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Design of Metal Hydride Pressure Vessel

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Abstract. This article describes the issue of hydrogen storage in the structure of metallic alloys and then solves the design and structural analysis in ANSYS Static Structural of low-pressure metal hydride steel vessel for hydrogen storage in metallic alloy based on MnTiVFeZr used for mobile applications.

Keywords: *hydrogen, pressure vessel, metalhydride, static structural*

1 Introduction

New technologies and new vehicle propulsion concepts need to be considered for the development of modern transport systems that meet the ambitious targets for reducing greenhouse gas emissions set out in the Paris Agreement from the end of 2015. In addition to the contractually agreed and accelerating need to contribute to significant emission reductions, such developments would help to replace fossil fuel energy, in which most countries around the world are highly dependent on imports. Thus, fossil fuels cannot be part of a sustainable transport system. A promising technological concept that meets the above requirements is the use of hydrogen in combination with fuel cells and an electric engine. In comparing with battery electric vehicles, hydrogen vehicles could be operated for much longer distances without refuelling. But such a concept of hydrogen-based mobility will only be successfully implemented in the existing market if hydrogen can be stored safely, quickly, and technically advanced, in an economically efficient and environmentally friendly way. [1] [4].

One of the solutions for hydrogen storage is the use of metal hydride alloys, which work on the principle of absorption into the structure of the metal alloy. This type of hydrogen storage is low-pressure, where working pressures range from 1 bar to 3 MPa. A metal hydride can also bind hydrogen into its structure at room temperatures. Considering these advantages that this hydrogen storage provides, this method of hydrogen storage is considered a suitable candidate for solving the problem of hydrogen storage in mobile applications [3].

1.1 Hydrogen storage in metal hydrides

As part of the solution of this work, the Hydralloy® alloy was chosen, the composition of which is based on MnTiVFeZr.

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For the design, an alloy in the form of a powder is considered, the grain size of which ranges from 0-2 mm. In Fig. 1. shows a PCI curve of three repeated measurements of the applied MH alloy at room temperature.

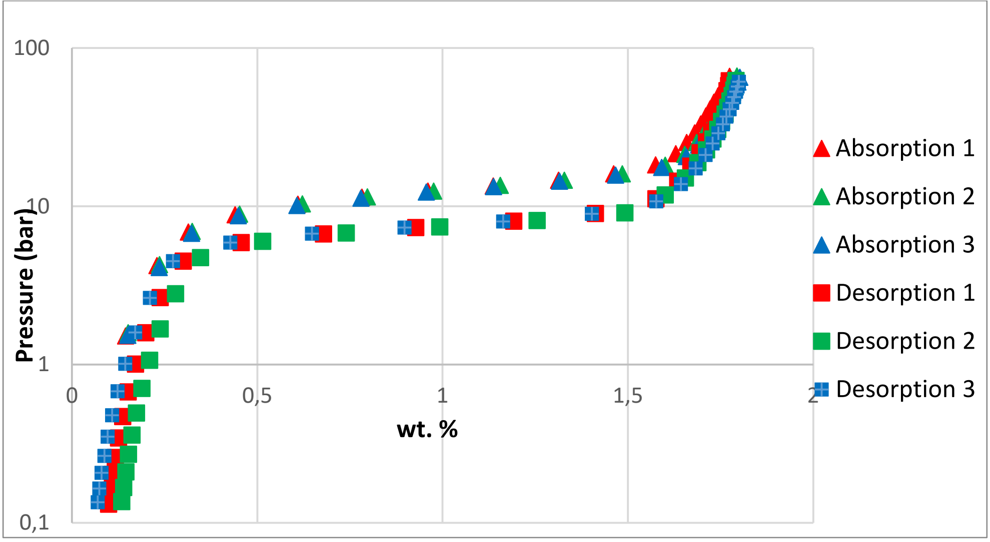

Fig. 1. PCI absorption and desorption curve of Hydralloy® alloy at room temperature.

It can be seen from the PCI curves that the capacity of the stored hydrogen at a temperature of 20 °C and a pressure of $65 \cdot 10^5$ Pa expresses the ratio of the weight of absorbed hydrogen to the weight of the alloy at the level of 1.8 %. Hydrogen is absorbed into the structure of the MH alloy at a pressure of $11.95 \cdot 10^5$ Pa. Hydrogen desorption from the structure of the MH alloy occurs at a pressure of $7.33 \cdot 10^5$ Pa.

