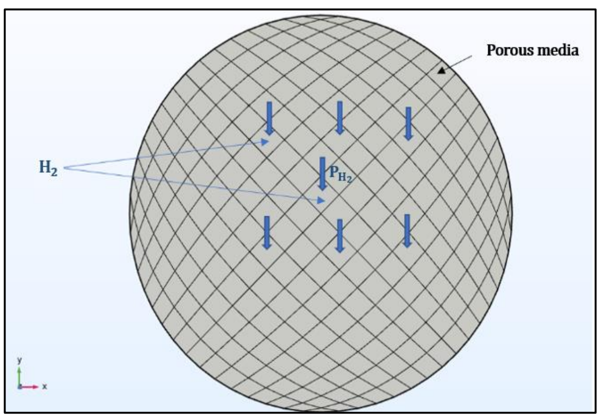


Figure 1. Schematic section view of the hydrogen absorption in a porous media

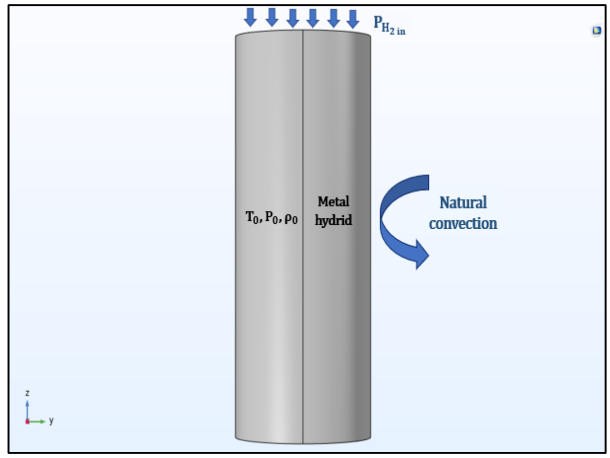


Figure 2. The geometry of the model

To simplify the numerical model, the following assumptions are considered [13, 14, 15, 16, 17]:

i. The gas phase (hydrogen) is pure.
ii. The tank is considered in three dimensions (3D).
iii. The media are in local thermal equilibrium between gas and solid.
iv. The validity of Darcy's law. ²z
v. The radiative transfer in the porous medium is neglected.
vi. The hydrogen inlet temperature and pressure are maintained constant ($T_0$ and $P_0$).

The equations governing the hydriding process are discussed in detail below.

### 2.1 Energy conservation

According to the [14, 18] heat transfer modeling can be simplified by setting a temperature variable for the system (Eq. (1)).

$$(\rho C_p)_{eff}\frac{\partial T}{\partial t} + \rho_g C_{pg} \upsilon_g \nabla T = \nabla(\lambda_{eff}\nabla T) + S_m \quad (1)$$

Where the effective heat capacity, $(\rho C_p)_{eff}$, is given by Eq. (2):

$$(\rho C_p)_{eff} = \epsilon\rho_g C_{pg} + (1-\epsilon)\rho_s C_{ps} \quad (2)$$

The effective thermal conductivity can be written as:

$$\lambda_{eff} = \epsilon\lambda_g + (1-\epsilon)\lambda_s \quad (3)$$

The heat source term $S_m$ is equal to:

$$S_m = (1-\epsilon).\parallel \Delta H \parallel.\frac{\partial\rho_s}{\partial t} \quad (4)$$

With, ϵ is the porosity of the medium studied and $\frac{\partial\rho_s}{\partial t}$ is the amount of hydrogen absorbed by the metal as a function of time.

In the case of absorption [19]:

$$\frac{\partial \rho_s}{\partial t} = C_a . e^{\frac{-E_a}{RT}} . ln\left(\frac{P}{P_{eq}}\right)(\rho_{ss} - \rho_s) \quad (5)$$

With $P_{eq}$ is the equilibrium pressure.

### 2.2 Mass conservation

For gaseous media (hydrogen):

$$\epsilon \frac{\partial \rho_{H2}}{\partial t} + div(\rho_{H2}\overrightarrow{\upsilon_{H2}}) = -\dot{m} \quad (6)$$

Where, $\rho_{H2}$ is the density of gas (hydrogen) and $\upsilon_{H2}$ is the velocity field of the gas (hydrogen).

