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Dynamic modeling and simulation of hydrogen supply capacity from a metal hydride tank

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ABSTRACT

The current study presents a modeling of a $LaNi_5$ metal hydride-based hydrogen storage tank to simulate and control the dynamic processes of hydrogen discharge from a metal hydride tank in various operating conditions. The metal hydride takes a partial volume in the tank and, therefore, hydrogen discharge through the exit of the tank was driven by two factors; one factor is compressibility of pressurized gaseous hydrogen in the tank, i.e. the pressure difference between the interior and the exit of the tank makes hydrogen released. The other factor is desorption of hydrogen from the metal hydride, which is subsequently released through the tank exit. The duration of a supposed full load supply is evaluated, which depends on the initial tank pressure, the circulation water temperature, and the metal hydride volume fraction in the tank. In the high pressure regime, the duration of full load supply is increased with increasing circulation water temperature while, in the low pressure regime where the initial amount of hydrogen absorbed in the metal hydride varies sensitively with the metal hydride temperature, the duration of full load supply is increased and then decreased with increasing circulation water temperature. PID control logic was implemented in the hydrogen supply system to simulate a representative scenario of hydrogen consumption demand for a fuel cell system. The demanded hydrogen consumption rate was controlled adequately by manipulating the discharge valve of the tank at a circulation water temperature not less than a certain limit, which is increased with an increase in the tank exit pressure.

1. Introduction

Metal hydrides have been receiving a great attention as a means of hydrogen storage, energy conversion materials such as heat pumps, refrigerators, heat engines [1–8]. In the context of hydrogen storage and supply capacity to power generation systems driven by hydrogen as a fuel, e.g. fuel cell driven automobiles, a particular interest lies in the effective hydrogen storage capabilities of metal hydrides due to their high volumetric density and prompt reversibility at relatively low pressures and moderate temperature ranges, which gives several advantages over other hydrogen storage methods

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Nomenclature

A_{th}	throttle area at the tank exit, m^2
C_a	constant for hydrogen desorption rate, 1/s
C_{pg}	specific heat of H_2, J/kg/K
C_{ps}	specific heat of metal hydride, J/kg/K
C_{pw}	specific heat of water, J/kg/K
d_e	exit port diameter of tank, m
D	diameter, m
E_a	activation energy, J/mol
ΔH	heat of reaction, J/kg_{H_2}
L	length, m
$\dot{m}_{MH}$	mass flow rate of hydrogen desorbed from the metal hydride, kg/s
$\dot{m}_{out}$	mass flow rate of hydrogen leaving the tank, kg/s
$\dot{m}_w$	circulation water flow rate, kg/min
M_e	Mach number at the tank exit
P	pressure, Pa
R_u	universal gas constant, J/mol K
U	overall heat transfer coefficient, W/m^2 K
V	volume, m^3
α_1, α_2, β	constant in Eq. (6)
γ	specific heat ratio
ε	porosity of metal hydride
ϕ, ϕ_0	constant in Eq. (6)
ρ_{s0}	density of empty metal hydride, kg/m^3
ρ_{ss}	density of saturated metal hydride, kg/m^3

Subscripts

e	exit of the tank
eq	equilibrium
MH	metal hydride
tank	metal hydride tank
w	circulation water
0	reference

utilizing high-pressure vessels or cryogenic techniques [1]. Research associated with metal hydrides may be categorized into the following three regimes. The first is related to the development of the metal hydride material with an enhanced storage capacity. The second is related to quantitatively detailed analyses of heat and mass transfer inside a metal hydride for a detailed characterization of hydrogen absorption and desorption processes. The third is related to dynamic performance analyses of hydrogen discharge process from a metal hydride subsystem in an energy conversion system equipped with metal hydrides, e.g. a fuel cell system. A variety of numerical studies have been conducted taking into account heat and mass transfer with reaction kinetics inside a metal hydride to examine the internal transfer mechanisms and/or optimize the operation characteristics [9–14]. Though numerical simulation techniques have been getting more and more intricate, they still rely on some assumptions about the key parameters, which significantly influence the overall performances, such as heat transfer coefficients and reaction kinetic variables. Thus, these intricate simulations lead to enhanced, yet often similar, conclusions with accuracy being compromised by computation time, particularly, in case of multi-dimensional simulations. On the other hand, numerous studies on the performance analysis of a metal hydride subsystem which serves as a part of an integrated fuel cell system have been demonstrated by some researchers [15–19]. Macdonald and Rowe [15] investigated the performance of a metal hydride which is thermally coupled with a fuel cell system. They simulated hydrogen gas pressure in a metal hydride tank for a pulsed hydrogen demand load using a simplified P–C curve where the equilibrium pressure is only a function of temperature. Førde et al.[16] experimentally investigated hydrogen supply capacity of a metal hydride storage unit which is thermally integrated with a fuel cell stack through a common water circulation loop. Their results showed that it was possible to utilize the full hydrogen storage capacity of the metal hydride hydrogen storage unit only when the metal hydride temperature was kept above a certain temperature by utilizing the waste heat from the fuel cell stack via water circulation loop.

The objective of the study is to demonstrate the dynamic response of hydrogen discharge from a metal hydride tank, and evaluate the effects of key operating parameters on the performance of hydrogen supply capacity. As the model presented here is developed as a part of a larger model of the dynamics of a fuel cell system, a lump model with a minimum number of modeling parameters was presented using MATLAB SIMULINK, instead of using a multi-dimensional model that requires many physical parameters, to specifically focus on the overall dynamic response of hydrogen discharge for operational ranges of pressure and temperature. Empirical fits of the P–C–T curve were utilized to model the desorption characteristics of the metal hydride. PID control logic was also implemented in the hydrogen supply system to demonstrate how the operation parameters affect the capacity of hydrogen supply for a representative scenario of hydrogen consumption demand for a fuel cell system. The sections that follow consist of the mathematical modeling in Section 2 and the results in Section 3. For detailed results and discussions, Section 3.1 describes basic characteristics of hydrogen discharge processes taking into account two mechanisms that drive hydrogen discharge. Section 3.2 conducts parametric studies to examine the dependence of hydrogen discharge characteristics upon the initial tank pressure, the circulation water temperature and flow rate, the overall heat transfer coefficient, and the metal hydride volume fraction in the tank. Finally, Section 3.3 demonstrates dynamic responses of hydrogen discharge processes using PID control logic for oscillating cycles of hydrogen demand to examine the controllability of hydrogen discharge rate for various operation conditions.

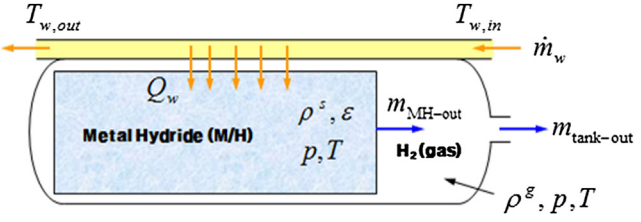

Fig. 1 – Schematic of a metal hydride tank.