Since the absorption of hydrogen into the intermetallic structure of the metal alloy results in the release of heat, it is necessary to dissipate the generated heat. The amount of heat released depends on the type of alloy used, for example in the case of an MH alloy based on LaCeNi, 1 MJ of heat is released when 1 m^3 of molecular hydrogen is absorbed. This heat can be used within the vehicle or other mobile heating device. When desorbing hydrogen from the structure of an MH alloy, it is necessary to bring the same amount of heat. Based on the above facts, in addition to the design of MH storage tanks, it is also necessary to consider the design of temperature management, which allows heat to be removed, but also supplied [3] [4].

2 Design of metalhydride pressure vessel for hydrogen storage

The design of the vessel must be based on the standard STN EN 13322-2. This standard provides a specification for gas transport cylinders, the design and manufacture of refillable steel transported welded gas cylinders in this case the medium by which the container will be filled is hydrogen. This European Standard describes the minimum requirements for the design, material, manufacturing processes and manufacturing tests of stainless steel transport cylinders with a water volume in the range of 0.5 to 150 litters for liquefied dissolved and compressed gases. The standard is only applicable to stainless steel cylinders with a maximum tensile strength up to $1100 \cdot 10^6$ Pa. The construction of the vessel consists of two main parts first is primary pressure vessel in which metal hydride powder is located and casing (Fig. 2.). Between the primary pressure vessel and the casing, there is an interspace space in which the coolant flows. For the construction of the metal hydride vessel, stainless steel type 1.4404 or 316L was chosen with mechanical properties listed in Tab. 1. The use of the steel type is prescribed by the standard [1]

Table 1. Mechanical properties of stainless steel 1.4404.

0.2% Re (MPa)	200
Rm (MPa)	500-700
ρ (kg·m^3)	8000
μ	0,3
E (MPa)	$2.1 \cdot 10^5$

where Re - Yield strength (MPa), Rm - structural strength (MPa), ρ - density (kg·m^3), μ - Poisson's number (-) a E - Young modulus of elasticity (MPa).

The tank can be cooled by active and passive modules. The active cooling module is the cooling liquid in this case water, which is in the interspace between the primary pressure vessel and the casing. The passive cooling module is located inside the primary tank and is a heat transfer intensifier which serves to increase the heat dissipation from the tank core in the direction of the fins to the wall of the primary tank where the tank is water cooled. [2]

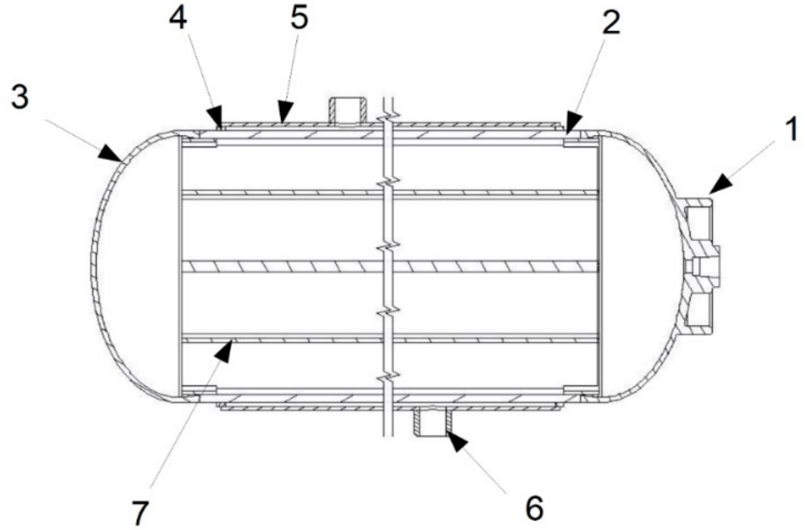

Fig. 2. Design of MH vessel with primary pressure vessel and casing.
1 - cylindrical part of the primary pressure vessel, 2 - elliptical bottom with hole and flange NPT1/4", 3 - elliptical bottom, 4 - flange for casing, 5 - cyllindrical part of casing, 6 - flange G1/2, which serves as a coolant supply, 7 - heat transfer intensifier.