For solid media (metal hydride):

$$(1 - \epsilon)\frac{\partial \rho_s}{\partial t} = -\dot{m} \quad (7)$$

Where, $\rho_s$ the density of solide (bed) and $\dot{m}$ the mass transferred from the gas phase to the solid in function of time.

The gas density $\rho_{H2}$ is described by the equation:

$$(1 - \epsilon)\frac{\partial \rho_s}{\partial t} = -\dot{m} \quad (8)$$

### 2.3 Momentum conservation

According to Darcy's law the hydrogen gas velocity within the thank is:

$$V_{H2} = \frac{k}{\mu_{H2}}\vec{\nabla}_P \quad (9)$$

Where, k is the intrinsic permeability of the porous medium ($m^2$), and $\mu_{H2}$ is the dynamic viscosity of the fluid (Pa.s).

### 2.4 Kinetics reaction

The absorption kinetic of a hydride metal is related to the amount of hydrogen absorbed by the metal over time can be expressed as:

$$\frac{\partial \rho_s}{\partial t} = C_a\, exp\left(-\frac{E_a}{RT}\right) ln\left(\frac{P}{P_{eq}}\right)(\rho_{sat} - \rho_s) \quad (10)$$

The equilibrium pressure $P_{eq}$ is calculated using the Van't Hof relation via the following term [19]:

$$ln\left(\frac{P_{eq}}{P_0}\right) = A - \frac{B}{T} \quad (11)$$

With A and B are Van't Hoff constants having the values of 12.95 and 3731.42 respectively [19].

### 2.5 Initial and boundary conditions

Initially "t = $t_0$", the temperature, pressure and hydride density are assumed to be constant (Figure 2).

$$T(t_0, r, z) = T_0 \quad (12)$$

$$P(t_0, r, z) = P_0 \quad (13)$$

$$\rho(t_0, r, z) = \rho_0 \quad (14)$$

At the hydrogen inlet (Figure 2):

$$T(x, y, t) = T_0 \quad (15)$$

$$P(x, y, t) = P_0 \quad (16)$$

The lateral cooling wall (Figure 2):

$$h_{conv}(T - T_0) \quad (17)$$

### 2.6 Modeling parameters

The thermophysical proprieties of the LaNi5 and $H_2$ used in this study are succinctly presented in Table 1.

Table 1. Thermophysical proprieties of the metal hydride (LaNi5), hydrogen ($H_2$) and other parameters used in the simulations [13, 14, 16, 17, 20, 21].

| | |
|---|---|
| $P_{in}$ | 8 [bar] |
| $T_{in}$ | 293 [K] |
| $M_{H2}$ | 2.01588 [g/mol] |
| $\lambda_{H2}$ | 0.24 [W/m. K] |
| $\rho_{H2}$ | 0.0838 [kg/m$^3$] |
| $Cp_{H2}$ | 14.890 [J/mol. K] |
| $P_0$ | 1 [bar] |
| $T_0$ | 293 [K] |
| $h_{conv}$ | 1650 [W/ (m².K)] |
| $k_{hyd}$ | 2.4 [W/ (m.K]] |
| $\epsilon$ | 0.5 |
| $Cp_s$ | 419 [J/kg. K] |
| k | $3\times10^{-12}$ [m²] |
| $\rho_{sat}$ | 8520 [kg/m$^3$] |
| $\rho_s$ | 8400 [kg/m$^3$] |
| $Cp_{air}$ | 1005 [J/kg. K] |
| $k_{air}$ | 0.025 [W/(m².K)] |
| $Cp_{H2O}$ | 4180 [J/kg. K] |
| $k_{H2O}$ | 0.598 [W/(m². K)] |
| $T_c$ | 293 [K] |
| R | 0.02 [m] |
| $E_a$ | 21170 [J/mol] |
| $C_a$ | 59.187 [1/s] |
| ΔH | 30 [kJ/kg] |
| $R_g$ | 8.314 [J/(mol. K)] |

## 2.7 Cooling strategies

In order to enhance the cooling efficiency of the storage tank, a novel approach was contemplated. This entailed the incorporation of internal cooling tubes withing the metal hydride, as illustrated in Figure 3 (b and c). While maintaining the original geometry of the tank, two cooling tubes with a radius of 0.02 m were integrated.

