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The development of a computational platform to design and simulate on-board hydrogen storage systems

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ABSTRACT

A computational platform is developed in the Modelica® language within the Dymola™ environment to provide a tool for the design and performance comparison of on-board hydrogen storage systems. The platform has been coupled with an open source library for hydrogen fueling stations to investigate the vehicular tank within the frame of a complete refueling system. The two technologies that are integrated in the platform are solid-state hydrogen storage in the form of metal hydrides and compressed gas systems. In this work the computational platform is used to compare the storage performance of two tank designs based on the tubular tank configuration with $Ti_{1.1}CrMn$ as the absorbing alloy. Results show that a shell and tube layout with metal hydride tubes of 2 mm inner diameter achieves the desired refueling time of 3 min and store a maximum of 3.1 kg of hydrogen in a 126 L tank, corresponding to a storage capacity four times larger than a tube-in-tube solution of the same size. The volumetric and gravimetric densities of the shell and tube are 2.46% and 1.25% respectively. The dehydriding ability of this solution is proven to withstand intense discharging conditions.

Introduction

The transportation sector accounts for approximately 14% of the global emissions of greenhouse gases (GHGs), two thirds of which come from road transportation, which is entirely dependent upon fossil fuels and was responsible for 112 million metric tons of equivalent CO_2 in 2014 [1]. Therefore, a clean alternative to current gasoline cars can provide a substantial benefit in terms of GHG reduction and global warming mitigation. One of these clean technologies is the fuel cell electric vehicle (FCEV). Despite the recent commercialization of FCEVs [2,3], many challenges have yet to be overcome in order to establish a solid ground for a significant market penetration of such a technology. The development of an effective solution for on-board hydrogen storage is one of the main technical tasks that need to be tackled [4,5].

This study presents the Hydrogen Storage and Design Platform (HySDeP), which is intended to serve as a simulation tool to design and compare different vehicular storage options with respect to targets based upon storage and fueling efficiencies, providing a starting point for a comprehensive model library that includes the main on-board storage solutions.

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Attention is given to solutions that involve hydrogen storage in metal hydride tanks and compressed hydrogen gas (CHG) vessel with an integrated phase change material (PCM) as the passive cooling system. A set of libraries is implemented in the modeling platform to select among different material compositions, kinetic equations, heat exchanger configurations and to enable the tailoring of the analysis according to the user needs. An ongoing effort is focusing on expanding such libraries and also including other types of tank configurations. The next step in this direction is to use the developed models to design MH tanks based on the chamber layout and different heat exchanger configurations that can be selected from a wide library. In addition, the effect of performance degradation over charging/discharging cycles is planned to be included in the next platform version.

Reliable computational models are developed to describe hydriding and dehydriding reactions as well as melting and solidification processes that occur in the metal hydride tank and novel compressed-hydrogen vessel respectively [6,7]. For the former, these models are used to quantify the main design parameter, being the critical metal hydride thickness, for the tank/heat-exchanger system as described in the *Heat exchanger designs* Section and in more detail in Ref. [6], wherein a verification of the model is also provided. Only the main results that refer to the MHSS are here presented, as the analysis of the CHG system was discussed in Ref. [7].

This work focuses on the charging and discharging processes of MHSSs to investigate the storage performance of two tank/heat-exchanger systems implemented in HySDeP. The gravimetric and volumetric densities, storage capacity as well as time of refueling/discharging are evaluated to select the most promising layout. Finally, a sensitivity analysis on the main geometrical parameters is carried out to address the advantages and limitations of each configuration and identify strategies for further improvement.

Methods

In this section we describe the methodology used to design the computational platform and set up the charging and discharging analyses presented in this work. In addition, it is made possible to couple the platform with the hydrogen refueling station library presented in Ref. [8] to investigate the different storage options within the frame of a complete refueling system. The platform can be freely downloaded from the github repository of the *DTU-TES* group [9].

Design of the simulation platform

The design approach of the platform is based on three criteria, such as:

- flexibility;
- user friendliness;
- ease of third party development.

These concepts are chosen to make the platform work as both a design/simulation tool for users and a well-structured environment for model developers. This means that the platform should be designed to adapt the needs of different users and should be based on an efficient and clear architecture in order to ease the code modification. In order to make the use of the platform as straightforward as possible for both types of end-users, its design is based on a multi-level architecture.

The first level corresponds to the *macro*-models representing the main physical components. Such components correspond to containers within which multiple nested sub-models are defined to perform intermediate calculation tasks. These sub-models represent the second level of hierarchy. The user should have direct access only to the *macro*-components. This occurs via the graphical interface, through which the domain of investigation and the values for the input parameters can be defined. To simplify the user interaction with the platform, the number of macro-models is limited to three, namely *Ambient*, *Refueling station* and the tank system. The developer should have access to both levels in order to modify the structure and operation of the platform. Different *if* -scenarios guide the user through the model set up, enabling the selection of various options and thus, the tailoring of the analysis based on specific needs. The first choice the user is asked to take, refers to which storage system should be investigated: MHSS or CHG-tank with or without PCM.

The component hierarchy should be implemented with preference for constructs that keep the modeling approach as simple and intuitive as possible. In Modelica® the above preference translates in the use of *inner/outer* and port/connector elements rather than nested *extends* constructs to exchange constant and variables between models. In addition, the code should be well commented to ease the understanding of all the implemented features. A reference list is included at the end of each component code to make transparent the source of equations, thermo-physical properties, thermal models and assumptions. These aspects are of fundamental importance as the platform should in principle allow for its use and modification by different users, including both company employees and researchers. In Fig. 1 the platform structure is shown in view of its *macro*-components and main implemented features.

Fig. 1 should be read as a black box scheme where the main components and information flows are presented. A more detailed description of the sub-models contained inside each *macro*-component can be found in Ref. [10], whereas the entries of the libraries presented in such a figure are reported in Appendix A. The ambient model serves as the environment where the user defines the ambient conditions in terms of pressure and temperature (i.e. p_{amb} and T_{amb}) that are passed to the refueling station and tank models. In the refueling station the user selects the hydrogen temperature at the tank inlet. In addition, if the PCM-tank is selected as the investigated system, the tank type (e.g. Type III or IV) and the initial pressure should also be given as inputs. These two parameters are used together with p_{amb} and T_{amb} to determine the appropriate refueling protocol, which, in turn, defines the fueling pressure ramp for CHG storage systems according to SAE J2601 as discussed in Ref. [7].

In the tank model all the equations concerning energy and mass balances, kinetics and heat transfer are solved (see Appendix B and Refs. [6,7]). This occurs according to the model