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Lumped parameter model for charge–discharge cycle of adsorptive hydrogen storage system

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ABSTRACT

We present a lumped parameter model for an adsorptive hydrogen storage system based on activated carbon. The model simply employs general mass balance and energy balance equations resulted from the fundamental conservation equations of thermodynamics. A modified Dubinin–Astakhov isotherm and a variable isosteric heat of adsorption are adopted in the lumped parameter model to improve validity for whole charge–discharge cycle. The lumped parameter model is implemented in Matlab/Simulink platform and applied to simulate charge–discharge cycle of the hydrogen storage system. Thermal averaging temperature is used to fill the gap between the multi-dimensional models, such as 0D model of Matlab/Simulink and 2D model of Comsol. The model is well validated by two sets of validation tests with the coolants of ice water and room temperature water respectively. The lumped parameter model is efficient and also accurate for predicting performance of adsorptive hydrogen storage system. Parametric studies are conducted to analyze the validity of the variable isosteric heat of adsorption, the practicality of heat transfer coefficient and the effect of hydrogen storage pressure.

1. Introduction

Adsorptive hydrogen storage on activated carbon is considered to be promising for distribution application because of its high gravimetric density, reasonable volumetric density and relatively low cost [1]. Heat and mass transfer related issues during hydrogen storage became worldwide research hotspot.

Various multi-dimensional simulation models are developed to describe the hydrogen storage process. Hermosilla-Lara et al. [2] developed a two-dimensional (2D) model of an activated carbon packed bed storage tank based on Fluent to describe the charge process. Momen et al. [3] analyzed the thermal effect during hydrogen charging in packed activated carbon tank by both experimental and numerical approaches. They reported that heat of adsorption took an important role even for moderately adsorbing activated carbon. The authors of current paper improved the model of Hermosilla-Lara by taking the tank wall into account and using D–A adsorption model, and then built models of the adsorptive hydrogen storage system to simulate charge process of activated carbon hydrogen storage based on Fluent [4] and Comsol [5] respectively. They further improved their model by using realistic geometry instead of the simplified one, and then used it to simulate charge and discharge cycle of activated carbon hydrogen storage [6]. Delahaye et al. [7] reported a 2D model of adsorptive hydrogen storage tank and performed simulations of the charge process of the tank. They pointed out that a model including tank wall is preferred and proposed solutions to improve the performance of the hydrogen storage system.

Multi-dimensional models are proved to be capable of well describing the pressure variation and temperature distribution in the tank. Compared with multi-dimensional models, lumped models are more suitable for system level investigation, for instance to evaluate the performance of hydrogen storage system applied on a fuel-cell vehicle or a renewable energy system. In addition, simulations based on lumped model are much faster than finite element simulations. Kumar et al. [8] designed system level models for sorption-based storage units, including both cryo-adsorption storage and metal hydride-based storage. They incorporated the system level models with detailed transport models to study their performance under representative drive cycle. Raju et al. [9] developed a system simulation model for a residential wind hybrid power system, where a compressed hydrogen storage system is integrated with a wind turbine and a fuel cell.

Many efforts have been paid on the lumped modeling of metal hydride storage systems. Gambini et al. [10] performed a detailed analysis of low-temperature, metal hydride-based hydrogen storage systems and built a model to predict the performance of metal

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Nomenclature

ΔH	isosteric heat of adsorption, J/mol
c_s	specific heat of adsorbent, J/(kg K)
c_p	constant-pressure specific heat of hydrogen, J/(kg K)
c_{va}	constant-volume specific heat of adsorbed phase hydrogen, J/(kg K)
c_{vg}	constant-volume specific heat of gaseous phase hydrogen, J/(kg K)
c_w	specific heat capacity of tank wall, J/(kg K)
h_f	heat transfer coefficient, W/(m^2 K)
$\dot{H}_i$	inflow enthalpy flow rate, W
h_i	specific enthalpy of inflow hydrogen, J/kg
$\dot{H}_e$	outflow enthalpy flow rate, W
h_e	specific enthalpy of outflow hydrogen, J/kg
m_a	mass of hydrogen in adsorbed phase, kg
m_g	mass of hydrogen in gaseous phase, kg
m_s	mass of adsorbent, kg
m_t	total mass of hydrogen, kg
m_w	mass of tank wall, kg
$\dot{m}_i$	inflow mass flow rate, kg/s
$\dot{m}_e$	outflow mass flow rate, kg/s
M_{H_2}	mole mass of hydrogen, kg/mol
n_a	absolute adsorption amount per unit adsorbent, mol/kg
n_0	limit adsorption amount per unit adsorbent, mol/kg
p	lumped pressure, Pa
p_0	saturated pressure, Pa
p_i	initial pressure, Pa
$\dot{Q}_a$	rate of heat of adsorption generation, W
$\dot{Q}_e$	rate of heat transfer, W
R	universal gas constant, J/(mol K)
T	lumped temperature, K
T_f	temperature of coolant, K
T_i	initial temperature, K
$\overline{T}_C$	thermal averaging temperature, K
U	total internal energy of hydrogen storage system, J
V	capacity of hydrogen storage tank, m^3
V_g	volume for gaseous hydrogen, m^3
$\dot{W}$	rate of shaft work, W
Z	compressibility factor