For this process, two heat transfer fluids were used: air and water. These fluids were chosen because of their specific heat transfer properties, abundance, and their common use in cooling applications. The aim of this study is to evaluate the effectiveness of the aforementioned approach using two distinct fluids, compared with the case of a basic tank which cools solely by natural convection. A schematic of the different configurations is presented in Figure 3. The cooling tubes, which are supposed isotherm (Figure 3):

$$T(t,r,z) = T_0 \quad (18)$$

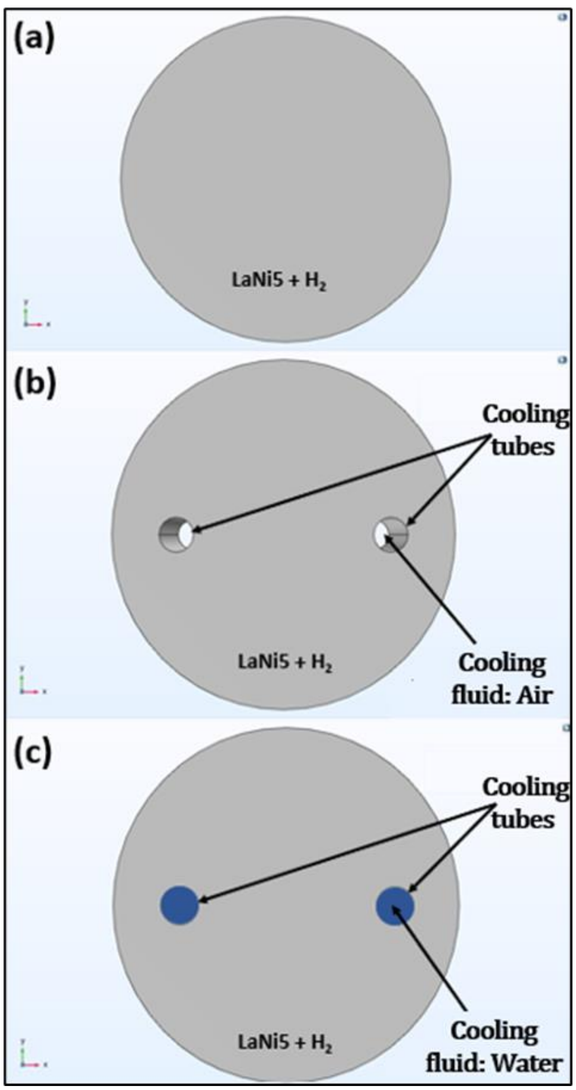


Figure 3. Schematic section view of the tank equipped with two cooling tubes. (a) basic tank, (b) tank with two air-filled cooling tubes and (c) tank with two water-filled cooling tubes

## 3. Results and discussion

In this section, we determine the variation of temperature and pressure as a function of time during the absorption process in hydrogen storage tanks. Then, we will provide a comparative assessment of the temperature variation in the tank for the various proposed cooling techniques.

## 3.1 Temperature evolution

Figure 4 shows the temperature variation as a function of time at a specific measuring point within the tank. A rapid increase in temperature can be observed, reaching the maximum value (345 K), attributed to the exothermic nature of as the hydriding reaction of the intermetallic. Then, after this rapid increase, the temperature gradually decreases towards ambient temperature (to 298 K). Our results align with those reported in the literature [12].

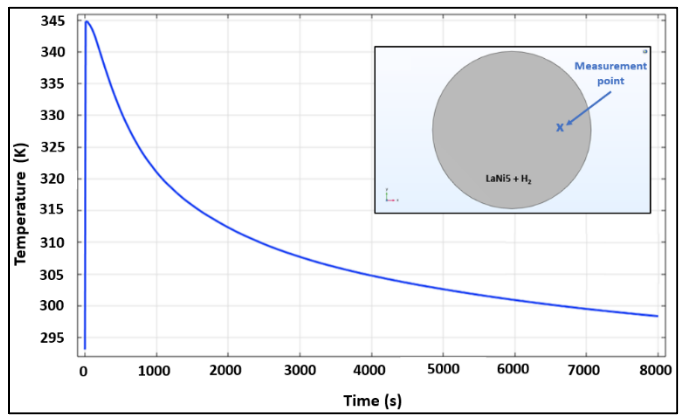


Figure 4. Temperature variation as a function of time during absorption

The spatio-temporal evolution of the temperature inside the thank from 0 to 4000 is shown in the Figure 5. The temperature rises rapidly, reaching a maximum value of 345 K, followed by a gradual descent to reach a peak temperature of 330 K after 4000 s.