2.1 Design of primary pressure vessel

2.1.1 Calculation of the cylindrical wall thickness of the primary pressure vessel

The wall thickness of the cylindrical shell according to the standard must not be less than calculated using the following formula [7]:

$$a = \frac{D}{2} \cdot \left(1 - \sqrt{\frac{10 \cdot F \cdot J \cdot R_e - \sqrt{3} \cdot p_h}{10 \cdot F \cdot J \cdot R_e}} \right) \qquad (mm) \qquad (1)$$

where: a - calculated minimum tank shell thickness (mm), J - stress reduction factor (-), F - design stress factor (-), Re - calculated yield strength of the material used (MPa), p_h - test hydraulic pressure above atmospheric (bar).

When designing the vessel, the diameter of the primary pressure vessel was 159 mm. Based on Annex A of STN EN 13322-2, the stress reduction factor J is 1 because the butt weld of the closure is considered. The design stress factor F is 0.77 based on the standard. To calculate the minimum thickness, the value of the yield strength Re is limited to a maximum of 0.85·Rg. The calculated value of the yield strength is 425 MPa and the tensile strength Rg of the stainless steel 1.4404 is 500 MPa. The test hydraulic pressure above atmospheric is 47 bar. After substituting all the above constants into equation (1), we get calculated minimum thickness, which is 1 mm.

2.1.2 Design of the bottoms of MH vessel

Standard STN EN 13322-2 prescribes two types of bottoms for closing the vessel, namely torispherical and ellipsoidal. In this work, an ellipsoidal bottom is considered, and the following conditions apply to this type of bottom [7]:

$$H \geq 0.192 \cdot D \qquad (mm) \qquad (2)$$

$$h \geq 4 \cdot b \qquad (mm) \qquad (3)$$

where D - outer diameter of the vessel (mm), h - height of the cylindrical part of the bottom (mm), b - minimum thickness of the cylindrical bottom (mm), H - outer height of the arched part of the bottom (mm).

After substituting the diameter into equation (2), we get the calculated outer height of the arched part of the bottom, which is 30 mm. The value of the outer height of the arched part of the bottom was chosen to be 50 mm.

The wall thickness of the bottom must not be less than the thickness calculated using the following equation [7]:

$$b = a_1 \cdot C \qquad (mm) \qquad (4)$$

where a_1 - value calculated in accordance with the calculated minimum wall thickness of the cylindrical shell of the primary pressure vessel (J = 1), C- shape factor, the value of which must be obtained from the graphs given in the standard STN EN 13322-2.

The value of the shape factor is 0.7 based on the standard. Subsequently, the value of the shape factor is substituted to the equation of the minimum thickness of the bottom of the container (4), whereby the minimum thickness of the bottom is 0.7 mm.

After substituting the equation of the minimum bottom thickness into equation (3), the calculated height of the cylindrical part of the arched bottom is obtained and is 2.8 mm. The selected height of the arched part of the bottom of the tank is 20 mm.

2.1.3 Minimum wall thickness of the MH vessel

In addition to equations (1) and (4), the condition must be that the selected thicknesses of the cylindrical part and the bottom of the primary pressure vessel must not be less than the following relationship [7]:

$$D \geq 150mm, a = b = \frac{D}{250} + 0.7 \text{ with absolute minimum of } \mathit{1.5\ mm} \tag{5}$$

After substituting the outer diameter of 159 mm of the primary container into equation (5), a value of 1.324 mm is obtained, so that the absolute minimum thicknesses of the bottom and the cylindrical part of the primary container are 1.5 mm. The selected thickness of the primary pressure vessel is 4.5mm and of the bottom is 3mm.

2.1.4 Design of casing for MH vessel

The casing in the MH vessel serves as an accessory because it is not exposed to the same pressure as in the primary pressure vessel. The standard also stipulates that the vessel must be made of steel compatible with the steel of the primary pressure vessel, meaning that the material from which the casing will be made is stainless steel 1.4404 or 316L. The design of the casing for the MH vessel is shown in Fig. 2.

Each accessory must be designed in such a way that it is possible to check the welds, meaning that the parts of the primary vessel must not be longitudinally welded but must be seamless. The individual parts of the casing can be made using longitudinal welds.

