ARTICLE IN PRESS

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2018) 1–13

Available online at www.sciencedirect.com

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journal homepage: www.elsevier.com/locate/he

Design tool for estimating chemical hydrogen storage system characteristics for light-duty fuel cell vehicles☆

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ARTICLE INFO

Article history:
Received 18 January 2018
Received in revised form
12 March 2018
Accepted 13 March 2018
Available online xxx

Keywords:
Fuel cell vehicle
Chemical hydrogen storage
Ammonia borane
Alane
System model

ABSTRACT

The U.S. Department of Energy (DOE) developed a vehicle Framework model to simulate fuel cell-based light-duty vehicle operation for various hydrogen storage systems. This transient model simulates the performance of the storage system, fuel cell, and vehicle for comparison to Technical Targets established by DOE for four drive cycles/profiles. Chemical hydrogen storage models have been developed for the Framework for both exothermic and endothermic materials. Despite the utility of such models, they require that material researchers input system design specifications that cannot be estimated easily. To address this challenge, a design tool has been developed that allows researchers to directly enter kinetic and thermodynamic chemical hydrogen storage material properties into a simple sizing module that then estimates system parameters required to run the storage system model. Additionally, the design tool can be used as a standalone executable file to estimate the storage system mass and volume outside of the Framework model. These models will be explained and exercised with the representative hydrogen storage materials exothermic ammonia borane (NH_3BH_3) and endothermic alane (AlH_3).

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Introduction

Fuel cell powered automobiles offer the potential for increased fuel efficiency, reduced dependency on foreign oil, and elimination of emissions such as pollutants or greenhouse gases. One of the challenges of fuel cell vehicles is onboard storage of the hydrogen fuel. Both high-pressure gaseous hydrogen (350–700 bar) and cryogenic liquid hydrogen storage (20 K) methods have been implemented [1,2]. To reduce the temperature and pressure limitations of storing neat hydrogen under these conditions, three material-based storage

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https://doi.org/10.1016/j.ijhydene.2018.03.090
0360-3199/© 2018 Published by Elsevier Ltd on behalf of Hydrogen Energy Publications LLC.

Please cite this article in press as: Brooks KP, et al., Design tool for estimating chemical hydrogen storage system characteristics for light-duty fuel cell vehicles, International Journal of Hydrogen Energy (2018), https://doi.org/10.1016/j.ijhydene.2018.03.090

alternatives have been developed: 1) adsorbents [3–5], 2) metal hydrides [6–9], and 3) chemical hydrogen storage (CHS) materials [10–15]. These material-based storage alternatives provide not only more reasonable pressure and temperature conditions but often improved gravimetric and volumetric storage density of the hydrogen [2]. The challenge of these storage materials is that they must address not only gravimetric and volumetric considerations, but also durability and efficiency during refueling, startup, and operations. Technical Targets developed by the U.S. Department of Energy (DOE) provide metrics for comparison of hydrogen storage materials in an automotive system [16,17]. Although these metrics were developed in the United States, they provide a means of comparing key requirements of any hydrogen storage system. Their primary applicability is for light-duty vehicles, but the results can be expanded into other vehicle and portable uses as well as stationary power applications.

A challenge of the Technical Targets is that they are based on automotive system characteristics (e.g. startup time, transient response, delivery pressure, and efficiency) rather than on materials. As a result, when new a hydrogen storage material is developed, it is difficult use its properties to determine if it will meet all of the system Technical Targets. Material developers generally measure capacity, thermodynamics, and kinetic properties, but may not be in a position to estimate the gravimetric and volumetric capacity of the hydrogen storage system and its performance under a variety of transient conditions and ambient temperatures.

DOE established the Hydrogen Storage Engineering Center of Excellence (HSECoE) to address the engineering aspects of material-based hydrogen storage [6]. The center was not engaged in development of new hydrogen storage materials themselves. Instead it addressed engineering system design challenges associated with currently available hydrogen storage materials. This work focuses on CHS materials assessed as part of the HSECoE. CHS materials are defined as materials that release hydrogen by breaking chemical bonds. Once these bonds have reacted to produce hydrogen, the material must be removed from the system and regenerated before it can be reused [2]. This differs from other hydrogen storage material that can be regenerated with neat hydrogen directly onboard the vehicle. CHS materials must be removed from the vehicle to be regenerated.

The HSECoE addressed engineering of storage materials specifically for light-duty vehicles. The work involved identifying, developing, and experimentally evaluating critical components of the storage system on a bench scale. Where possible, efforts were made to reduce the system mass, volume, and cost through value engineering of tanks, heat exchangers, and balance-of-plant components. Hydrogen storage system models then were developed and validated using Simulink® simulation software that could be integrated into a light-duty fuel cell vehicle Framework model [18]. The purpose of the Framework model is to provide insight into overall system performance under a variety of drive-cycle scenarios [19]. HSECoE then used the experimental work performed on a bench scale to validate the models.

In 2015, CHS material properties required for automotive applications were documented by Semelsberger and Brooks who estimated material properties of the hydrogen storage materials that would be required to meet DOE Technical Targets [20]. The hydrogen capacity, kinetics, reaction enthalpy, and other chemical properties necessary to meet the targets were estimated to provide guidance to material researchers.

The CHS system design [6] and its associated Simulink model [21] for a light-duty vehicle represent two promising CHS materials: ammonia borane (AB), an exothermic material, and alane, an endothermic material. Both of these materials have been considered extensively for hydrogen storage [10–15]. The Simulink model was developed to simulate the performance of the hydrogen storage system in a light-duty fuel cell vehicle for a set of four drive cycles or transient speed profiles described previously [22]: 1) a highway cycle (UDDS + HWFET), 2) an aggressive cycle (US06), 3) a cold-start cycle (FTP), and 4) a hot cycle (SC03). Validation of the model against experimental data also is described. Earlier stages of development of this CHS model also have been documented previously [23,24].

The purpose of this current work is to describe the development and utility of a System Design Tool as a preprocessor to the storage system and vehicle-level model previously presented. Because material developers may not be able to determine the CHS system design information to input into the Framework model, we have developed a System Design Tool to make initial estimates for these design parameters available to material developers. The tool provides an estimate of the total system mass and volume and the size of the individual components that feed into the Hydrogen Storage Model and the Framework model. It also estimates the control parameters required for a particular hydrogen storage material.

The System Design Tool bridges the gap between the thermodynamic and kinetic information generally measured by hydrogen storage material developers and the information needed to exercise the light-duty fuel cell vehicle Framework model and demonstrate a material that adequately meets the requirements for an automotive hydrogen storage system.

Chemical hydrogen storage system design

The CHS system design developed is flexible and adaptable to a wide range of fluid-phase materials. It has the flexibility to operate with slurries and neat fluids, and with only minor system modifications, it can be operated with both endothermic and exothermic materials. The current model assumes the materials react when through thermolysis or homogeneous catalysis heated. The system process flow and its components are shown in Fig. 1.

Hydrogenated slurry is loaded on the vehicle where it is stored in a volume-displacement tank. This style of tank has a membrane separating the feed and product within a single tank (TNK-1). As fresh slurry is loaded into the tank, the membrane displaces spent slurry out of the tank and back to the filling/transfer station for reprocessing. During system operation when hydrogen is being generated, the fresh slurry is transported from the feed side of the tank through the process and then back into the spent slurry side of the volume-displacement tank. The advantage of using a volume-displacement tank is that the overall tank volume is reduced by a factor of two.

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