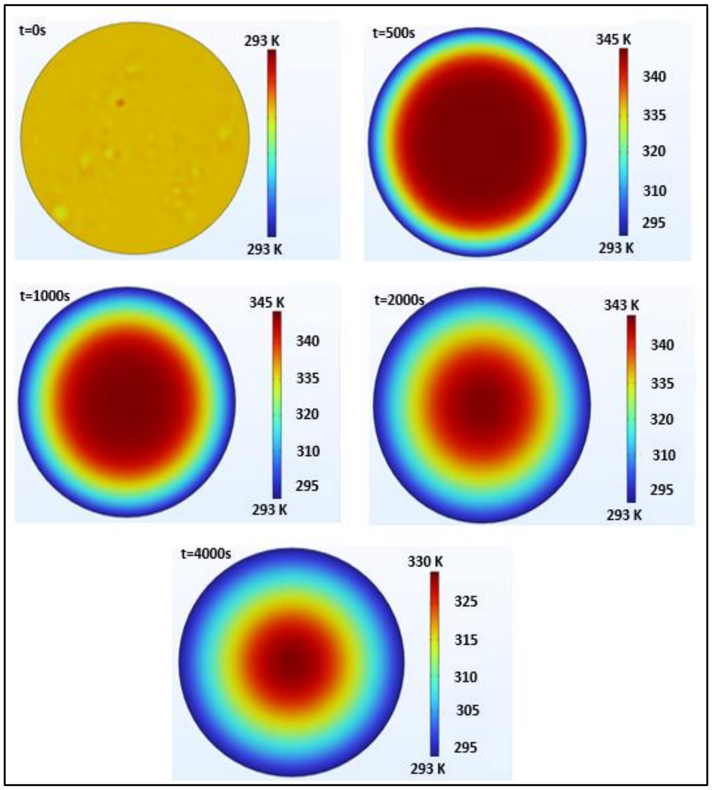


Figure 5. Spatio-temporal temperature variation

### 3.2 Pressure evolution

Figure 6 illustrates the temporal variation of hydrogen pressure within the hybrid bed. It is observed that the pressure increases rapidly until it reaches a steady state corresponding to the set pressure. This rapid and uniform stabilization of pressure is observed throughout the entire hybrid zone, leading to the conclusion that $H_2$ percolation times are extremely short [22].

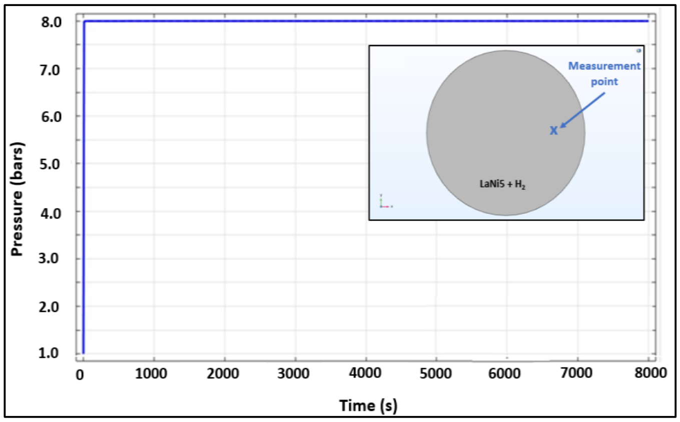


Figure 6. Temperature Pressure variation as a function of time

### 3.3 Effect of the tubes cooling

Figure 7 illustrated the temperature field reigning inside the tank from 0 s to 4000 s in three different configurations ((a) basic tank, (b) tank with two air-filled cooling tubes and (c) tank with two water-filled cooling tubes). We can observe the rapid growth of the temperature in the hydride bed at the start for all three tank configurations. Then, they decrease progressively as the kinetics of the hydriding reaction slow. However, the rate in which the temperature goes down shows a marked disparity between configurations with cooling tubes and those without, where cooling is based solely on the peripheral wall of the tank. We observe a rapid increase, reaching a maximum value of 345 K for t = 500 s, both for the configuration without cooling tubes and for that with air-filled tubes. However, in the case of the configuration with water-filled tubes, a slightly lower maximum temperature of 344 K is observed. Thereafter, it gradually decreases to reach a temperature of 330 K after 4000 s in the case of the tank without cooling tubes, while for the configurations with cooling tubes filled with air and water, the corresponding temperatures after 4000 s are 319 K and 318 K, respectively.