The use of bottoms to close the casing is not considered, but the use of flanges is considered, which describe the size of the primary container with their inner diameter [7].

3 Strength calculation of the designed MH vessel

The investigated metal hydride container must be divided into n finite elements. The finite element network (Fig. 3) consists of approximately 200,000 volumetric finite elements with quadratic approximation and 500,000 nodal points. The mechanical properties of the stainless steel material were used to solve the strength calculation (Tab. 1). The next step of the simulation is the creation of boundary conditions. The boundary conditions applied to the investigated model are [5]:

1. The force acting on the wall surface of the vessel resulting from the weight of the powdered metal hydride was replaced by the equivalent action of the hydrostatic pressure of a fictitious liquid with the same density of 7 000 $kg \cdot m^{-3}$ [6].
2. The pressure on the inner surfaces of the examined tank was set to an operating pressure of 3 MPa later to a maximum test hydraulic pressure of 4.7 MPa.
3. The pressure on the outer walls of the tank at a level of 0.5 MPa is considered.
4. At the same time, a condition with hydrostatic pressure and density of 1 000 $kg \cdot m^{-3}$ is applied to surfaces that are in contact with the coolant.
5. The self-weight condition of the metal hydride container is applied.
6. The applied cylindrical bonds with the circumference describing the size of the metal hydride container. The bond at the container valve has removed radial and

axial displacements and the bond at the closed end of the container has removed degrees of freedom only in the radial direction.

7. A temperature condition of 60 °C is considered. It is the borderline temperature at which Hydralloy® metalhydride can absorb hydrogen into its structure.

3.1. Results of strength calculation simulation

The first simulation is set at an internal pressure of 3 MPa, which represents the operating pressure. After setting the boundary conditions of the simulation, the results were obtained. The results of this simulation are shown in Tab. 2. In the second simulation, the internal pressure was adjusted to 4.7 MPa, which represents the maximum test hydraulic pressure above atmospheric. The results of this simulation are shown in Tab. 3.

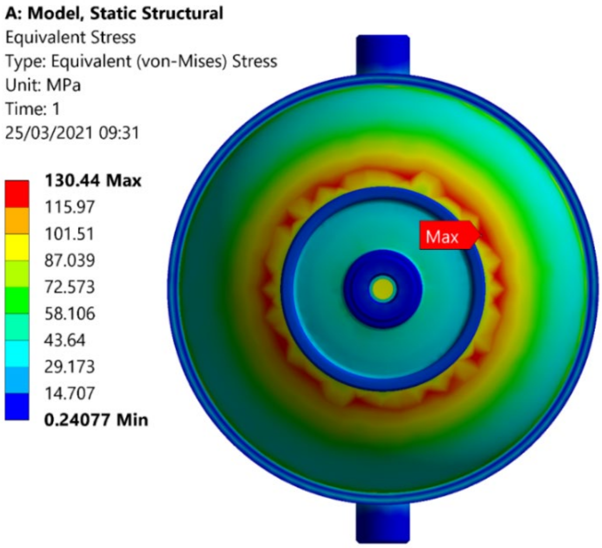

Fig. 3. Equivalent Von Misses stress on MH vessel.

Table 2. Resulting values of the MH vessel at internal pressure 3 MPa.

Total deformation	0.06 mm
Directional deformation in y direction	0.04 mm
Directional deformation in x direction	0.01 mm
Equivalent Von Misses stress	83.6 MPa

Table 3. Resulting values of the MH vessel at internal pressure 4.7MPa.

Total deformation	0.09 mm
Directional deformation in y direction	0.07 mm
Directional deformation in x direction	0.02 mm
Equivalent Von Misses stress	130.9 MPa

4 Conclusion

Simulations in the Ansys Static Structural program showed that the MH vessel, which was designed according to the standard STN EN 13322-2, meets the requirements for operating parameters, as the equivalent Von Misses stress at an operating pressure of 3 MPa and at maximum test hydraulic pressure of 4.7 MPa did not exceed the yield strength of the selected material. With the help of simulations, the shape of the selected bottom was also verified based on the standard. The selected wall thicknesses of the structure were verified by simulation to support the strength of the vessel. By combining the stress calculation and the standard, the ideal characteristic dimensions of the vessel were chosen. The next step is to design an efficient cooling of the container during the absorption of hydrogen into the metal alloy structure.

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