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Charge-discharge cycle thermodynamics for compression hydrogen storage system

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ABSTRACT

Knowledge of the evolution of the thermodynamic properties of hydrogen storage systems, such as temperature and pressure, is required in order to evaluate and optimize their performance. The thermodynamic models of hydrogen storage systems are based on the mass and energy balance equations. They can be expressed, for high level analysis, as lumped parameter or zero-dimensional models, which are represented as a set of ordinary differential equations. We present a simple thermodynamic model that can predict the charging and discharging of gaseous hydrogen, which allows, in specific situations, for analytical solutions of the temperature and the pressure as a function of time, and can be used to validate more detailed numerical models. From the analytical solution, the final hydrogen temperature of refueling can be expressed as a weighted average of initial, inflow and ambient temperatures. The weighted factors are related to other refueling parameters, such as initial mass, initial pressure, refueling time, refueling mass rate, average pressure ramp rate (APRR), final mass, final pressure, etc. This work may be extended to adsorption-based or metal hydride hydrogen storage system. The analytical solutions can be used for sensitivity studies of hydrogen fueling standard.

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Introduction

Compression hydrogen storage is currently the preferred method for storing hydrogen in fuel cell vehicles due to its simple tank structure and fast refueling process. Knowledge of the evolution of thermodynamic properties, such as pressure and temperature of hydrogen storage systems, is important in order to evaluate and optimize system

performance and to compare the efficiency of various storage strategies (such as compression storage and materials-based storage) [1].

There are two types of models for simulating hydrogen storage systems: distributed parameter models and lumped parameter models. Distributed parameter models can be multidimensional. Multidimensional (2D or 3D) heat and mass transfer analysis, based on computational fluid dynamics (CFD), has been widely used to study hydrogen storage

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Nomenclature

a_f	heat transfer coefficient between hydrogen and ambient fluid, $W/m^2/K$
A_s	internal surface area of tank, m^2
c_p	specific heat at constant pressure, $J/kg/K$
c_v	specific heat at constant volume, $J/kg/K$
h	specific enthalpy of hydrogen, J/kg
h_{in}	specific enthalpy of inflow hydrogen, J/kg
h_{out}	specific enthalpy of outflow hydrogen, J/kg
h_∞	specific enthalpy of either inflow or outflow hydrogen, J/kg
m	mass of hydrogen mass in tank, kg
m_0	initial hydrogen mass, kg
\dot{m}	hydrogen mass flow rate, an algebraic quantity, $\dot{m} = \dot{m}_{in}$ for charge process, $\dot{m} = -\dot{m}_{out}$ for discharge process, kg/s
\dot{m}_{in}	hydrogen mass inflow rate for charge, kg/s
\dot{m}_{out}	hydrogen mass outflow rate for discharge, kg/s
\dot{m}^*	pseudo mass flow rate, $\dot{m}^* = a_f A_s / c_v$, kg/s
M_{H_2}	molecular weight of hydrogen, $M_{H_2} = 2.0159 \times 10^{-3} \text{ kg/mol}$
p	pressure of hydrogen in tank, MPa
p_0	initial pressure, MPa
\dot{p}	average pressure ramp rate (APRR), MPa/min
q	specific heat inflow, $q = \dot{Q} / \dot{m}$, J/kg
\dot{q}	specific heat inflow rate, $\dot{q} = \dot{Q} / m_0$, W/kg
\dot{Q}	heat inflow rate, $\dot{Q} = a_f A_s (T_f - T)$, W
R	universal gas constant, $R = 8.314 \text{ J/K/mol}$
t	time, s
t^*	characteristic time, $t^* = m_0 / \dot{m}$ for charge/discharge processes $t^* = m_0 / \dot{m}^*$ for dormancy processes, s
T	temperature of hydrogen in tank, K
T_0	initial temperature in tank, K
T_f	temperature of ambient fluid, K
T^*	characteristic temperature, K
T_∞	constant inflow or outflow hydrogen temperature, K
u	specific internal energy, J/kg
u^*	specific energy (enthalpy and heat) inflow $u^* = h + q$, J/kg
V_t	internal volume of tank, m^3
Z	compressibility factor
<i>Greek symbols</i>	
α	dimensionless heat transfer coefficient, $\alpha = \dot{m}^* / \dot{m} = a_f A_s / c_v / \dot{m}$
γ	ratio of specific heats, $\gamma = c_p / c_v$
μ	fraction of initial mass over total mass of hydrogen, $\mu = m_0 / m$
τ	dimensionless time, $\tau = t / t^*$

systems based on high pressure compression [2], adsorption in activated carbons [3] and in metal-organic framework [4], and absorption in metal hydride [5]. These distributed parameter models [2–5] can give detailed information on the temperature and density and velocity distributions in the hydrogen storage tank. They are, however, numerically intensive and

cannot be used efficiently, in general, to perform detailed sensitivity analysis and detailed system simulations.

In order to estimate the overall performance of hydrogen storage systems, a top-level thermodynamic analysis based on simplified models is necessary. Lumped parameter models are simple (0D) thermodynamic models based on the mass and energy balance equations, which are derived from basic principles of mass and energy conservation. They predict volume-averaged properties, from which representative system temperatures and other properties can be efficiently estimated. Ahluwalia et al. analyzed the dynamics of cryogenic hydrogen storage [6] and cryo-adsorption hydrogen storage [7] in insulated pressure vessels for automotive applications. Kumar et al. developed a lumped parameter model for cryo-adsorber hydrogen storage tank [8]. A lumped parameter model for charge–discharge cycle of adsorptive hydrogen storage system was developed in Ref. [9], and applied to a cryo-adsorptive hydrogen storage system [10]. These lumped parameter models [6–10] were solved numerically and used for parametric studies. Numerical solutions and parametric studies cannot, by themselves, lead to physically meaningful engineering correlations for hydrogen storage systems. The thermodynamic analysis of lumped parameter models is of great importance for validating numerical models and establishing engineering correlations for hydrogen storage systems. Yang et al. carried out analyses for basic thermodynamic processes involving hydrogen [11] and a thermodynamic analysis of hydrogen tank during refueling process [12].

The current work will extend thermodynamic analyses to whole charge–discharge cycle, which includes four processes: charging, dormancy after charging, discharge and dormancy after discharge. We use a global thermodynamic model to describe the whole charge–discharge cycle. In this work, the analytical solution of a lumped parameter model is used as benchmarks to test and validate numerical methods and models of hydrogen storage system, and to fit final hydrogen temperatures under different refueling conditions. As an example, we use the analytical solution to validate a Matlab/Simulink model of a generation 2 or 3 tank with volume of 151L developed by Lawrence Livermore National Laboratory (LLNL) [13]. The Matlab/Simulink results are compared with the analytical solutions for whole charge–discharge cycle under three different boundary conditions. Both results agree very well.

Another possible application of this approach would be to establish engineering correlations to predict the final temperature after charging hydrogen storage systems. For example, for safety reasons, the gas temperature in the hydrogen tank after refueling is limited to 85 °C. Many experiments have been performed to determine the final gas temperature in the hydrogen tank under different refueling conditions [15–17]. Numerical simulations [18] based on computational fluid dynamics (CFD) have been performed and compared with experiments. This approach could provide a simple correlation between the final gas temperature and the refueling parameters. As second example, we express the final gas temperature as function of initial and final mass based on the analytical solution for the charging process [14]. By this way, we are able to express the experimental data with less number of parameters which are meaningful physically. This

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