Greek symbols

α	enthalpic factor, J/mol
β	entropic factor, J/(mol K)
ε_b	activated carbon bed porosity
ρ	density, kg/m^3

hydride hydrogen storage devices in fuel cell based energy systems. Raju et al. [11] established a system simulation model for high-pressure metal hydride hydrogen storage systems based on Matlab/Simulink. They analyzed both the refueling and drive cycle of the hydrogen storage system. Visaria et al. [12] studied the influence of the heat transfer and kinetics parameters on the design of heat exchangers for hydrogen storage in high-pressure metal hydrides. They found that fill time is influenced more from thermal conductivity of the metal hydride and the coolant's temperature than from the contact resistance.

Metal hydride storage systems store hydrogen by chemisorption while adsorptive hydrogen storage systems, such as activated carbon (AC) and metal-organic framework (MOF) hydrogen storage system, store hydrogen by physical adsorption. Different principles of hydrogen conservation determine that different adsorption isotherms are applied on these systems. Kumar et al. [13] fitted excess adsorption data of MOF-5 powder to a Langmuir isotherm and developed a quasi-static lumped parameters model for cryo-adsorption of hydrogen on MOF-5 to describe slower processes of hydrogen storage cycle. They pointed out that the temperature gradients within bed during slow processes are expected to be negligible. Kumar et al. [14] developed a generalized model for a cryo-adsorber and analyzed the 1-D results for the isobaric refueling period. A multi-cartridge annular bed design was found to be helpless to enhance the heat and mass transfer processes. Saha et al. [15] experimentally analyzed the adsorption isotherms of *n*-butane on pitch based activated carbon (Maxsorb III) at 298–328 K and 0.02–0.3 MPa and successfully used Dubinin–Astakhov (D–A) adsorption isotherm model to describe all the isotherm experimental data. Richard et al. [16,17] adapted D–A model to describe hydrogen, nitrogen, and methane adsorption isotherms on activated carbon (AX-21) at high pressures and supercritical temperature. Good agreement was observed between modified D–A model and experimental excess adsorption isotherms.

Most lumped models or system level models have been developed based on thermodynamic relations [13,14,18,19]. In these models, a series of ordinary differential equations and differential expressions were developed based on thermodynamic relations of the system. The gases phase density and the adsorption density are obtained through governing equations involving the time derivatives of temperature and pressure, and the isobaric temperature derivative and the isothermal pressure derivative of gaseous density or adsorption density.

In this paper, we develop a lumped parameter model using modified D–A model and conduct system analysis for adsorptive hydrogen storage system. Instead of constant isosteric heat of adsorption, variable isosteric heat of adsorption is adopted to improve validity. The lumped parameter model simply employs general mass balance and energy balance equations resulted from the fundamental conservation equations of thermodynamics. It is implemented numerically in the Matlab/Simulink platform (Ver. 2009b), so there is no need to derive analytically a number of complex expressions for different thermodynamic processes, such as the time derivatives of temperature and pressure, and the temperature and pressure derivatives of mass and energy.

The whole charge–discharge cycle is studied based on the Simulink model. The concept of thermal averaging temperature is used to fill the gap between the multi-dimensional models, such as 0D model Matlab/Simulink and 2D Comsol finite element model. Thermal averaging temperature results computed by Comsol model (Ver. 3.6) are assumed as reference average temperatures, considering that the Comsol model can well describe the temperature distribution during the whole charge–discharge cycle [6]. The model is well validated by two sets of validation tests equipped with two different free convection cooling systems which use ice water and room temperature (RT) water as the coolants respectively.

2. Lumped parameter model

2.1. Model assumptions

In order to develop a lumped parameter model for an adsorption-based hydrogen storage system, the following assumptions are made.