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Measurement of boundary conditions for numerical solution of temperature fields of metal hydride containers

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ABSTRACT

The presented paper describes the measurement of boundary conditions while cooling a metal hydride (MH) container with the $La_{0.85}Ce_{0.15}Ni_5$ alloy. Results are subsequently used for 3D simulation of thermal field in the container during the process of hydrogen absorption. To solve the complicated flow of cooling medium among individual pressure receptacles, ANSYS CFX simulation tool is used and the finite volume method is applied. The same simulation tool is used to describe heat conduction in the metal alloy and the container. For the given construction of the container, uniform distribution of stored hydrogen can be expected among individual receptacles. For cooling the system, cooling radiator is used which is based on Peltier elements. The radiator also enables, in case of desorption, to warm the container. By measuring flows of working substances and the relevant temperatures, it is possible to obtain, by subsequent analysis of temperature flows, the resulting value of the internal heat source. This internal heat source creates a temperature gradient in the container, which impedes exact determination of Pressure Concentration Isotherm curves that should be ideally measured at constant temperature. In addition, measuring in combination with numerical calculations offers a closer look at the absorption process directly in the hydrogen manufacturing plant where, using the alternative energy source, hydrogen is produced and subsequently stored. The results enable to optimize the cooling process in MH hydrogen storage equipment of similar construction and indicate problems with meeting the requirements of the American Department of Energy (DOE).

1. Introduction

Price fluctuations in fossil fuel markets, their limited resources, geopolitical tensions and rising energy consumption define at the moment important position of renewable energy sources (RES). Therefore, the area of RES is, understandably, one of the priorities of European, national and global energy policies. Currently, attention is also directed to the production of hydrogen from renewable energy sources. The production of electricity by photovoltaic panels, or wind turbines, respectively, is marked by instabilities caused by unstable natural conditions. As a result, those sources represent a significant burden for the electricity transmission and supply system.

There are two options to overcome the variability in performance of photovoltaic and wind power: transfer of the energy use or energy storage. Electrical energy can be stored only if it is converted into another form of energy. One possible way is to produce and store hydrogen.

The essential advantage of hydrogen against electricity is the possibility of hydrogen storage: nevertheless the

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low density of hydrogen makes its storage difficult. The volumetric energetic density of hydrogen is relatively low and high pressures must be used for the common way of storage in pressure vessels. By the use of metal hydrides (MH) lowering of the pressures can be reached at energetic densities even higher than in case of liquid hydrogen storage. This form of hydrogen storage is also safer than the classical ones. A commonly accessible type of MH is the intermetallic alloy $LaNi_5$, especially its related alloys with cerium (Ce) addition.

$LaNi_5$ has the working pressure in the range of 1–10 bars and the temperature of 20–60 °C, which are values compatible with the selected types of high pressure electrolyzers and fuel cells [1,2]. The US Department of Energy established in 2012, under the "FCT Program's multiyear Research, Development and Demonstration Plan", number of parameters representing technological objectives for efficient usage of mobile hydrogen storage tanks to be achieved in 2020. One of them is the minimum time for storage of 5 kg hydrogen, which was set to 3.3 min. The minimum weight capacity should reach 5.5 wt% and the minimum volume capacity 0.04 kg H_2/L of system [3,4]. An interesting objective is also the cost of the storage system of $333/kg of H_2 stored. Achieving this price is problematic, given the significant number of laboratory investigated alloys based on La, Mn, Cr and V, especially for its higher price, or difficult and highly expensive preparation.

Hydrogen absorption is a complex process. It consists of the adsorption of hydrogen on the surface of the alloy, followed by catalytic dissociation of the hydrogen molecule and subsequent diffusion of the hydrogen atoms into intermetallic structure of the metal. This process is accompanied by the generation of considerable amounts of heat [5]. The value for the alloy $LaNi_5$ is −30.8 kJ of heat per mole of the stored hydrogen [6,7]. Due to the heat transfer in the powder form of metalhydride, the adsorption of the hydrogen requires to cool the tank. Despite efforts to improve the geometry while designing the storage tanks, significant temperature gradients are generated. Problematic measuring of the heat field inside the tanks led number of authors to numerical solution of hydrogen absorption while simulating cooling media [8,9]. Freni et al. [1] presented a 3D model in COMSOL Multiphysics for $LaNi_5$ simulation at different setups of the cooling system. The used mathematical model calculated with the law of conservation of energy and mass for fluids, and with the hydrogen diffusion via powdered alloy using Darcy's law. It also described the kinetics of adsorption as a function of difference between the local and the equilibrium pressures.

The main objective of this article is to describe the linking and the measurement of the boundary conditions of the MH container placed in the hydrogen production plant where hydrogen is produced from the renewable energy sources. The measurement is founded on calorimetric determination of heat, using device based on the Peltier's elements, and by measuring the relevant temperatures. Based on findings, the internal source of heat (generated in the tank) is specified. Results of the measurement of the boundary conditions dependent on time of the real hydrogen absorption are subsequently used as input data to 3D simulation using the simulation tool ANSYS CFX [10–14]. This tool uses the finite volume methodology in order to deal with the cooling water flow and the heat transfer in individual parts of the reservoir to determine the non-stationary temperature field during the hydrogen absorption. Obtained results allow to optimize the cooling of the reservoir and to quantify more accurately the temperature used to define the PCI (Pressure Concentration Isotherm).

2. Description of the experimental measuring system

The measuring system is a part of the Laboratory of hydrogen technologies, which serves for a comprehensive research of issues related to the storage of energy obtained from a renewable source in form of hydrogen, and its subsequent transformation into electric energy. The laboratory is designed to operate as an insular energy system. Solar energy is converted into electricity by means of photovoltaic panels, placed on a steel structure above the roof of the building, with the surface vector oriented to the southwest. The photovoltaic system consists of 12 pieces of Sanyo HIT 250 panels. This are hybrid photovoltaic (PV) panels, in which the monocrystalline silicon is coated with a layer of amorphous silicon. The combination of the monocrystalline with the amorphous silicon allows for more efficient transformation of solar radiation, in particular of its diffusion component. Amorphous panels show sufficient efficiency even in low light conditions. PV modules are connected in two rows of six panels, each with a power of 250 Wp (total power of 3 kWp). Interconnection of PV panels is the series/parallel. This setup ensures a sufficient voltage for backup batteries charging and also reduces power losses. Electric energy is accumulated in batteries, or it is further consumed in the electrolyzer to produce hydrogen. Batteries are maintenance-free with the electrolyte fixed in AGM glass fiber. Two batteries are connected in series, with a total electrical capacity of 24.3 kW h. Batteries of the hydrogen accumulation system serve for storage of energy from PV panels that is not directly consumed by the connected electrolyzer and analyzer. In case there is a problem with weather conditions, causing a temporary restriction of the production of electricity from solar panels, the batteries are able to cover the consumption of the electrolyzer for about one hour in full operation mode. Charging of batteries is made by the inverter SunnyIsland 2224 which also ensures keeping a stable frequency within the insular energy system. Another inverter, the SunnyBoy 5000 with P_{max} = 5 kW, is used to regulate and deliver electric power from the PV panels. This inverter enables connection of the transformed energy into the insular energy system. The main objective of the PV panels and inverters is to transform solar energy into electric energy which is used to feed the electrolyzers. For correct functioning of the generator it is necessary to ensure continuous supply of deionized water which is prepared in the deionizer SolPure 7. Water for generation of hydrogen must have its specific conductivity of 0.5 $\mu S\ cm^{-1}$. The deionizer itself is capable of delivering water with a conductivity below 0.1 $\mu S\ cm^{-1}$.