The presence of cooling tubes in the storage tank reduces the time required to cool the hydride bed, which in turn reduces the hydriding time. This approach considerably increases the heat exchange surface area within the tank. The cooling tubes also enable the heat to be dispersed more efficiently.

The use of water as a coolant is highly effective due to its excellent heat transfer properties, making it an efficient cooling medium. Nonetheless meticulous selection of materials for the design of cooling tubes is imperative to mitigate potential issues such as corrosion and leaks, thereby ensuring the enduring robustness of the envisaged cooling system. However, it's worth noting that in some cases, air may be preferable to water as a cooling medium. While water is highly efficient for heat transfer, it can also present additional challenges in terms of corrosion and maintenance, especially if the construction materials are not compatible with water. Conversely, utilizing air as a coolant offers a more straightforward and potentially more reliable alternative, exhibiting reduced susceptibility to operational issues. This can be particularly advantageous in applications where water-related risks are high or where simplicity and ease of maintenance are priorities.

Therefore, considering that there is only a 1 K temperature difference between air cooling and liquid cooling, opting for air cooling may be more effective compared to the potential issues associated with using water.

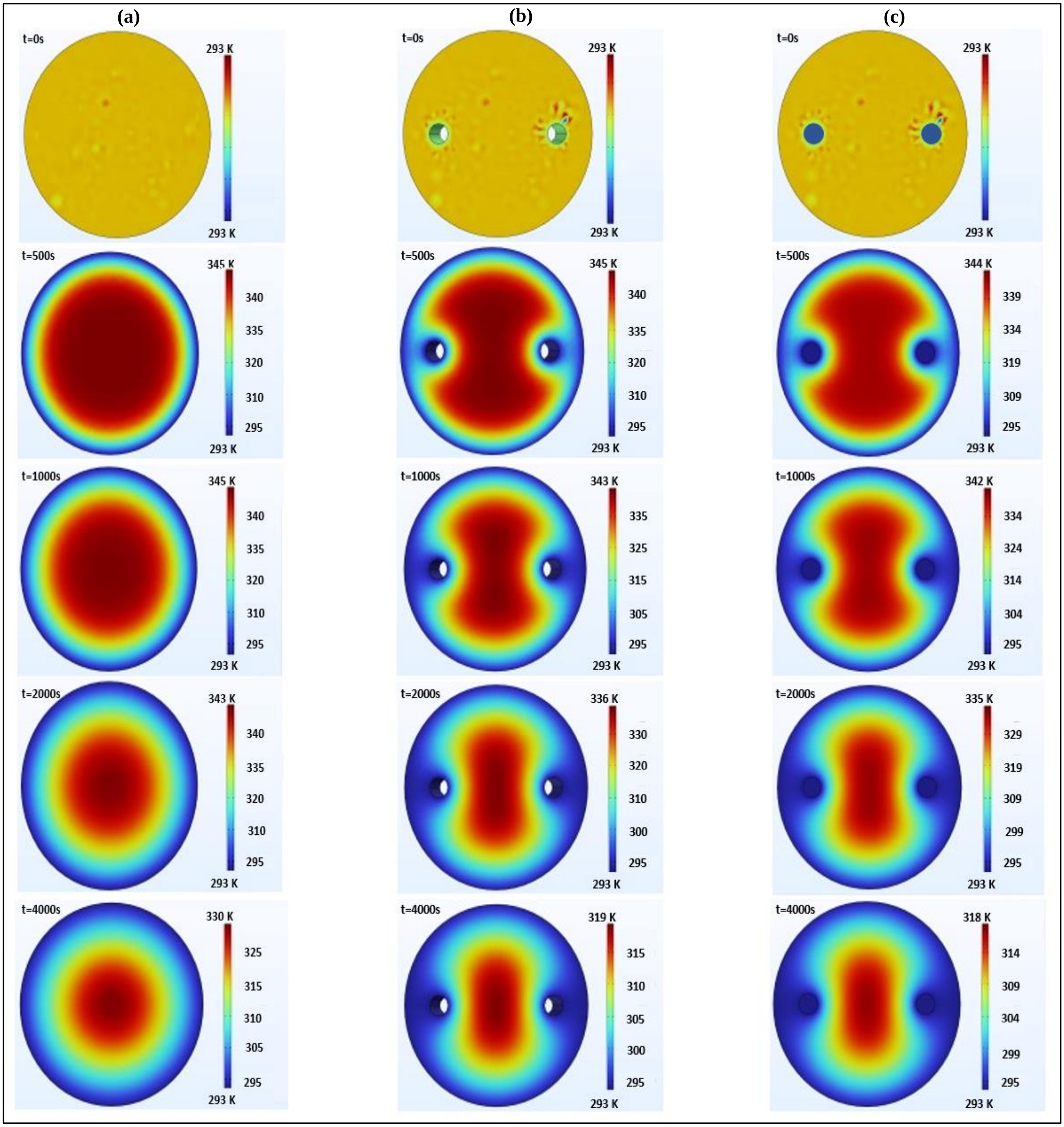


Figure 7. Variation of the temperature in function of time during absorption for different configurations: (a) basic tank, (b) tank with two air-filled cooling tubes and (c) tank with two water-filled cooling tubes

## 4. Conclusions

This study contributes to a better understanding of hydrogen storage in tanks, in particular the hydrogen absorption process with different designs of the cooling system. A three-dimensional mathematical model describes how heat and mass transfer in metal hydride are carried out. The results showed a substantial and swift generation of heat during the hydrogen absorption. Furthermore, this study compares cooling solutions for solid hydrogen storage tanks. It offers different approaches to controlling the temperature and thus ensuring safe hydrogen storage. Incorporating cooling tubes filled with air significantly enhances heat transfer within the tank.

There are many perspectives and avenues for achieving our study:

i. Desorption phenomenon: In the current work we have studied the phenomenon of hydrogen adsorption. Subsequently, a systematic examination of hydrogen desorption kinetics is envisaged for future research. This will involve examining the influence of key parameters including temperature, pressure, material characteristics and surface morphology on the desorption process (a Model utilizing COMSOL Multiphysics is currently under development).

Incorporating phase-change materials (PCMs) within hydrogen tank facilitates the storage of hydrogen at elevated densities and reduced temperatures when compared to high-pressure and cryogenic tanks. The integration of a PCM is an important part of the thermal management of the tanks and offers several important advantages, such as the recovery of excess heat and the maintenance of temperature at optimum levels. There are many perspectives and avenues for achieving our study.

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## Nomenclature

| | |
|---|---|
| $P_{in}$ | Inlet pressure of hydrogen |
| $T_{in}$ | Inlet temperature of hydrogen |
| $M_{H2}$ | Molecular mass of hydrogen |
| $\lambda_{H2}$ | Heat conductivity of the $H_2$ gas |
| $\rho_{H2}$ | Density of the $H_2$ gas |
| $Cp_{H2}$ | Specific heat of $H_2$ gas |
| $P_0$ | Initial pressure |
| $T_0$ | Initial temperature |
| $h_{conv}$ | Heat convection coefficient |
| $k_{hyd}$ | Specific heat of the solid |
| $\epsilon$ | Permeability of the metal |
| $Cp_s$ | Specific heat of the solide |
| $k$ | Permeability of the metal |
| $\rho_{sat}$ | Saturated metal hydride density |
| $\rho_s$ | $H_2$-free metal hydride density |
| $Cp_{air}$ | Specific heat of air |
| $k_{air}$ | Heat conductivity of air |
| $Cp_{H2O}$ | Specific heat of $H_2O$ |
| $k_{H2O}$ | Heat conductivity of air |
| $T_c$ | Cooling tubes temperature |
| $R$ | Annular disc unit radius |
| $E_a$ | Activation energy for absorption |
| $C_a$ | Absorption rate constant |
| $\Delta H$ | Reaction heat of formation |
| $R_g$ | Universal gas constant |

## Conflict of Interest Statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## CRediT Author Statement

**Mohand-Ouyahia Bousseksou:** Writing- review & editing, supervision, project leader, Methodology & software, **Yucai Lin:** Formal analysis.

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